Full wwPDB X-ray Structure Validation Report (i)

Aug 30, 2023 – 02:57 AM EDT

PDB ID	:	3NBZ
Title	:	Crystal structure of the HIV-1 Rev NES-CRM1-RanGTP nuclear export complex (crystal I)
Authors	:	Guttler, T.; Madl, T.; Neumann, P.; Deichsel, D.; Corsini, L.; Monecke, T.; Ficner, R.; Sattler, M.; Gorlich, D.
Deposited on	:	2010-06-04
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

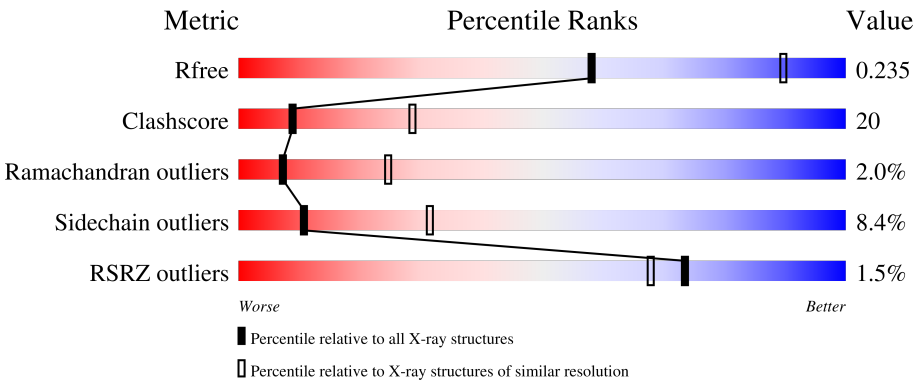
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1073	% 58% 34% • •
1	D	1073	% 57% 35% • •
2	B	362	2% 42% 33% 6% 20%
2	E	362	2% 45% 32% • 19%

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Mol	Chain	Length	Quality of chain
3	C	176	% 61% 31% 6%
3	F	176	% 56% 37% 5%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 25144 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Exportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1038	8394	5387	1411	1543	53	0	0	0
1	D	1038	8394	5387	1411	1543	53	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q6P5F9
A	0	SER	-	expression tag	UNP Q6P5F9
D	-1	GLY	-	expression tag	UNP Q6P5F9
D	0	SER	-	expression tag	UNP Q6P5F9

- Molecule 2 is a protein called Snurportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	291	2339	1491	403	430	15	0	0	0
2	E	293	2354	1500	405	434	15	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP O95149
B	0	SER	-	expression tag	UNP O95149
B	1	PRO	-	expression tag	UNP O95149
B	2	VAL	-	expression tag	UNP O95149
B	3	PRO	-	expression tag	UNP O95149
B	4	LEU	-	expression tag	UNP O95149
B	5	GLN	-	expression tag	UNP O95149
B	6	LEU	-	expression tag	UNP O95149

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Chain	Residue	Modelled	Actual	Comment	Reference
B	7	PRO	-	expression tag	UNP O95149
B	8	PRO	-	expression tag	UNP O95149
B	9	LEU	-	expression tag	UNP O95149
B	10	GLU	-	expression tag	UNP O95149
B	11	ARG	-	expression tag	UNP O95149
B	12	LEU	-	expression tag	UNP O95149
B	13	THR	-	expression tag	UNP O95149
B	14	LEU	-	expression tag	UNP O95149
E	-1	GLY	-	expression tag	UNP O95149
E	0	SER	-	expression tag	UNP O95149
E	1	PRO	-	expression tag	UNP O95149
E	2	VAL	-	expression tag	UNP O95149
E	3	PRO	-	expression tag	UNP O95149
E	4	LEU	-	expression tag	UNP O95149
E	5	GLN	-	expression tag	UNP O95149
E	6	LEU	-	expression tag	UNP O95149
E	7	PRO	-	expression tag	UNP O95149
E	8	PRO	-	expression tag	UNP O95149
E	9	LEU	-	expression tag	UNP O95149
E	10	GLU	-	expression tag	UNP O95149
E	11	ARG	-	expression tag	UNP O95149
E	12	LEU	-	expression tag	UNP O95149
E	13	THR	-	expression tag	UNP O95149
E	14	LEU	-	expression tag	UNP O95149

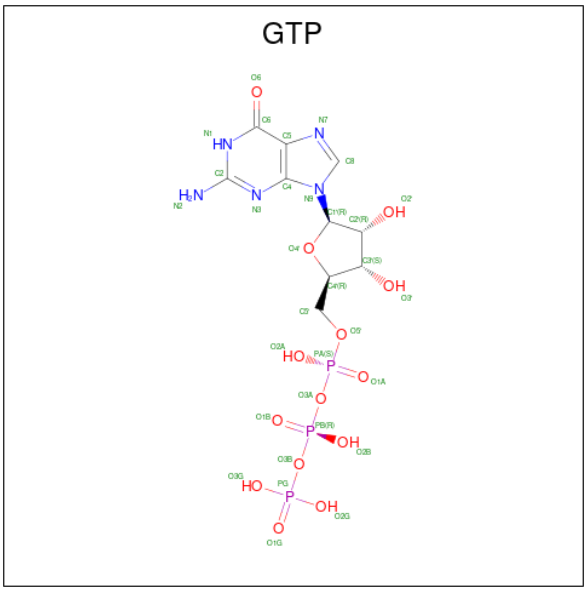
- Molecule 3 is a protein called GTP-binding nuclear protein Ran.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	173	1405	914	246	240	5	0	0	0
			Total	C	N	O	S			
3	F	173	1405	914	246	240	5	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	69	LEU	GLN	engineered mutation	UNP P62826
F	69	LEU	GLN	engineered mutation	UNP P62826

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	C	1	32	10	5	14	3	0	0
4	F	1	32	10	5	14	3	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	C	1	1	1	0	0
5	F	1	1	1	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
6	C	1	1	1	0	0
6	D	1	1	1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	237	237	237	0	0

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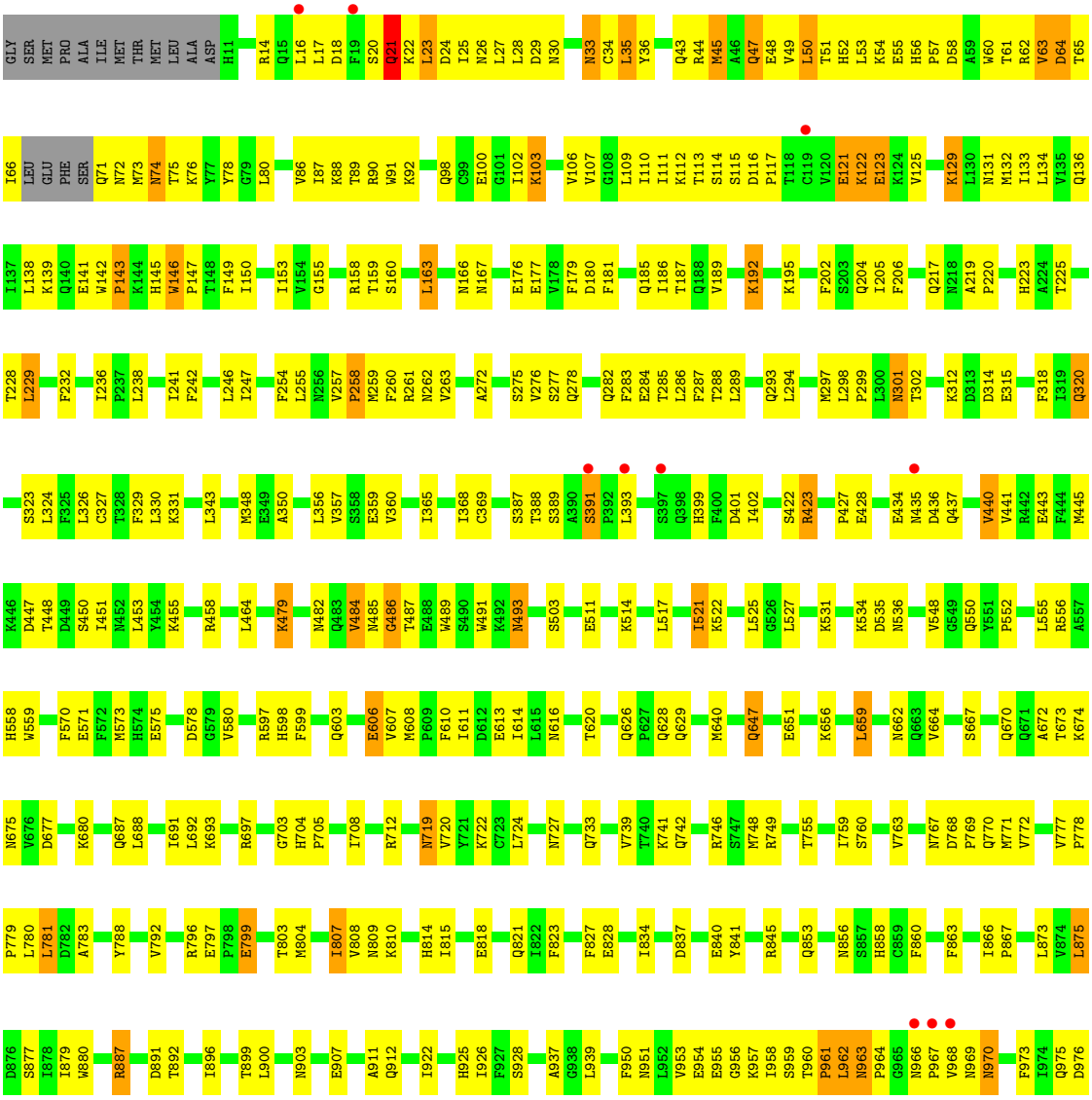
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	B	94	94	94	0	0
			Total	O		
7	C	53	53	53	0	0
			Total	O		
7	D	279	279	279	0	0
			Total	O		
7	E	71	71	71	0	0
			Total	O		
7	F	51	51	51	0	0

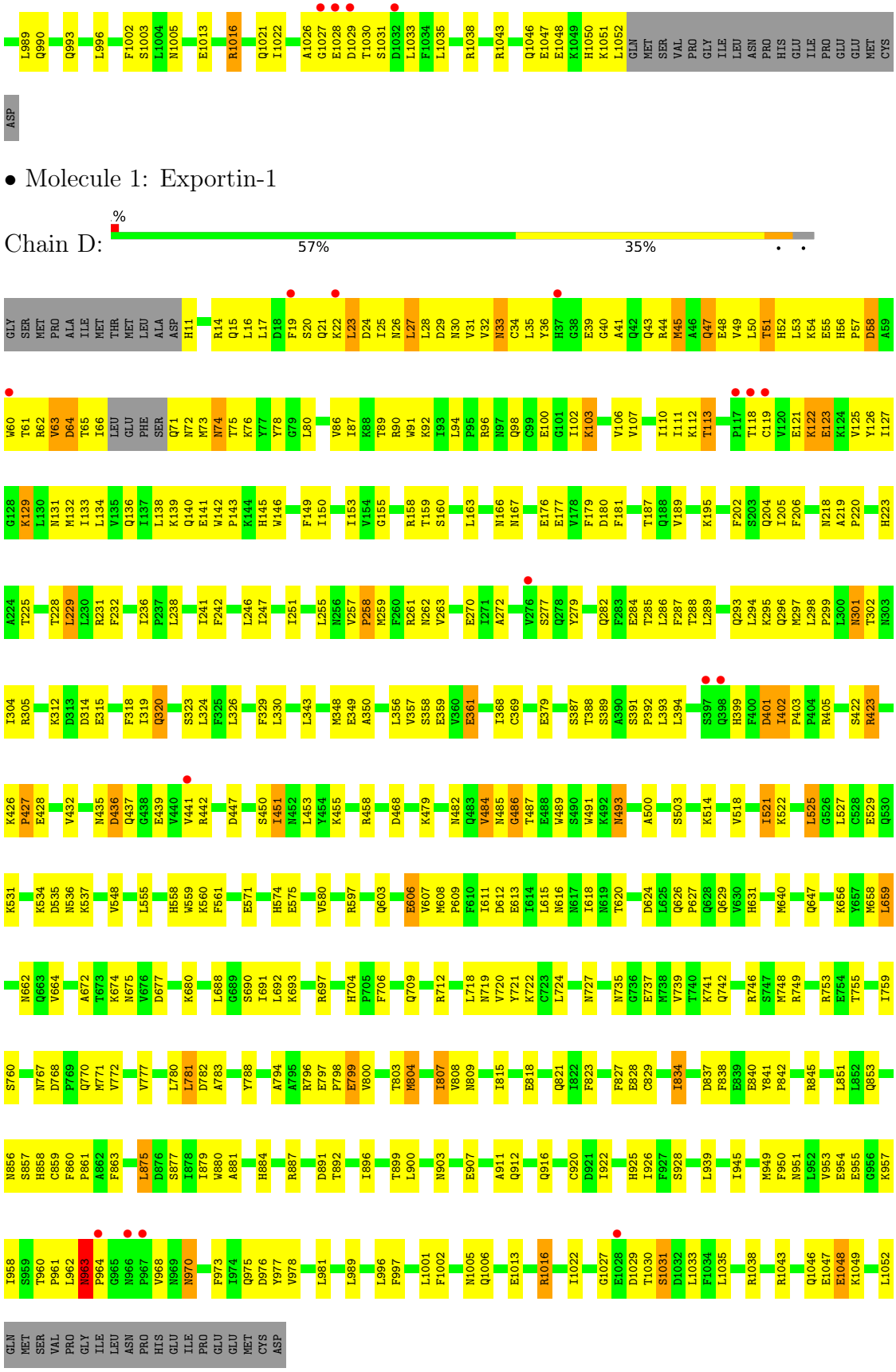
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Exportin-1

Chain A:



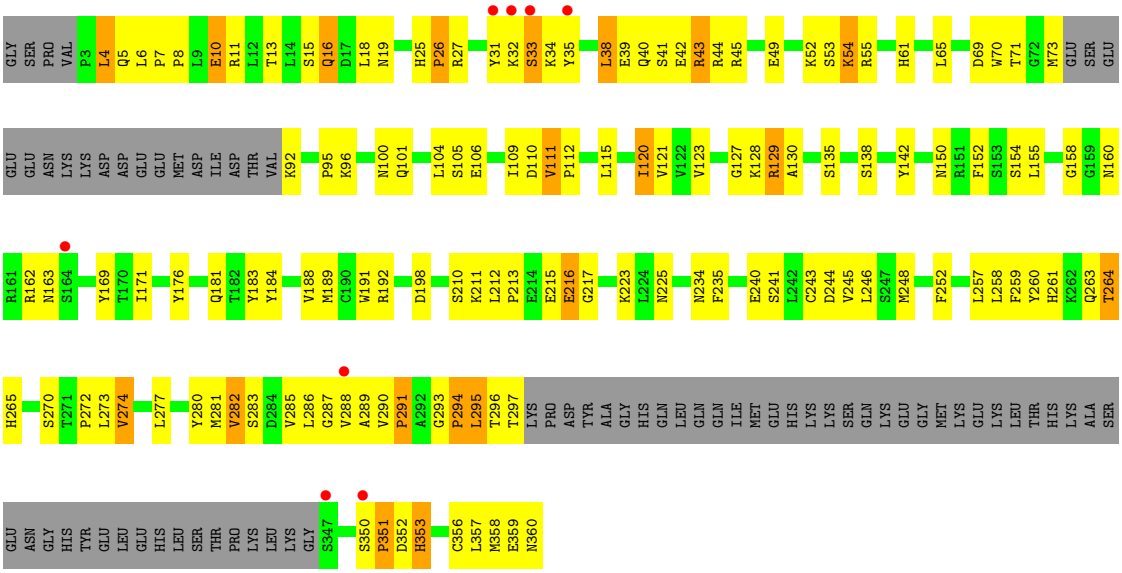


• Molecule 1: Exportin-1

Chain D: % 57% 35%

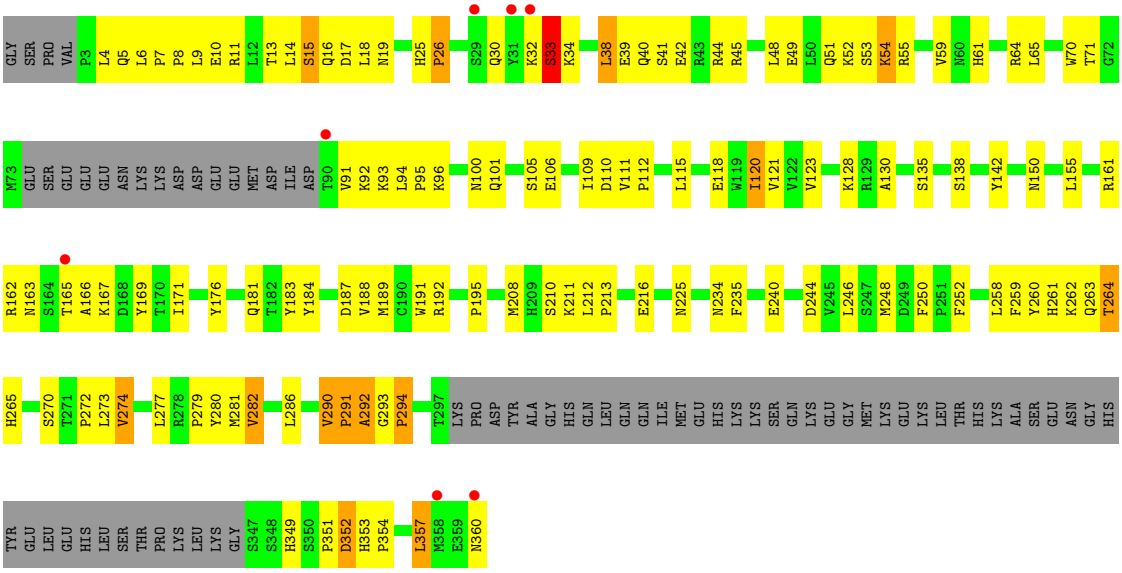
• Molecule 2: Snurportin-1

Chain B:



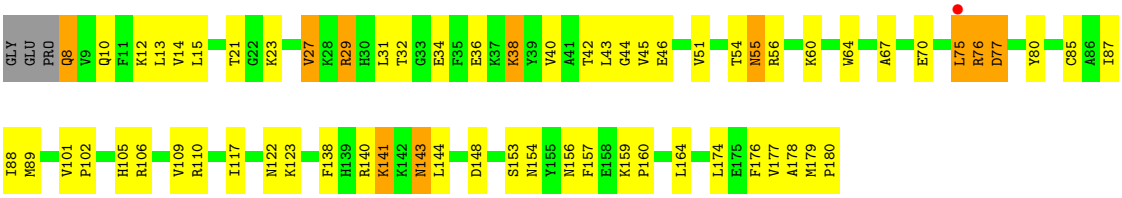
- Molecule 2: Snurportin-1

Chain E:



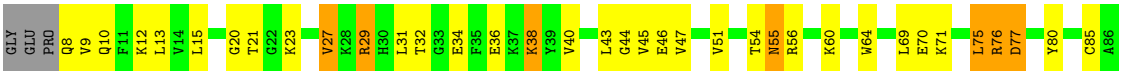
- Molecule 3: GTP-binding nuclear protein Ran

Chain C:



• Molecule 3: GTP-binding nuclear protein Ran

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.66Å 224.62Å 164.02Å 90.00° 100.82° 90.00°	Depositor
Resolution (Å)	38.90 – 2.80 38.90 – 2.80	Depositor EDS
% Data completeness (in resolution range)	90.1 (38.90-2.80) 81.4 (38.90-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.6.1_357	Depositor
R, R_{free}	0.226 , 0.285 0.226 , 0.235	Depositor DCC
R_{free} test set	5702 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	40.3	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 40.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.119 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	25144	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, GTP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.31	0/8566	0.47	0/11604
1	D	0.31	0/8566	0.48	0/11604
2	B	0.34	0/2404	0.53	0/3263
2	E	0.34	0/2419	0.53	0/3283
3	C	0.32	0/1440	0.48	0/1945
3	F	0.32	0/1440	0.49	0/1945
All	All	0.32	0/24835	0.49	0/33644

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8394	0	8460	325	0
1	D	8394	0	8460	347	0
2	B	2339	0	2295	114	0
2	E	2354	0	2311	110	0
3	C	1405	0	1434	52	0
3	F	1405	0	1434	62	0
4	C	32	0	12	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	32	0	12	2	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	237	0	0	17	0
7	B	94	0	0	7	0
7	C	53	0	0	6	0
7	D	279	0	0	22	0
7	E	71	0	0	3	0
7	F	51	0	0	6	0
All	All	25144	0	24418	992	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (992) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:290:VAL:H	2:E:291:PRO:HD3	1.09	1.10
2:B:52:LYS:HZ3	2:B:264:THR:HA	1.17	1.08
2:E:52:LYS:HZ3	2:E:264:THR:HA	1.18	1.02
1:D:45:MET:HE3	3:F:44:GLY:HA3	1.46	0.98
1:A:131:ASN:HD21	1:A:166:ASN:HD21	1.12	0.95
1:D:964:PRO:HG2	1:D:968:VAL:HB	1.49	0.94
1:D:131:ASN:HD21	1:D:166:ASN:HD21	1.11	0.94
2:B:52:LYS:NZ	2:B:264:THR:HA	1.84	0.93
2:E:52:LYS:NZ	2:E:264:THR:HA	1.84	0.92
2:B:43:ARG:HG3	2:B:44:ARG:H	1.35	0.91
1:D:55:GLU:HG2	1:D:56:HIS:H	1.37	0.90
1:A:961:PRO:HG2	1:A:973:PHE:HD2	1.35	0.88
1:A:964:PRO:HD2	1:A:968:VAL:HG21	1.55	0.88
1:A:45:MET:HE3	3:C:44:GLY:HA3	1.54	0.88
3:C:31:LEU:HD12	3:C:32:THR:HG23	1.54	0.87
1:A:719:ASN:HD21	2:B:358:MET:HB2	1.38	0.87
2:E:290:VAL:N	2:E:291:PRO:HD3	1.90	0.87
2:B:158:GLY:HA2	2:B:163:ASN:HD22	1.38	0.87
1:D:435:ASN:HB2	1:D:439:GLU:HB2	1.55	0.86
1:A:962:LEU:C	1:A:964:PRO:HD3	1.95	0.86
1:A:673:THR:HB	7:A:1090:HOH:O	1.77	0.84
3:F:31:LEU:HD12	3:F:32:THR:HG23	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:105:SER:HB3	2:B:274:VAL:HG22	1.59	0.83
1:D:20:SER:O	1:D:21:GLN:HG2	1.78	0.83
1:A:20:SER:HB2	1:A:22:LYS:HE2	1.59	0.82
1:A:807:ILE:HD11	1:A:815:ILE:HD12	1.60	0.82
1:D:1033:LEU:HD12	7:D:1305:HOH:O	1.78	0.81
1:D:996:LEU:HD12	1:D:1033:LEU:HD11	1.62	0.81
1:A:719:ASN:ND2	2:B:358:MET:HB2	1.96	0.81
2:E:290:VAL:H	2:E:291:PRO:CD	1.92	0.80
1:D:100:GLU:HA	1:D:103:LYS:CD	2.12	0.80
1:D:797:GLU:HG3	1:D:799:GLU:HG2	1.62	0.80
1:A:229:LEU:HD11	1:A:246:LEU:HD11	1.64	0.80
1:D:737:GLU:OE1	1:D:794:ALA:HB1	1.82	0.79
1:A:966:ASN:N	1:A:967:PRO:HD2	1.97	0.79
2:B:19:ASN:ND2	2:B:38:LEU:H	1.81	0.79
2:E:292:ALA:C	2:E:294:PRO:HD3	2.02	0.79
1:A:1043:ARG:O	1:A:1047:GLU:HG2	1.82	0.79
1:D:760:SER:HB3	1:D:803:THR:HG23	1.65	0.79
1:D:693:LYS:O	1:D:697:ARG:HG2	1.82	0.78
1:A:962:LEU:HB3	1:A:964:PRO:CD	2.13	0.78
3:C:21:THR:HG21	3:C:89:MET:HB3	1.66	0.77
1:A:797:GLU:HG3	1:A:799:GLU:HG2	1.65	0.77
2:E:19:ASN:ND2	2:E:38:LEU:H	1.82	0.77
3:F:117:ILE:HB	3:F:144:LEU:HD22	1.66	0.77
2:B:4:LEU:HB3	2:B:6:LEU:HD13	1.67	0.76
2:B:19:ASN:HD21	2:B:38:LEU:H	1.34	0.76
1:D:807:ILE:HD11	1:D:815:ILE:HD12	1.64	0.76
1:A:724:LEU:HD12	1:A:748:MET:HG2	1.68	0.76
3:C:55:ASN:HD21	3:C:174:LEU:HD12	1.50	0.76
2:E:19:ASN:HD21	2:E:38:LEU:H	1.34	0.76
1:A:247:ILE:HD12	1:A:247:ILE:H	1.49	0.76
1:D:755:THR:O	1:D:759:ILE:HG13	1.84	0.76
3:F:55:ASN:HD21	3:F:174:LEU:HD12	1.51	0.76
2:B:216:GLU:HG2	2:B:217:GLY:H	1.50	0.76
1:A:760:SER:HB3	1:A:803:THR:HG23	1.67	0.75
1:D:113:THR:HG22	1:D:119:CYS:SG	2.26	0.75
1:A:92:LYS:HD2	1:A:1026:ALA:HA	1.67	0.75
2:B:243:CYS:SG	2:B:288:VAL:HG13	2.26	0.75
1:D:100:GLU:HA	1:D:103:LYS:HD2	1.69	0.75
1:A:33:ASN:HB3	1:A:44:ARG:HG3	1.68	0.75
2:B:4:LEU:CB	2:B:6:LEU:HD13	2.17	0.75
1:A:14:ARG:HH22	1:A:16:LEU:HD22	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:LEU:HD11	1:D:246:LEU:HD11	1.68	0.75
2:B:38:LEU:HD22	2:B:40:GLN:H	1.52	0.75
2:B:4:LEU:HD22	2:B:6:LEU:HD22	1.67	0.75
1:A:755:THR:O	1:A:759:ILE:HG13	1.86	0.75
2:B:290:VAL:N	2:B:291:PRO:HD3	2.02	0.75
1:A:680:LYS:HE3	1:A:727:ASN:OD1	1.87	0.74
1:D:25:ILE:HD12	1:D:25:ILE:H	1.52	0.74
1:A:887:ARG:HD3	1:A:937:ALA:HB3	1.68	0.74
1:A:961:PRO:HG2	1:A:973:PHE:CD2	2.20	0.74
1:D:1031:SER:HB2	7:D:1299:HOH:O	1.87	0.74
1:D:964:PRO:CG	1:D:968:VAL:HB	2.17	0.73
3:F:21:THR:HG21	3:F:89:MET:HB3	1.70	0.73
1:A:223:HIS:NE2	1:A:263:VAL:HG21	2.03	0.73
1:A:35:LEU:C	1:A:36:TYR:HD1	1.92	0.73
1:D:961:PRO:HG2	1:D:973:PHE:HD2	1.54	0.73
1:A:25:ILE:HD12	1:A:25:ILE:H	1.53	0.73
2:E:25:HIS:ND1	2:E:26:PRO:HD2	2.03	0.72
1:A:962:LEU:HB3	1:A:964:PRO:HD2	1.69	0.72
1:A:100:GLU:HA	1:A:103:LYS:HD2	1.69	0.72
1:A:389:SER:HB3	7:A:1218:HOH:O	1.89	0.72
1:D:356:LEU:O	1:D:359:GLU:HG2	1.89	0.72
1:D:963:ASN:N	1:D:964:PRO:HD3	2.04	0.72
1:A:491:TRP:HE1	1:A:536:ASN:HD22	1.38	0.72
1:D:56:HIS:N	1:D:57:PRO:HD3	2.04	0.72
3:C:117:ILE:HB	3:C:144:LEU:HD22	1.72	0.72
2:E:18:LEU:HD13	2:E:38:LEU:HD12	1.72	0.72
2:E:38:LEU:HD22	2:E:40:GLN:H	1.55	0.71
1:D:60:TRP:HZ2	1:D:102:ILE:HD13	1.55	0.71
2:B:25:HIS:ND1	2:B:26:PRO:HD2	2.06	0.71
2:E:55:ARG:HD2	2:E:91:VAL:HG21	1.72	0.71
1:D:33:ASN:HB3	1:D:44:ARG:HG3	1.73	0.71
1:A:722:LYS:HD2	1:A:783:ALA:HA	1.73	0.71
1:D:960:THR:CG2	1:D:964:PRO:HD2	2.21	0.70
1:D:970:ASN:N	1:D:970:ASN:HD22	1.87	0.70
2:E:105:SER:HB3	2:E:274:VAL:HG22	1.72	0.70
1:A:33:ASN:CB	1:A:44:ARG:HG3	2.21	0.70
2:B:11:ARG:HD3	2:B:35:TYR:HE2	1.57	0.70
4:C:217:GTP:O3G	7:C:183:HOH:O	2.09	0.70
1:A:55:GLU:HG2	1:A:56:HIS:H	1.55	0.70
1:D:1016:ARG:HH11	1:D:1016:ARG:CG	2.05	0.69
1:D:491:TRP:HE1	1:D:536:ASN:HD22	1.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:GLU:HB2	1:D:145:HIS:HB2	1.74	0.69
1:D:724:LEU:HD12	1:D:748:MET:HG2	1.73	0.69
1:D:809:ASN:HA	1:D:858:HIS:HD2	1.57	0.69
1:A:356:LEU:O	1:A:359:GLU:HG2	1.93	0.69
1:A:56:HIS:N	1:A:57:PRO:HD3	2.08	0.69
1:D:722:LYS:HD2	1:D:783:ALA:HA	1.75	0.69
1:D:247:ILE:HD12	1:D:247:ILE:H	1.57	0.68
1:A:556:ARG:O	1:A:598:HIS:HE1	1.75	0.68
3:C:143:ASN:N	3:C:143:ASN:HD22	1.91	0.68
1:D:33:ASN:CB	1:D:44:ARG:HG3	2.23	0.68
1:D:45:MET:O	1:D:49:VAL:HG23	1.94	0.68
3:F:56:ARG:HD3	3:F:174:LEU:HD13	1.74	0.68
1:D:30:ASN:HB3	1:D:47:GLN:HE22	1.58	0.68
3:F:141:LYS:H	3:F:141:LYS:HD2	1.59	0.68
3:C:141:LYS:H	3:C:141:LYS:HD2	1.58	0.68
3:F:143:ASN:N	3:F:143:ASN:HD22	1.91	0.68
1:A:970:ASN:N	1:A:970:ASN:HD22	1.90	0.68
1:D:458:ARG:HG3	1:D:503:SER:HB2	1.76	0.68
1:D:664:VAL:HB	1:D:691:ILE:HD11	1.74	0.67
1:A:30:ASN:HB3	1:A:47:GLN:HE22	1.58	0.67
1:D:11:HIS:N	1:D:44:ARG:HH22	1.93	0.67
1:D:55:GLU:HB3	1:D:57:PRO:HD3	1.75	0.67
2:E:293:GLY:N	2:E:294:PRO:HD3	2.09	0.67
1:A:141:GLU:HB2	1:A:145:HIS:HB2	1.75	0.67
1:D:30:ASN:HB3	1:D:47:GLN:NE2	2.10	0.67
1:A:954:GLU:O	1:A:955:GLU:HG3	1.95	0.66
1:D:697:ARG:HD3	7:D:1093:HOH:O	1.94	0.66
1:D:393:LEU:HD23	1:D:394:LEU:N	2.11	0.66
1:A:436:ASP:HB3	7:A:1310:HOH:O	1.94	0.66
1:A:853:GLN:NE2	1:A:892:THR:HG23	2.09	0.66
1:D:436:ASP:O	1:D:437:GLN:HG2	1.96	0.66
1:D:611:ILE:HD13	1:D:640:MET:HE2	1.77	0.66
1:D:954:GLU:O	1:D:955:GLU:HG3	1.96	0.66
3:C:75:LEU:HD12	3:C:75:LEU:N	2.10	0.66
1:A:693:LYS:O	1:A:697:ARG:HG2	1.97	0.65
1:A:45:MET:O	1:A:49:VAL:HG23	1.96	0.65
2:B:45:ARG:HA	2:B:273:LEU:HD11	1.77	0.65
1:A:704:HIS:CD2	1:A:767:ASN:H	2.14	0.65
1:A:739:VAL:O	1:A:742:GLN:HG2	1.96	0.65
1:D:285:THR:O	1:D:289:LEU:HB2	1.96	0.65
3:F:75:LEU:HD12	3:F:75:LEU:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1016:ARG:CG	1:A:1016:ARG:HH11	2.10	0.65
1:D:132:MET:HE3	1:D:132:MET:O	1.96	0.65
1:D:704:HIS:CD2	1:D:767:ASN:H	2.15	0.64
3:F:92:VAL:N	7:F:683:HOH:O	2.26	0.64
1:A:30:ASN:HB3	1:A:47:GLN:NE2	2.12	0.64
2:E:45:ARG:HA	2:E:273:LEU:HD11	1.79	0.64
1:A:458:ARG:HG3	1:A:503:SER:HB2	1.79	0.64
1:A:241:ILE:O	1:A:247:ILE:HD11	1.97	0.64
1:D:153:ILE:HG13	1:D:167:ASN:OD1	1.96	0.64
1:D:1016:ARG:NH1	1:D:1016:ARG:HG2	2.13	0.64
1:D:241:ILE:O	1:D:247:ILE:HD11	1.98	0.64
1:D:781:LEU:HD21	1:D:821:GLN:HG2	1.79	0.63
1:A:132:MET:HE3	1:A:132:MET:O	1.98	0.63
1:A:781:LEU:HD21	1:A:821:GLN:HG2	1.79	0.63
1:D:131:ASN:HD21	1:D:166:ASN:ND2	1.92	0.63
1:D:720:VAL:HG23	1:D:724:LEU:HD23	1.80	0.63
1:A:167:ASN:ND2	7:A:1207:HOH:O	2.32	0.63
1:D:962:LEU:C	1:D:964:PRO:HD3	2.18	0.63
1:A:285:THR:O	1:A:289:LEU:HB2	1.97	0.63
1:A:1021:GLN:HE22	1:A:1033:LEU:HD22	1.63	0.63
1:A:389:SER:N	1:A:401:ASP:OD1	2.31	0.63
1:D:225:THR:HA	1:D:228:THR:HG22	1.81	0.63
1:D:55:GLU:CG	1:D:56:HIS:H	2.08	0.63
1:A:664:VAL:HB	1:A:691:ILE:HD11	1.79	0.63
1:D:103:LYS:HE3	7:D:1276:HOH:O	1.98	0.63
1:D:293:GLN:O	1:D:297:MET:HG3	1.98	0.63
3:F:10:GLN:HB3	3:F:60:LYS:HB3	1.81	0.63
1:A:133:ILE:O	1:A:136:GLN:HB2	1.98	0.63
7:A:1208:HOH:O	2:B:127:GLY:HA2	1.97	0.63
2:B:52:LYS:HE2	2:B:265:HIS:H	1.63	0.63
1:A:107:VAL:O	1:A:111:ILE:HG12	1.98	0.62
3:F:32:THR:OG1	3:F:34:GLU:HG2	1.98	0.62
1:D:626:GLN:H	1:D:629:GLN:NE2	1.97	0.62
2:E:290:VAL:N	2:E:291:PRO:CD	2.59	0.62
1:A:314:ASP:HB2	7:A:1259:HOH:O	1.99	0.62
2:E:65:LEU:HD12	2:E:171:ILE:HD13	1.81	0.62
1:D:223:HIS:NE2	1:D:263:VAL:HG21	2.14	0.62
1:A:255:LEU:HD23	1:A:255:LEU:O	2.00	0.62
3:F:122:ASN:O	3:F:123:LYS:HB2	1.98	0.62
1:D:574:HIS:CE1	7:D:1267:HOH:O	2.52	0.62
1:D:675:ASN:HD21	1:D:677:ASP:HB2	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:899:THR:HG22	1:D:903:ASN:HD21	1.64	0.61
2:B:65:LEU:HD23	2:B:70:TRP:HH2	1.65	0.61
1:D:357:VAL:HG12	1:D:369:CYS:SG	2.40	0.61
3:F:123:LYS:HE2	4:F:217:GTP:C4	2.35	0.61
1:A:225:THR:HA	1:A:228:THR:HG22	1.82	0.61
2:B:285:VAL:O	2:B:286:LEU:HD23	2.00	0.61
2:B:26:PRO:HG2	2:B:109:ILE:HD11	1.83	0.61
3:C:56:ARG:HD3	3:C:174:LEU:HD13	1.81	0.61
7:D:1351:HOH:O	2:E:351:PRO:HB2	2.00	0.61
2:E:61:HIS:HE1	2:E:101:GLN:HE22	1.49	0.61
1:A:35:LEU:HD11	7:C:234:HOH:O	2.00	0.61
1:A:35:LEU:O	1:A:36:TYR:HD1	1.83	0.61
1:A:626:GLN:H	1:A:629:GLN:NE2	1.99	0.61
1:D:107:VAL:O	1:D:111:ILE:HG12	2.00	0.61
1:D:561:PHE:HB2	2:E:6:LEU:HD12	1.83	0.61
1:A:106:VAL:O	1:A:110:ILE:HG13	2.01	0.61
1:A:809:ASN:HA	1:A:858:HIS:HD2	1.66	0.60
2:E:52:LYS:HE2	2:E:265:HIS:H	1.63	0.60
1:A:558:HIS:ND1	2:B:4:LEU:HD23	2.16	0.60
2:B:154:SER:O	2:B:160:ASN:HB3	2.02	0.60
1:D:960:THR:HG21	1:D:964:PRO:HD2	1.83	0.60
2:E:95:PRO:HG2	2:E:100:ASN:O	2.01	0.60
1:A:293:GLN:O	1:A:297:MET:HG3	2.00	0.60
2:B:111:VAL:HG21	2:B:286:LEU:HD22	1.84	0.60
1:D:32:VAL:O	1:D:36:TYR:HD1	1.85	0.60
1:A:720:VAL:HG23	1:A:724:LEU:HD23	1.82	0.60
3:F:138:PHE:HA	3:F:141:LYS:HE3	1.83	0.60
2:B:43:ARG:HG3	2:B:44:ARG:N	2.14	0.60
1:D:100:GLU:HA	1:D:103:LYS:HD3	1.81	0.60
1:D:739:VAL:O	1:D:742:GLN:HG2	2.02	0.60
1:A:962:LEU:HB3	1:A:964:PRO:HD3	1.84	0.60
1:A:16:LEU:HG	1:A:16:LEU:O	2.02	0.59
1:A:320:GLN:O	1:A:323:SER:HB2	2.02	0.59
1:A:485:ASN:O	1:A:487:THR:N	2.35	0.59
1:A:957:LYS:HZ3	1:A:961:PRO:HG3	1.67	0.59
2:E:65:LEU:HD23	2:E:70:TRP:HH2	1.68	0.59
1:D:255:LEU:HD23	1:D:255:LEU:O	2.02	0.59
2:B:8:PRO:HA	2:B:10:GLU:OE1	2.02	0.59
1:D:11:HIS:N	1:D:44:ARG:NH2	2.51	0.59
1:D:853:GLN:NE2	1:D:892:THR:HG23	2.17	0.59
3:C:23:LYS:O	3:C:27:VAL:HG13	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1016:ARG:HH11	1:D:1016:ARG:HG2	1.64	0.59
2:E:100:ASN:HB3	7:E:465:HOH:O	2.02	0.59
1:D:55:GLU:HG2	1:D:56:HIS:N	2.12	0.59
1:D:680:LYS:HE3	1:D:727:ASN:OD1	2.03	0.59
1:A:357:VAL:HG12	1:A:369:CYS:SG	2.43	0.59
1:A:441:VAL:HG12	1:A:628:GLN:NE2	2.18	0.59
1:D:119:CYS:SG	1:D:127:ILE:HD11	2.43	0.59
1:A:428:GLU:HG2	7:A:1176:HOH:O	2.02	0.58
1:A:482:ASN:HA	1:A:486:GLY:HA3	1.84	0.58
1:D:957:LYS:HZ3	1:D:961:PRO:HG3	1.68	0.58
2:B:61:HIS:HE1	2:B:101:GLN:HE22	1.51	0.58
1:D:428:GLU:HG3	7:D:1239:HOH:O	2.03	0.58
1:D:950:PHE:O	1:D:953:VAL:HB	2.03	0.58
2:E:163:ASN:O	2:E:165:THR:HG23	2.02	0.58
2:B:112:PRO:HD2	2:B:115:LEU:HD13	1.85	0.58
2:B:18:LEU:HD13	2:B:38:LEU:HD12	1.85	0.58
2:E:16:GLN:O	2:E:16:GLN:HG2	2.02	0.58
1:A:401:ASP:OD2	1:A:401:ASP:N	2.37	0.58
1:A:724:LEU:HD12	1:A:748:MET:CG	2.33	0.58
1:D:324:LEU:CD2	1:D:368:ILE:HD13	2.33	0.58
1:D:803:THR:O	1:D:807:ILE:HG23	2.03	0.58
1:D:62:ARG:HB2	1:D:62:ARG:CZ	2.32	0.58
1:A:139:LYS:HE2	1:A:177:GLU:HB3	1.86	0.58
2:B:41:SER:O	2:B:45:ARG:HG3	2.03	0.58
3:C:10:GLN:HB3	3:C:60:LYS:HB3	1.85	0.58
2:E:176:TYR:HB2	2:E:183:TYR:CE1	2.38	0.58
2:E:349:HIS:NE2	2:E:351:PRO:HG3	2.19	0.58
1:A:662:ASN:HD22	1:A:712:ARG:HH21	1.51	0.58
2:B:176:TYR:HB2	2:B:183:TYR:CE1	2.39	0.58
1:D:662:ASN:HD22	1:D:712:ARG:NH2	2.01	0.58
1:A:675:ASN:HD21	1:A:677:ASP:HB2	1.68	0.57
1:A:966:ASN:N	1:A:967:PRO:CD	2.67	0.57
1:D:489:TRP:CE2	1:D:531:LYS:HE2	2.39	0.57
1:A:899:THR:HG22	1:A:903:ASN:HD21	1.69	0.57
3:F:92:VAL:HG13	7:F:683:HOH:O	2.03	0.57
1:A:962:LEU:HD13	1:A:968:VAL:HB	1.86	0.57
1:D:482:ASN:HA	1:D:486:GLY:HA3	1.86	0.57
1:D:607:VAL:HG13	1:D:608:MET:HG2	1.86	0.57
1:A:58:ASP:O	1:A:62:ARG:HG2	2.04	0.57
1:A:489:TRP:CE2	1:A:531:LYS:HE2	2.39	0.57
1:A:55:GLU:HB3	1:A:57:PRO:HD3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:GLN:CG	1:D:21:GLN:O	2.53	0.57
2:B:277:LEU:HD22	2:B:281:MET:HE2	1.86	0.57
1:D:399:HIS:HB3	1:D:401:ASP:H	1.69	0.57
1:D:534:LYS:HE3	1:D:575:GLU:OE2	2.04	0.57
1:D:1016:ARG:HH11	1:D:1016:ARG:CB	2.18	0.57
3:F:77:ASP:HA	3:F:80:TYR:CD2	2.40	0.57
1:A:957:LYS:HZ1	1:A:961:PRO:HB3	1.70	0.57
1:A:996:LEU:HD12	1:A:1033:LEU:HD21	1.85	0.57
1:D:529:GLU:HG3	2:E:11:ARG:HH21	1.70	0.57
1:D:963:ASN:N	1:D:964:PRO:CD	2.67	0.57
2:E:354:PRO:HB2	2:E:357:LEU:HD23	1.86	0.57
1:D:996:LEU:CD1	1:D:1033:LEU:HD11	2.33	0.56
2:B:4:LEU:O	2:B:5:GLN:HB2	2.05	0.56
3:C:29:ARG:HB3	3:C:157:PHE:CZ	2.39	0.56
1:A:662:ASN:HD22	1:A:712:ARG:NH2	2.03	0.56
2:B:95:PRO:HG2	2:B:100:ASN:O	2.06	0.56
1:A:704:HIS:HB3	7:A:1262:HOH:O	2.05	0.56
1:A:1016:ARG:HH11	1:A:1016:ARG:CB	2.17	0.56
3:C:77:ASP:HA	3:C:80:TYR:CD2	2.41	0.56
3:C:88:ILE:HG21	3:C:101:VAL:HG13	1.86	0.56
2:E:112:PRO:HD2	2:E:115:LEU:HD13	1.88	0.56
1:A:788:TYR:CE1	1:A:796:ARG:HB3	2.41	0.56
1:A:803:THR:O	1:A:807:ILE:HG23	2.05	0.56
1:D:437:GLN:HG3	1:D:753:ARG:NH1	2.20	0.56
1:D:970:ASN:N	1:D:970:ASN:ND2	2.53	0.56
1:D:295:LYS:HD2	1:D:349:GLU:OE2	2.06	0.56
1:D:299:PRO:HG2	1:D:302:THR:CG2	2.35	0.56
1:D:103:LYS:O	1:D:107:VAL:HG23	2.06	0.56
2:E:13:THR:HG22	2:E:15:SER:H	1.70	0.56
2:E:277:LEU:HD22	2:E:281:MET:HE2	1.88	0.56
1:A:299:PRO:HG2	1:A:302:THR:CG2	2.35	0.55
2:B:129:ARG:NH2	7:B:361:HOH:O	2.37	0.55
3:C:55:ASN:ND2	3:C:174:LEU:HD12	2.21	0.55
1:D:435:ASN:ND2	1:D:441:VAL:HG11	2.21	0.55
2:E:279:PRO:HB2	2:E:294:PRO:HB2	1.87	0.55
1:A:258:PRO:O	1:A:261:ARG:HG2	2.06	0.55
1:A:1051:LYS:HG2	1:A:1052:LEU:HG	1.88	0.55
1:A:1016:ARG:NH1	1:A:1016:ARG:HG2	2.21	0.55
1:D:66:ILE:HG21	1:D:72:ASN:ND2	2.21	0.55
2:E:8:PRO:HA	2:E:10:GLU:OE1	2.06	0.55
1:A:511:GLU:HA	1:A:514:LYS:HE3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:950:PHE:O	1:A:953:VAL:HB	2.05	0.55
1:A:951:ASN:HA	1:A:1005:ASN:HD22	1.71	0.55
1:D:957:LYS:HZ1	1:D:961:PRO:HB3	1.71	0.55
1:D:1043:ARG:HA	1:D:1046:GLN:HB3	1.86	0.55
1:A:17:LEU:HG	1:A:20:SER:HB2	1.89	0.55
1:A:275:SER:HB2	7:A:1167:HOH:O	2.05	0.55
2:B:155:LEU:O	7:B:417:HOH:O	2.18	0.55
3:C:55:ASN:N	3:C:55:ASN:HD22	2.04	0.55
1:D:238:LEU:HD22	1:D:242:PHE:HE2	1.71	0.55
1:D:680:LYS:HB2	1:D:680:LYS:NZ	2.21	0.55
1:D:103:LYS:NZ	1:D:103:LYS:CB	2.70	0.55
1:D:961:PRO:HD3	1:D:970:ASN:ND2	2.22	0.55
2:E:55:ARG:HD2	2:E:91:VAL:CG2	2.37	0.55
1:A:150:ILE:HD12	1:A:153:ILE:HD11	1.89	0.55
1:D:139:LYS:HE2	1:D:177:GLU:HB3	1.89	0.55
1:D:50:LEU:O	1:D:53:LEU:HG	2.07	0.54
1:A:324:LEU:CD2	1:A:368:ILE:HD13	2.37	0.54
1:D:219:ALA:HB3	1:D:220:PRO:HD3	1.90	0.54
1:D:837:ASP:O	1:D:845:ARG:NH2	2.40	0.54
2:B:27:ARG:HG3	2:B:31:TYR:HD1	1.71	0.54
1:D:493:ASN:N	1:D:493:ASN:HD22	2.04	0.54
1:A:963:ASN:N	1:A:964:PRO:HD3	2.22	0.54
3:F:55:ASN:ND2	3:F:174:LEU:HD12	2.22	0.54
2:B:65:LEU:HD12	2:B:171:ILE:HD13	1.89	0.54
2:B:283:SER:HB2	2:B:290:VAL:HG22	1.90	0.54
1:D:121:GLU:O	1:D:123:GLU:N	2.41	0.54
1:D:529:GLU:HB3	7:D:1106:HOH:O	2.07	0.54
1:A:27:LEU:HD21	1:A:75:THR:HG23	1.89	0.54
1:A:493:ASN:N	1:A:493:ASN:HD22	2.03	0.54
1:A:892:THR:O	1:A:896:ILE:HG13	2.08	0.54
1:A:957:LYS:NZ	1:A:961:PRO:HB3	2.23	0.54
1:D:1016:ARG:CG	1:D:1016:ARG:NH1	2.67	0.54
3:C:32:THR:OG1	3:C:34:GLU:HG2	2.06	0.54
1:D:284:GLU:HG3	1:D:343:LEU:HD11	1.89	0.54
1:D:485:ASN:O	1:D:487:THR:N	2.41	0.54
1:D:892:THR:O	1:D:896:ILE:HG13	2.08	0.54
2:E:135:SER:HB3	2:E:169:TYR:HB3	1.90	0.54
1:A:272:ALA:HB1	1:A:329:PHE:HD1	1.73	0.54
3:F:55:ASN:HD22	3:F:55:ASN:N	2.05	0.54
1:A:284:GLU:HG3	1:A:343:LEU:HD11	1.89	0.54
1:D:103:LYS:HZ3	1:D:103:LYS:HB3	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:HIS:N	1:D:57:PRO:CD	2.71	0.53
1:D:106:VAL:O	1:D:110:ILE:HG13	2.08	0.53
1:D:320:GLN:O	1:D:323:SER:HB2	2.09	0.53
1:A:129:LYS:O	1:A:133:ILE:HG13	2.09	0.53
1:A:962:LEU:O	1:A:963:ASN:HB2	2.08	0.53
2:B:43:ARG:HG3	2:B:44:ARG:HG3	1.90	0.53
1:D:450:SER:O	1:D:453:LEU:HB3	2.08	0.53
1:D:167:ASN:ND2	7:D:1160:HOH:O	2.41	0.53
1:A:484:VAL:HA	1:A:527:LEU:HD13	1.89	0.53
1:A:276:VAL:O	1:A:276:VAL:HG22	2.08	0.53
1:A:741:LYS:HA	1:A:746:ARG:HH11	1.74	0.53
1:D:202:PHE:CZ	1:D:236:ILE:HG21	2.44	0.53
2:E:264:THR:HG23	2:E:273:LEU:HD22	1.90	0.53
1:A:50:LEU:O	1:A:53:LEU:HG	2.08	0.53
1:A:647:GLN:NE2	7:A:1263:HOH:O	2.42	0.53
1:A:925:HIS:O	1:A:928:SER:HB3	2.08	0.53
2:B:69:ASP:OD2	2:B:71:THR:HG23	2.08	0.53
3:F:179:MET:HG3	3:F:179:MET:O	2.08	0.53
1:D:860:PHE:HE1	1:D:900:LEU:CD1	2.22	0.53
1:D:205:ILE:HG22	1:D:206:PHE:N	2.23	0.53
1:D:951:ASN:HA	1:D:1005:ASN:HD22	1.73	0.53
2:E:15:SER:C	2:E:17:ASP:H	2.12	0.53
1:D:514:LYS:NZ	1:D:558:HIS:HE1	2.07	0.53
1:D:30:ASN:CB	1:D:47:GLN:NE2	2.73	0.52
1:D:788:TYR:CE1	1:D:796:ARG:HB3	2.44	0.52
3:C:122:ASN:O	3:C:123:LYS:HB2	2.09	0.52
1:D:960:THR:HG21	1:D:964:PRO:O	2.10	0.52
1:D:149:PHE:O	1:D:153:ILE:HG22	2.09	0.52
1:D:437:GLN:HG3	1:D:753:ARG:NH2	2.24	0.52
2:E:286:LEU:O	2:E:286:LEU:HG	2.09	0.52
1:A:970:ASN:N	1:A:970:ASN:ND2	2.57	0.52
2:B:158:GLY:HA2	2:B:163:ASN:ND2	2.18	0.52
2:B:288:VAL:HG12	2:B:289:ALA:N	2.23	0.52
1:D:361:GLU:CD	1:D:361:GLU:H	2.11	0.52
1:D:574:HIS:ND1	7:D:1267:HOH:O	2.34	0.52
1:D:627:PRO:O	1:D:631:HIS:ND1	2.42	0.52
1:A:121:GLU:O	1:A:123:GLU:N	2.43	0.52
1:A:1016:ARG:CG	1:A:1016:ARG:NH1	2.71	0.52
2:B:288:VAL:CG1	2:B:289:ALA:N	2.72	0.52
1:D:401:ASP:O	1:D:403:PRO:HD3	2.10	0.52
1:D:975:GLN:HG2	1:D:1002:PHE:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:75:LEU:HD12	3:F:75:LEU:H	1.74	0.52
1:A:219:ALA:HB3	1:A:220:PRO:HD3	1.92	0.52
1:A:534:LYS:HE3	1:A:575:GLU:OE2	2.09	0.52
1:A:860:PHE:HE1	1:A:900:LEU:CD1	2.23	0.52
1:D:50:LEU:C	1:D:52:HIS:H	2.13	0.52
1:D:548:VAL:O	1:D:555:LEU:HD11	2.09	0.52
1:D:857:SER:HB2	7:D:1087:HOH:O	2.10	0.52
1:A:177:GLU:OE1	1:A:177:GLU:HA	2.09	0.51
2:B:13:THR:HG21	7:B:408:HOH:O	2.09	0.51
1:D:179:PHE:CE1	1:D:195:LYS:HG2	2.45	0.51
1:A:232:PHE:O	1:A:236:ILE:HG23	2.10	0.51
3:C:123:LYS:HE2	4:C:217:GTP:C4	2.45	0.51
3:C:138:PHE:HA	3:C:141:LYS:HE3	1.92	0.51
1:D:616:ASN:OD1	1:D:656:LYS:HE3	2.10	0.51
1:A:1003:SER:HA	1:A:1046:GLN:OE1	2.10	0.51
2:B:294:PRO:O	2:B:295:LEU:HD23	2.11	0.51
1:D:96:ARG:HH21	1:D:145:HIS:HB3	1.75	0.51
1:D:134:LEU:O	1:D:138:LEU:HG	2.10	0.51
2:E:38:LEU:HD22	2:E:39:GLU:H	1.76	0.51
4:C:217:GTP:O3G	4:C:217:GTP:O2B	2.28	0.51
1:D:887:ARG:HB2	1:D:887:ARG:CZ	2.40	0.51
1:A:301:ASN:H	1:A:301:ASN:HD22	1.57	0.51
2:B:135:SER:HB3	2:B:169:TYR:HB3	1.93	0.51
1:A:853:GLN:HE21	1:A:892:THR:HG23	1.73	0.51
2:B:38:LEU:HD22	2:B:39:GLU:H	1.75	0.51
2:E:44:ARG:NH1	2:E:272:PRO:HG3	2.26	0.51
2:E:210:SER:C	2:E:211:LYS:HD2	2.31	0.51
1:A:769:PRO:HB2	1:A:814:HIS:CE1	2.46	0.51
2:B:191:TRP:CD1	2:B:192:ARG:HG3	2.45	0.51
1:D:27:LEU:HD21	1:D:75:THR:HG23	1.91	0.51
1:A:35:LEU:HD12	7:C:561:HOH:O	2.10	0.51
1:D:912:GLN:CD	1:D:958:ILE:HG12	2.32	0.51
1:A:47:GLN:HG2	1:A:48:GLU:N	2.25	0.51
1:A:131:ASN:ND2	1:A:166:ASN:HD21	1.95	0.51
1:A:434:GLU:HB3	1:A:440:VAL:CG1	2.41	0.51
1:A:548:VAL:O	1:A:555:LEU:HD11	2.11	0.51
3:C:75:LEU:HD12	3:C:75:LEU:H	1.74	0.51
1:A:767:ASN:HB2	7:A:1166:HOH:O	2.12	0.50
1:A:611:ILE:HD13	1:A:640:MET:HE2	1.92	0.50
1:A:912:GLN:CD	1:A:958:ILE:HG12	2.32	0.50
1:D:17:LEU:HB3	1:D:22:LYS:HE2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:ILE:O	1:D:251:ILE:HG13	2.12	0.50
1:D:662:ASN:HD22	1:D:712:ARG:HH21	1.59	0.50
1:D:840:GLU:O	1:D:841:TYR:HB2	2.09	0.50
1:A:55:GLU:HG2	1:A:56:HIS:N	2.25	0.50
1:A:55:GLU:C	1:A:57:PRO:HD3	2.30	0.50
1:A:35:LEU:C	1:A:36:TYR:CD1	2.79	0.50
1:A:856:ASN:HB2	1:A:863:PHE:HE1	1.75	0.50
1:D:258:PRO:O	1:D:261:ARG:HG2	2.11	0.50
1:A:55:GLU:CG	1:A:56:HIS:H	2.18	0.50
1:A:963:ASN:N	1:A:964:PRO:CD	2.75	0.50
3:C:29:ARG:HB3	3:C:157:PHE:HZ	1.75	0.50
1:D:155:GLY:O	1:D:159:THR:HG23	2.12	0.50
1:D:899:THR:HG22	1:D:903:ASN:ND2	2.26	0.50
1:D:957:LYS:NZ	1:D:961:PRO:HG3	2.26	0.50
1:A:185:GLN:HG2	1:A:186:ILE:HG13	1.93	0.50
2:B:285:VAL:HG12	2:B:286:LEU:CD2	2.41	0.50
1:D:435:ASN:OD1	1:D:441:VAL:HG21	2.12	0.50
1:D:877:SER:O	1:D:880:TRP:HB3	2.11	0.50
2:E:261:HIS:CD2	2:E:263:GLN:H	2.30	0.50
2:E:280:TYR:HB3	2:E:294:PRO:O	2.11	0.50
1:A:422:SER:C	1:A:423:ARG:HG2	2.32	0.50
1:A:841:TYR:O	1:A:845:ARG:HG3	2.12	0.50
1:D:961:PRO:HB2	1:D:973:PHE:HE2	1.76	0.50
1:D:962:LEU:HD23	1:D:964:PRO:HG3	1.94	0.50
1:A:20:SER:HB2	1:A:22:LYS:CE	2.37	0.50
1:D:27:LEU:HD23	1:D:27:LEU:C	2.31	0.50
1:D:103:LYS:NZ	1:D:103:LYS:HB3	2.26	0.50
1:D:299:PRO:HG2	1:D:302:THR:HG21	1.94	0.50
1:D:704:HIS:HD2	1:D:767:ASN:H	1.57	0.50
1:D:856:ASN:HB2	1:D:863:PHE:HE1	1.76	0.50
1:A:276:VAL:O	1:A:278:GLN:N	2.45	0.50
1:A:837:ASP:O	1:A:845:ARG:NH2	2.44	0.50
2:B:19:ASN:HB2	2:B:106:GLU:HB3	1.94	0.50
2:B:44:ARG:NH1	2:B:272:PRO:HG3	2.27	0.50
1:D:484:VAL:HA	1:D:527:LEU:HD13	1.93	0.50
3:F:141:LYS:HG3	7:F:407:HOH:O	2.11	0.50
1:A:287:PHE:HZ	1:A:350:ALA:HB2	1.77	0.49
1:D:14:ARG:HB3	1:D:16:LEU:HG	1.93	0.49
1:D:176:GLU:O	1:D:181:PHE:HD2	1.94	0.49
1:D:358:SER:O	1:D:423:ARG:NH1	2.45	0.49
1:D:741:LYS:HA	1:D:746:ARG:HH11	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:88:ILE:HG21	3:F:101:VAL:HG13	1.94	0.49
1:A:89:THR:HG22	1:A:90:ARG:HG3	1.94	0.49
2:B:55:ARG:NH2	7:B:404:HOH:O	2.44	0.49
2:E:155:LEU:HG	2:E:225:ASN:HB2	1.93	0.49
3:F:122:ASN:N	7:F:683:HOH:O	2.43	0.49
1:A:80:LEU:HD22	1:A:133:ILE:HD12	1.94	0.49
1:A:388:THR:O	1:A:389:SER:C	2.50	0.49
1:A:704:HIS:HD2	1:A:767:ASN:H	1.59	0.49
1:A:1016:ARG:HH11	1:A:1016:ARG:HB3	1.77	0.49
2:E:65:LEU:CD1	2:E:171:ILE:HD13	2.42	0.49
2:B:293:GLY:N	2:B:294:PRO:CD	2.74	0.49
3:C:85:CYS:HB2	3:C:164:LEU:HD22	1.94	0.49
3:F:29:ARG:HB3	3:F:157:PHE:CZ	2.47	0.49
1:D:521:ILE:HD11	2:E:7:PRO:HB2	1.93	0.49
1:D:961:PRO:HG2	1:D:973:PHE:CD2	2.42	0.49
1:A:389:SER:HB3	1:A:399:HIS:HE2	1.78	0.49
2:B:210:SER:C	2:B:211:LYS:HD2	2.33	0.49
1:D:55:GLU:HG2	1:D:56:HIS:ND1	2.28	0.49
1:D:437:GLN:HG3	1:D:753:ARG:CZ	2.42	0.49
2:E:290:VAL:HG12	2:E:290:VAL:O	2.13	0.49
1:A:393:LEU:HG	1:A:399:HIS:HA	1.94	0.49
3:C:15:LEU:HD12	3:C:87:ILE:O	2.13	0.49
3:C:153:SER:O	3:C:154:ASN:HB2	2.11	0.49
1:D:768:ASP:O	1:D:772:VAL:HG23	2.13	0.49
1:A:176:GLU:O	1:A:181:PHE:HD2	1.96	0.49
1:A:179:PHE:CE1	1:A:195:LYS:HG2	2.48	0.49
1:A:282:GLN:OE1	1:A:282:GLN:N	2.41	0.49
1:A:840:GLU:O	1:A:841:TYR:HB2	2.12	0.49
2:B:216:GLU:CG	2:B:217:GLY:H	2.23	0.49
1:D:74:ASN:N	1:D:74:ASN:HD22	2.09	0.49
7:D:1351:HOH:O	2:E:351:PRO:CB	2.58	0.49
1:A:56:HIS:N	1:A:57:PRO:CD	2.75	0.49
1:A:202:PHE:CZ	1:A:236:ILE:HG21	2.48	0.49
1:D:662:ASN:ND2	7:D:1111:HOH:O	2.46	0.49
1:A:30:ASN:CB	1:A:47:GLN:NE2	2.76	0.48
1:A:616:ASN:OD1	1:A:656:LYS:HE3	2.12	0.48
2:B:296:THR:O	2:B:297:THR:C	2.52	0.48
1:D:176:GLU:O	1:D:180:ASP:HB2	2.12	0.48
1:A:877:SER:O	1:A:880:TRP:HB3	2.13	0.48
2:B:104:LEU:HA	7:B:361:HOH:O	2.13	0.48
2:B:353:HIS:ND1	2:B:353:HIS:N	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:67:ALA:HB1	7:C:395:HOH:O	2.12	0.48
3:F:15:LEU:HD12	3:F:87:ILE:O	2.12	0.48
1:A:299:PRO:HG2	1:A:302:THR:HG21	1.95	0.48
1:D:518:VAL:O	1:D:522:LYS:HG3	2.13	0.48
1:A:294:LEU:O	1:A:298:LEU:N	2.44	0.48
1:A:599:PHE:HB2	1:A:640:MET:HG2	1.94	0.48
1:A:50:LEU:C	1:A:52:HIS:H	2.17	0.48
1:A:55:GLU:HG3	1:A:90:ARG:NH2	2.29	0.48
1:D:559:TRP:NE1	1:D:606:GLU:OE1	2.46	0.48
2:E:165:THR:O	2:E:167:LYS:N	2.45	0.48
1:A:772:VAL:O	1:A:777:VAL:HG23	2.13	0.48
1:D:631:HIS:CD2	1:D:693:LYS:HB3	2.47	0.48
1:A:720:VAL:O	1:A:724:LEU:HD23	2.14	0.48
1:A:961:PRO:HB2	1:A:973:PHE:HE2	1.79	0.48
1:D:287:PHE:HZ	1:D:350:ALA:HB2	1.79	0.48
1:D:432:VAL:HG22	7:D:1136:HOH:O	2.12	0.48
1:A:66:ILE:HG21	1:A:72:ASN:ND2	2.28	0.48
1:A:286:LEU:HD12	1:A:286:LEU:O	2.13	0.48
2:B:25:HIS:HD2	2:B:281:MET:CE	2.27	0.48
2:B:130:ALA:HA	2:B:142:TYR:O	2.14	0.48
2:B:215:GLU:HB3	7:B:417:HOH:O	2.14	0.48
2:B:285:VAL:HG12	2:B:286:LEU:HD23	1.96	0.48
1:D:326:LEU:O	1:D:330:LEU:HG	2.13	0.48
3:F:177:VAL:O	3:F:178:ALA:HB3	2.14	0.48
1:A:18:ASP:C	1:A:20:SER:H	2.17	0.48
1:A:74:ASN:N	1:A:74:ASN:HD22	2.10	0.48
1:A:391:SER:O	1:A:399:HIS:CD2	2.67	0.48
2:B:19:ASN:HD21	2:B:38:LEU:N	2.06	0.48
1:D:30:ASN:CB	1:D:47:GLN:HE22	2.26	0.48
2:E:128:LYS:HB3	7:E:364:HOH:O	2.12	0.48
1:D:160:SER:HB3	1:D:163:LEU:HB2	1.95	0.48
1:D:324:LEU:HD21	1:D:368:ILE:HD13	1.96	0.48
1:D:451:ILE:O	1:D:455:LYS:HG2	2.14	0.48
2:E:191:TRP:CD1	2:E:192:ARG:HG3	2.48	0.48
3:F:23:LYS:O	3:F:27:VAL:HG13	2.14	0.48
2:B:282:VAL:HG12	2:B:283:SER:N	2.29	0.47
3:C:177:VAL:O	3:C:178:ALA:HB3	2.14	0.47
1:D:324:LEU:HD23	1:D:368:ILE:HD13	1.95	0.47
2:E:61:HIS:CE1	2:E:101:GLN:HE22	2.28	0.47
3:F:85:CYS:HB2	3:F:164:LEU:HD22	1.95	0.47
1:A:112:LYS:NZ	1:A:112:LYS:HB3	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:609:PRO:HD2	1:D:612:ASP:OD2	2.14	0.47
1:A:450:SER:O	1:A:453:LEU:HB3	2.14	0.47
1:A:1016:ARG:HH11	1:A:1016:ARG:HG2	1.75	0.47
2:B:259:PHE:O	2:B:274:VAL:HA	2.13	0.47
3:C:179:MET:HB3	3:C:180:PRO:HD2	1.96	0.47
1:D:25:ILE:HD12	1:D:25:ILE:N	2.24	0.47
1:D:1016:ARG:HH11	1:D:1016:ARG:HB3	1.77	0.47
2:E:5:GLN:O	2:E:5:GLN:HG2	2.13	0.47
1:A:973:PHE:CD1	1:A:973:PHE:C	2.84	0.47
2:B:73:MET:O	2:B:73:MET:HG2	2.15	0.47
3:C:143:ASN:N	3:C:143:ASN:ND2	2.61	0.47
1:D:294:LEU:O	1:D:298:LEU:N	2.44	0.47
1:D:706:PHE:CZ	1:D:709:GLN:HG2	2.50	0.47
7:D:1130:HOH:O	3:F:47:VAL:HB	2.14	0.47
2:E:30:GLN:O	2:E:33:SER:HA	2.14	0.47
2:B:52:LYS:CE	2:B:265:HIS:H	2.27	0.47
2:B:216:GLU:HG2	2:B:217:GLY:N	2.24	0.47
3:C:14:VAL:HG11	3:C:80:TYR:CD1	2.50	0.47
1:D:119:CYS:C	1:D:121:GLU:N	2.67	0.47
1:A:667:SER:O	1:A:670:GLN:HG2	2.13	0.47
3:C:36:GLU:OE2	3:C:38:LYS:HB2	2.14	0.47
1:D:724:LEU:HD12	1:D:748:MET:CG	2.41	0.47
1:A:324:LEU:HD21	1:A:368:ILE:HD13	1.96	0.47
3:C:21:THR:CG2	3:C:89:MET:HB3	2.40	0.47
3:C:42:THR:OG1	4:C:217:GTP:O1G	2.28	0.47
1:D:436:ASP:HB3	1:D:753:ARG:NH1	2.30	0.47
1:D:807:ILE:HG13	1:D:808:VAL:N	2.30	0.47
1:D:939:LEU:HD21	1:D:1016:ARG:HD2	1.95	0.47
2:E:19:ASN:HD21	2:E:38:LEU:N	2.06	0.47
2:E:19:ASN:HB2	2:E:106:GLU:HB3	1.97	0.47
2:E:244:ASP:O	2:E:248:MET:HG3	2.15	0.47
3:F:143:ASN:N	3:F:143:ASN:ND2	2.62	0.47
1:A:899:THR:HG22	1:A:903:ASN:ND2	2.29	0.47
1:D:89:THR:HG22	1:D:90:ARG:HG3	1.96	0.47
1:D:963:ASN:C	1:D:963:ASN:OD1	2.52	0.47
2:E:18:LEU:HD12	2:E:44:ARG:CZ	2.44	0.47
3:F:13:LEU:C	3:F:13:LEU:HD23	2.36	0.47
1:A:314:ASP:CB	7:A:1259:HOH:O	2.61	0.47
1:A:548:VAL:O	1:A:548:VAL:HG12	2.14	0.47
1:D:129:LYS:O	1:D:133:ILE:HG13	2.15	0.47
1:D:422:SER:C	1:D:423:ARG:HG2	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:925:HIS:O	1:D:928:SER:HB3	2.14	0.47
2:E:352:ASP:N	2:E:352:ASP:OD1	2.47	0.47
1:D:525:LEU:HD21	2:E:9:LEU:HA	1.97	0.47
1:A:43:GLN:HB2	1:A:44:ARG:NH1	2.31	0.46
1:A:103:LYS:NZ	1:A:103:LYS:HB3	2.29	0.46
1:A:149:PHE:O	1:A:153:ILE:HG12	2.15	0.46
1:A:276:VAL:HG23	1:A:283:PHE:CD2	2.50	0.46
2:B:25:HIS:CD2	2:B:281:MET:HE1	2.50	0.46
1:D:690:SER:HB2	7:D:1211:HOH:O	2.14	0.46
1:A:51:THR:HG22	1:A:51:THR:O	2.15	0.46
1:A:30:ASN:CB	1:A:47:GLN:HE22	2.28	0.46
1:A:856:ASN:ND2	1:A:860:PHE:HD1	2.12	0.46
3:C:45:VAL:HG22	3:C:46:GLU:N	2.30	0.46
1:D:559:TRP:CD2	1:D:603:GLN:HG3	2.50	0.46
1:A:961:PRO:HD3	1:A:970:ASN:ND2	2.31	0.46
2:B:52:LYS:HZ3	2:B:264:THR:CA	2.08	0.46
2:B:244:ASP:O	2:B:248:MET:HG3	2.15	0.46
1:D:17:LEU:HD23	1:D:19:PHE:H	1.80	0.46
1:D:47:GLN:HG2	1:D:48:GLU:N	2.29	0.46
1:D:51:THR:O	1:D:51:THR:HG22	2.16	0.46
1:D:71:GLN:HG3	1:D:72:ASN:N	2.30	0.46
1:D:112:LYS:O	1:D:112:LYS:HD3	2.15	0.46
1:D:286:LEU:HD12	1:D:286:LEU:O	2.15	0.46
1:D:426:LYS:HA	1:D:427:PRO:HD3	1.75	0.46
1:D:437:GLN:HG3	1:D:753:ARG:HH12	1.80	0.46
1:D:561:PHE:HB2	2:E:6:LEU:CD1	2.45	0.46
1:A:160:SER:HB3	1:A:163:LEU:HB2	1.96	0.46
2:B:261:HIS:CD2	2:B:263:GLN:H	2.34	0.46
1:D:92:LYS:HE3	1:D:140:GLN:OE1	2.15	0.46
1:D:500:ALA:O	1:D:503:SER:OG	2.28	0.46
1:D:664:VAL:CB	1:D:691:ILE:HD11	2.44	0.46
1:D:960:THR:HA	1:D:961:PRO:HD3	1.82	0.46
2:E:188:VAL:HG13	2:E:188:VAL:O	2.16	0.46
1:A:17:LEU:HG	1:A:22:LYS:HE2	1.97	0.46
1:A:139:LYS:CE	1:A:177:GLU:HB3	2.44	0.46
1:D:63:VAL:HA	1:D:76:LYS:HG2	1.97	0.46
1:D:521:ILE:HG13	1:D:522:LYS:N	2.31	0.46
1:D:664:VAL:HB	1:D:691:ILE:CD1	2.45	0.46
1:A:276:VAL:O	1:A:276:VAL:CG2	2.64	0.46
1:A:314:ASP:OD1	1:A:315:GLU:N	2.49	0.46
1:A:887:ARG:HA	1:A:887:ARG:HD2	1.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:966:ASN:H	1:A:967:PRO:HD2	1.75	0.46
2:B:61:HIS:CE1	2:B:101:GLN:HE22	2.31	0.46
1:D:122:LYS:O	1:D:123:GLU:O	2.34	0.46
1:D:177:GLU:OE1	1:D:177:GLU:HA	2.15	0.46
1:A:17:LEU:O	1:A:22:LYS:HG2	2.16	0.46
1:A:27:LEU:C	1:A:27:LEU:HD23	2.35	0.46
1:A:56:HIS:HE1	7:A:1301:HOH:O	1.97	0.46
3:C:55:ASN:ND2	3:C:55:ASN:H	2.13	0.46
1:D:537:LYS:HB3	2:E:14:LEU:HD23	1.96	0.46
2:E:38:LEU:CD1	2:E:44:ARG:HE	2.29	0.46
3:F:105:HIS:CE1	3:F:109:VAL:HG11	2.51	0.46
3:F:143:ASN:HD22	3:F:143:ASN:H	1.61	0.46
1:A:664:VAL:HB	1:A:691:ILE:CD1	2.46	0.46
1:A:768:ASP:O	1:A:772:VAL:HG23	2.16	0.46
1:A:975:GLN:HG2	1:A:1002:PHE:CE1	2.51	0.46
1:D:391:SER:HB2	7:D:1188:HOH:O	2.16	0.46
1:D:529:GLU:HG3	2:E:11:ARG:NH2	2.31	0.46
1:D:804:MET:HB3	1:D:851:LEU:HD13	1.98	0.46
2:E:259:PHE:O	2:E:274:VAL:HA	2.15	0.46
1:A:122:LYS:O	1:A:123:GLU:O	2.35	0.45
2:B:290:VAL:N	2:B:291:PRO:CD	2.77	0.45
1:D:127:ILE:HD12	1:D:127:ILE:H	1.80	0.45
1:D:139:LYS:CE	1:D:177:GLU:HB3	2.46	0.45
1:D:432:VAL:HG12	1:D:442:ARG:HG2	1.99	0.45
1:D:735:ASN:ND2	7:D:1269:HOH:O	2.47	0.45
1:D:1048:GLU:HG3	1:D:1048:GLU:O	2.15	0.45
1:A:100:GLU:HA	1:A:103:LYS:CD	2.42	0.45
1:A:659:LEU:HD22	1:A:659:LEU:HA	1.75	0.45
1:A:672:ALA:C	1:A:674:LYS:H	2.19	0.45
1:A:807:ILE:CD1	1:A:815:ILE:HD12	2.41	0.45
1:D:55:GLU:C	1:D:57:PRO:HD3	2.36	0.45
1:D:232:PHE:O	1:D:236:ILE:HG23	2.16	0.45
2:E:49:GLU:CB	2:E:52:LYS:HZ2	2.29	0.45
2:E:118:GLU:O	2:E:262:LYS:HG3	2.16	0.45
1:A:71:GLN:HG3	1:A:72:ASN:N	2.31	0.45
1:A:301:ASN:H	1:A:301:ASN:ND2	2.13	0.45
1:A:960:THR:HG22	1:A:963:ASN:H	1.82	0.45
1:D:51:THR:HB	1:D:78:TYR:OH	2.16	0.45
1:A:25:ILE:HD12	1:A:25:ILE:N	2.27	0.45
1:A:88:LYS:HD2	1:A:136:GLN:NE2	2.32	0.45
1:A:610:PHE:CD2	1:A:614:ILE:HD11	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:359:GLU:O	2:B:360:ASN:C	2.55	0.45
1:D:272:ALA:HB1	1:D:329:PHE:HD1	1.82	0.45
1:A:155:GLY:O	1:A:159:THR:HG23	2.16	0.45
2:B:246:LEU:HD11	2:B:282:VAL:HG11	1.97	0.45
2:B:277:LEU:CD2	2:B:281:MET:HE2	2.46	0.45
3:C:141:LYS:HD2	3:C:141:LYS:N	2.29	0.45
1:D:279:TYR:HD2	1:D:282:GLN:NE2	2.15	0.45
1:D:823:PHE:O	1:D:827:PHE:HB3	2.16	0.45
3:F:15:LEU:HD11	3:F:89:MET:HE3	1.99	0.45
2:B:53:SER:O	2:B:54:LYS:C	2.55	0.45
2:B:160:ASN:HD22	2:B:162:ARG:H	1.65	0.45
3:C:55:ASN:ND2	3:C:55:ASN:N	2.65	0.45
1:D:772:VAL:O	1:D:777:VAL:HG23	2.16	0.45
1:D:875:LEU:O	1:D:879:ILE:HD13	2.17	0.45
3:F:20:GLY:HA2	4:F:217:GTP:H5"	1.99	0.45
3:F:141:LYS:HD2	3:F:141:LYS:N	2.29	0.45
1:A:123:GLU:C	1:A:125:VAL:N	2.70	0.45
1:D:920:CYS:HB3	1:D:977:TYR:CE2	2.52	0.45
2:E:246:LEU:HD11	2:E:282:VAL:HG11	1.97	0.45
1:A:962:LEU:O	1:A:964:PRO:HD3	2.17	0.45
1:D:514:LYS:O	1:D:518:VAL:HG23	2.17	0.45
1:D:797:GLU:HA	1:D:798:PRO:HD2	1.85	0.45
1:D:807:ILE:CD1	1:D:815:ILE:HD12	2.40	0.45
2:E:130:ALA:HA	2:E:142:TYR:O	2.16	0.45
3:F:106:ARG:O	3:F:110:ARG:HG3	2.17	0.45
3:F:133:ALA:HA	3:F:136:ILE:HD12	1.99	0.45
1:A:879:ILE:HD12	1:A:879:ILE:N	2.31	0.45
2:B:350:SER:HA	2:B:351:PRO:HD3	1.73	0.45
1:D:80:LEU:HD22	1:D:133:ILE:HD12	1.99	0.45
1:D:142:TRP:N	1:D:143:PRO:HD2	2.32	0.45
2:E:176:TYR:HB2	2:E:183:TYR:CD1	2.52	0.45
3:F:177:VAL:HG21	3:F:179:MET:CE	2.47	0.45
1:A:559:TRP:CD2	1:A:603:GLN:HG3	2.51	0.45
1:A:687:GLN:O	1:A:691:ILE:HG13	2.17	0.45
3:C:106:ARG:O	3:C:110:ARG:HG3	2.17	0.45
1:D:301:ASN:H	1:D:301:ASN:ND2	2.14	0.45
3:F:56:ARG:HB2	3:F:174:LEU:HD11	1.98	0.45
1:D:777:VAL:O	1:D:780:LEU:HB2	2.17	0.44
1:D:838:PHE:HD1	1:D:884:HIS:CD2	2.35	0.44
1:A:962:LEU:HD12	1:A:973:PHE:HB2	2.00	0.44
3:C:148:ASP:HB2	7:C:198:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:GLN:HB2	1:D:44:ARG:NH1	2.32	0.44
1:D:922:ILE:O	1:D:926:ILE:HG12	2.17	0.44
1:D:548:VAL:O	1:D:548:VAL:HG12	2.17	0.44
1:A:189:VAL:HG11	1:A:1038:ARG:HB2	2.00	0.44
1:D:770:GLN:HG2	1:D:771:MET:N	2.31	0.44
1:D:841:TYR:O	1:D:845:ARG:HG3	2.18	0.44
1:D:962:LEU:HG	1:D:962:LEU:O	2.17	0.44
2:E:121:VAL:HA	2:E:258:LEU:O	2.17	0.44
2:E:349:HIS:CD2	2:E:351:PRO:HG3	2.53	0.44
1:A:142:TRP:N	1:A:143:PRO:HD2	2.33	0.44
1:A:205:ILE:HG22	1:A:206:PHE:N	2.33	0.44
1:A:399:HIS:HB3	1:A:401:ASP:OD2	2.16	0.44
2:B:49:GLU:HB3	2:B:52:LYS:HZ2	1.83	0.44
1:D:881:ALA:O	1:D:884:HIS:HB2	2.17	0.44
2:E:41:SER:O	2:E:45:ARG:HG3	2.17	0.44
1:A:521:ILE:HG13	1:A:522:LYS:N	2.32	0.44
2:B:121:VAL:HA	2:B:258:LEU:O	2.17	0.44
1:D:189:VAL:HG22	7:D:1253:HOH:O	2.18	0.44
1:D:314:ASP:OD1	1:D:315:GLU:N	2.51	0.44
1:D:659:LEU:HD22	1:D:659:LEU:HA	1.83	0.44
1:A:73:MET:HB2	1:A:122:LYS:HE3	1.99	0.44
1:A:103:LYS:NZ	1:A:103:LYS:CB	2.79	0.44
1:A:570:PHE:O	1:A:573:MET:HB2	2.18	0.44
2:B:38:LEU:CD1	2:B:44:ARG:HE	2.30	0.44
1:A:327:CYS:O	1:A:331:LYS:HB2	2.17	0.44
1:D:558:HIS:HB3	2:E:6:LEU:HD11	2.00	0.44
1:D:615:LEU:HD23	1:D:618:ILE:HD11	2.00	0.44
1:D:1013:GLU:HA	1:D:1016:ARG:HD3	2.00	0.44
2:E:25:HIS:ND1	2:E:26:PRO:CD	2.79	0.44
3:F:153:SER:O	3:F:154:ASN:HB2	2.17	0.44
1:D:436:ASP:HB3	1:D:753:ARG:HH12	1.82	0.43
2:E:25:HIS:HD2	2:E:281:MET:CE	2.31	0.43
2:E:353:HIS:HA	2:E:354:PRO:HD3	1.84	0.43
1:A:778:PRO:HB2	1:A:779:PRO:HD3	2.00	0.43
2:B:38:LEU:CD2	2:B:39:GLU:H	2.31	0.43
3:C:105:HIS:CE1	3:C:109:VAL:HG11	2.53	0.43
2:E:123:VAL:HG21	2:E:250:PHE:CZ	2.53	0.43
2:E:277:LEU:CD2	2:E:281:MET:HE2	2.48	0.43
3:F:29:ARG:NH1	7:F:634:HOH:O	2.51	0.43
1:A:87:ILE:O	1:A:91:TRP:HB2	2.18	0.43
1:A:149:PHE:CE2	1:A:153:ILE:HD13	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:GLU:HG3	1:A:343:LEU:HD21	2.00	0.43
1:A:887:ARG:HD3	1:A:937:ALA:CB	2.44	0.43
1:A:1013:GLU:HA	1:A:1016:ARG:HD3	2.00	0.43
2:B:25:HIS:CD2	2:B:281:MET:CE	3.02	0.43
2:E:162:ARG:O	2:E:163:ASN:ND2	2.51	0.43
1:A:61:THR:HA	1:A:64:ASP:HB2	1.99	0.43
1:A:176:GLU:O	1:A:180:ASP:HB2	2.18	0.43
1:A:875:LEU:O	1:A:879:ILE:HD13	2.18	0.43
2:B:241:SER:O	2:B:245:VAL:HG23	2.18	0.43
3:C:13:LEU:HD23	3:C:13:LEU:C	2.39	0.43
1:D:907:GLU:O	1:D:911:ALA:HB2	2.18	0.43
2:E:92:LYS:HE3	2:E:93:LYS:O	2.18	0.43
3:F:12:LYS:HE3	3:F:64:TRP:CE2	2.53	0.43
3:F:55:ASN:ND2	3:F:55:ASN:H	2.15	0.43
1:A:664:VAL:CB	1:A:691:ILE:HD11	2.48	0.43
1:A:763:VAL:O	1:A:810:LYS:HG2	2.18	0.43
1:A:956:GLY:HA3	7:A:1265:HOH:O	2.19	0.43
1:D:150:ILE:HD11	1:D:205:ILE:HD11	1.98	0.43
1:D:658:MET:O	1:D:662:ASN:HB2	2.19	0.43
1:D:997:PHE:O	1:D:1001:LEU:HG	2.18	0.43
1:A:103:LYS:O	1:A:107:VAL:HG23	2.19	0.43
1:A:1021:GLN:HE22	1:A:1033:LEU:CD2	2.29	0.43
3:C:143:ASN:HD22	3:C:143:ASN:H	1.64	0.43
1:D:39:GLU:HG3	1:D:40:GLY:N	2.34	0.43
1:D:624:ASP:HB3	7:D:1099:HOH:O	2.19	0.43
2:E:52:LYS:CE	2:E:265:HIS:H	2.29	0.43
3:F:55:ASN:ND2	3:F:55:ASN:N	2.66	0.43
1:A:116:ASP:OD1	1:A:117:PRO:HD2	2.18	0.43
1:A:238:LEU:HD22	1:A:242:PHE:HE2	1.83	0.43
1:A:437:GLN:NE2	1:A:746:ARG:HB3	2.34	0.43
1:A:990:GLN:HG2	1:A:993:GLN:OE1	2.19	0.43
1:D:24:ASP:O	1:D:28:LEU:HB2	2.18	0.43
1:D:521:ILE:HD11	2:E:7:PRO:HG2	2.00	0.43
1:D:675:ASN:ND2	1:D:677:ASP:HB2	2.31	0.43
1:D:680:LYS:HB2	1:D:680:LYS:HZ2	1.83	0.43
1:D:1006:GLN:CD	1:D:1049:LYS:HD2	2.39	0.43
2:E:42:GLU:HB2	2:E:110:ASP:OD1	2.19	0.43
3:F:21:THR:CG2	3:F:89:MET:HB3	2.45	0.43
1:A:35:LEU:HD21	7:C:234:HOH:O	2.17	0.43
1:A:63:VAL:HA	1:A:76:LYS:HG2	2.00	0.43
1:A:680:LYS:HB2	1:A:680:LYS:NZ	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:856:ASN:HD22	1:A:860:PHE:HD1	1.67	0.43
2:B:4:LEU:O	2:B:5:GLN:CB	2.66	0.43
2:B:120:ILE:HG13	2:B:260:TYR:HB2	2.01	0.43
1:D:61:THR:HA	1:D:64:ASP:HB2	2.00	0.43
1:D:91:TRP:HA	1:D:94:LEU:HD12	2.01	0.43
1:D:123:GLU:C	1:D:125:VAL:N	2.72	0.43
2:E:49:GLU:HB3	2:E:52:LYS:NZ	2.34	0.43
2:E:120:ILE:HG13	2:E:260:TYR:HB2	2.01	0.43
3:F:36:GLU:OE2	3:F:38:LYS:HB2	2.18	0.43
1:A:27:LEU:HD13	1:A:62:ARG:HH11	1.84	0.43
1:A:664:VAL:CG1	1:A:691:ILE:HD11	2.49	0.43
1:D:27:LEU:HD13	1:D:62:ARG:CZ	2.48	0.43
1:D:521:ILE:HD11	2:E:7:PRO:CB	2.49	0.43
1:D:664:VAL:CG1	1:D:691:ILE:HD11	2.49	0.43
2:E:49:GLU:C	2:E:51:GLN:H	2.20	0.43
1:A:939:LEU:HD21	1:A:1016:ARG:HD2	2.01	0.43
1:D:860:PHE:N	1:D:861:PRO:CD	2.82	0.43
1:D:962:LEU:O	1:D:963:ASN:CB	2.67	0.43
2:E:53:SER:O	2:E:54:LYS:C	2.58	0.43
3:F:55:ASN:HD22	3:F:55:ASN:H	1.67	0.43
1:A:51:THR:HB	1:A:78:TYR:OH	2.19	0.42
1:A:62:ARG:HA	1:A:62:ARG:HD3	1.74	0.42
1:A:559:TRP:NE1	1:A:606:GLU:OE1	2.52	0.42
1:A:770:GLN:HG2	1:A:771:MET:N	2.33	0.42
1:A:823:PHE:O	1:A:827:PHE:HB3	2.18	0.42
1:A:954:GLU:HB2	1:A:955:GLU:OE1	2.19	0.42
3:C:75:LEU:N	3:C:75:LEU:CD1	2.80	0.42
1:D:514:LYS:NZ	1:D:558:HIS:CE1	2.86	0.42
1:A:23:LEU:HD11	1:A:26:ASN:HB2	2.01	0.42
1:A:132:MET:O	1:A:136:GLN:HG2	2.19	0.42
1:A:479:LYS:HD2	7:A:1100:HOH:O	2.19	0.42
2:B:6:LEU:HA	2:B:7:PRO:HD3	1.88	0.42
2:B:212:LEU:N	2:B:213:PRO:CD	2.83	0.42
1:D:87:ILE:O	1:D:91:TRP:HB2	2.18	0.42
3:F:75:LEU:N	3:F:75:LEU:CD1	2.81	0.42
1:A:610:PHE:CE2	1:A:614:ILE:HD11	2.55	0.42
3:C:54:THR:HG22	3:C:176:PHE:CD1	2.54	0.42
1:D:58:ASP:HB2	1:D:62:ARG:HH21	1.84	0.42
1:D:611:ILE:HD13	1:D:640:MET:CE	2.48	0.42
2:E:94:LEU:HA	2:E:95:PRO:HD3	1.88	0.42
1:A:299:PRO:HG2	1:A:302:THR:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:GLU:HB3	1:A:440:VAL:HG12	2.00	0.42
1:A:704:HIS:HB3	1:A:705:PRO:HD3	2.01	0.42
2:B:45:ARG:HA	2:B:273:LEU:CD1	2.47	0.42
2:B:184:TYR:CZ	2:B:252:PHE:HD1	2.37	0.42
3:C:55:ASN:HD22	3:C:55:ASN:H	1.67	0.42
1:D:720:VAL:O	1:D:724:LEU:HD23	2.19	0.42
1:D:841:TYR:N	1:D:842:PRO:HD3	2.34	0.42
3:F:45:VAL:HG22	3:F:46:GLU:N	2.34	0.42
3:F:138:PHE:O	3:F:141:LYS:HD2	2.19	0.42
1:A:807:ILE:HG13	1:A:808:VAL:N	2.35	0.42
2:B:188:VAL:HG13	2:B:188:VAL:O	2.20	0.42
1:D:231:ARG:HH22	3:F:142:LYS:NZ	2.17	0.42
1:D:305:ARG:HG3	1:D:361:GLU:HG3	2.01	0.42
2:E:49:GLU:HB3	2:E:52:LYS:HZ2	1.83	0.42
2:E:187:ASP:HA	2:E:208:MET:SD	2.59	0.42
3:C:159:LYS:HB2	3:C:160:PRO:HD3	2.00	0.42
1:D:56:HIS:C	1:D:58:ASP:H	2.22	0.42
1:D:815:ILE:HG12	1:D:815:ILE:O	2.20	0.42
1:D:887:ARG:HE	3:F:94:SER:HB2	1.84	0.42
2:E:38:LEU:CD2	2:E:39:GLU:H	2.32	0.42
2:E:212:LEU:HB2	2:E:213:PRO:HD3	2.02	0.42
1:A:134:LEU:O	1:A:138:LEU:HG	2.19	0.42
2:B:15:SER:HB2	2:B:16:GLN:H	1.68	0.42
2:B:70:TRP:HB3	2:B:96:LYS:HD2	2.01	0.42
1:D:945:ILE:O	1:D:949:MET:HG3	2.20	0.42
2:E:48:LEU:HD11	7:E:408:HOH:O	2.20	0.42
1:A:56:HIS:CE1	7:A:1301:HOH:O	2.72	0.42
1:A:254:PHE:HB3	1:A:260:PHE:HB3	2.02	0.42
2:B:258:LEU:HD23	2:B:258:LEU:HA	1.90	0.42
1:D:23:LEU:HD11	1:D:26:ASN:HB2	2.02	0.42
1:D:964:PRO:CB	1:D:968:VAL:HB	2.49	0.42
2:E:184:TYR:CZ	2:E:252:PHE:HD1	2.38	0.42
1:A:907:GLU:O	1:A:907:GLU:HG3	2.20	0.42
2:B:42:GLU:HB2	2:B:110:ASP:OD1	2.20	0.42
1:D:17:LEU:HD22	1:D:20:SER:CB	2.50	0.42
1:D:402:ILE:H	1:D:402:ILE:HG12	1.71	0.42
1:D:973:PHE:CD1	1:D:973:PHE:C	2.91	0.42
1:A:262:ASN:OD1	1:A:318:PHE:HA	2.20	0.42
2:B:123:VAL:HG22	2:B:257:LEU:CD2	2.50	0.42
2:B:123:VAL:HG22	2:B:257:LEU:HD21	2.02	0.42
1:D:189:VAL:HG11	1:D:1038:ARG:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:834:ILE:O	1:D:845:ARG:NH2	2.53	0.42
1:D:954:GLU:C	1:D:955:GLU:HG3	2.39	0.42
1:D:978:VAL:O	1:D:981:LEU:HB3	2.20	0.42
1:A:777:VAL:O	1:A:780:LEU:HB2	2.21	0.41
1:D:60:TRP:CZ2	1:D:102:ILE:HD13	2.45	0.41
2:E:64:ARG:NH1	2:E:71:THR:H	2.18	0.41
1:A:651:GLU:HG2	1:A:708:ILE:HD12	2.02	0.41
1:A:907:GLU:O	1:A:911:ALA:HB2	2.19	0.41
1:D:299:PRO:HG2	1:D:302:THR:HG23	2.02	0.41
1:D:961:PRO:HB2	1:D:973:PHE:CE2	2.55	0.41
2:E:26:PRO:HG2	2:E:109:ILE:HD11	2.02	0.41
1:A:49:VAL:CG2	3:C:75:LEU:HD11	2.50	0.41
1:A:57:PRO:HA	1:A:60:TRP:CH2	2.55	0.41
1:A:360:VAL:HG11	1:A:365:ILE:HD12	2.03	0.41
1:A:464:LEU:HD23	1:A:464:LEU:HA	1.84	0.41
1:A:688:LEU:O	1:A:692:LEU:HG	2.19	0.41
1:A:733:GLN:HB2	1:A:792:VAL:HG11	2.03	0.41
2:B:43:ARG:CG	2:B:44:ARG:H	2.15	0.41
2:B:296:THR:O	2:B:297:THR:O	2.38	0.41
1:D:282:GLN:OE1	1:D:282:GLN:N	2.41	0.41
1:D:629:GLN:HE21	1:D:629:GLN:HB2	1.66	0.41
3:F:69:LEU:HD23	3:F:69:LEU:HA	1.81	0.41
3:F:114:ASN:ND2	7:F:590:HOH:O	2.54	0.41
1:A:324:LEU:HD23	1:A:368:ILE:HD13	2.02	0.41
1:A:856:ASN:ND2	1:A:860:PHE:CD1	2.88	0.41
1:D:304:ILE:CG2	1:D:319:ILE:HD13	2.50	0.41
1:D:672:ALA:C	1:D:674:LYS:H	2.24	0.41
1:D:797:GLU:HB3	1:D:800:VAL:HG23	2.02	0.41
1:D:807:ILE:HD11	1:D:815:ILE:CD1	2.44	0.41
2:E:40:GLN:HE22	2:E:42:GLU:HB3	1.86	0.41
1:A:451:ILE:O	1:A:455:LYS:HG2	2.20	0.41
2:B:27:ARG:HG3	2:B:31:TYR:CD1	2.53	0.41
1:D:296:GLN:HB3	7:D:1166:HOH:O	2.21	0.41
1:D:560:LYS:HA	1:D:560:LYS:HD2	1.85	0.41
3:F:100:ASN:HD22	3:F:100:ASN:HA	1.68	0.41
1:A:192:LYS:HB2	1:A:192:LYS:NZ	2.35	0.41
1:A:326:LEU:O	1:A:330:LEU:HG	2.20	0.41
1:A:445:MET:HB3	1:A:448:THR:HG23	2.03	0.41
1:A:821:GLN:NE2	7:A:1093:HOH:O	2.54	0.41
1:D:73:MET:SD	1:D:126:TYR:HB2	2.60	0.41
1:D:98:GLN:O	1:D:102:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:437:GLN:HG3	1:D:753:ARG:HH22	1.86	0.41
1:D:688:LEU:O	1:D:692:LEU:HG	2.20	0.41
1:A:21:GLN:H	1:A:21:GLN:HG2	1.33	0.41
1:A:98:GLN:O	1:A:102:ILE:HG12	2.20	0.41
1:A:115:SER:O	1:A:116:ASP:C	2.58	0.41
1:D:724:LEU:HD13	1:D:724:LEU:HA	1.87	0.41
1:A:146:TRP:N	1:A:147:PRO:CD	2.83	0.41
1:A:435:ASN:O	1:A:437:GLN:N	2.51	0.41
1:A:575:GLU:HG2	1:A:580:VAL:HG11	2.03	0.41
1:A:879:ILE:N	1:A:879:ILE:CD1	2.84	0.41
1:A:954:GLU:C	1:A:955:GLU:HG3	2.40	0.41
2:B:280:TYR:HA	2:B:294:PRO:CB	2.51	0.41
3:C:12:LYS:HE3	3:C:64:TRP:CE2	2.56	0.41
1:D:741:LYS:HG2	1:D:746:ARG:NH1	2.36	0.41
1:D:809:ASN:HA	1:D:858:HIS:CD2	2.47	0.41
1:D:840:GLU:O	1:D:845:ARG:NH1	2.53	0.41
1:D:859:CYS:C	1:D:861:PRO:HD2	2.41	0.41
2:E:25:HIS:CD2	2:E:281:MET:HE1	2.55	0.41
2:E:48:LEU:O	2:E:51:GLN:HB3	2.21	0.41
3:F:29:ARG:HB3	3:F:157:PHE:HZ	1.85	0.41
3:F:54:THR:HG22	3:F:176:PHE:CD1	2.56	0.41
1:A:873:LEU:HD12	1:A:873:LEU:HA	1.82	0.41
2:B:152:PHE:CD1	2:B:152:PHE:N	2.88	0.41
2:B:155:LEU:HG	2:B:225:ASN:HB2	2.02	0.41
1:D:119:CYS:C	1:D:121:GLU:H	2.23	0.41
1:D:218:ASN:OD1	1:D:220:PRO:HD2	2.20	0.41
1:D:284:GLU:HG3	1:D:343:LEU:HD21	2.02	0.41
1:A:550:GLN:O	1:A:552:PRO:HD2	2.20	0.40
1:A:866:ILE:HB	1:A:867:PRO:HD2	2.02	0.40
2:B:18:LEU:HD12	2:B:44:ARG:CZ	2.51	0.40
2:B:54:LYS:HD3	2:B:198:ASP:OD2	2.20	0.40
1:D:15:GLN:HA	1:D:22:LYS:HE3	2.03	0.40
1:D:388:THR:HG21	1:D:402:ILE:HD13	2.02	0.40
1:D:718:LEU:O	1:D:721:TYR:HB3	2.21	0.40
1:D:989:LEU:HD11	1:D:1022:ILE:HG22	2.04	0.40
2:E:15:SER:C	2:E:17:ASP:N	2.75	0.40
3:F:89:MET:HG3	3:F:120:CYS:HB2	2.03	0.40
1:D:270:GLU:OE2	1:D:270:GLU:HA	2.21	0.40
1:D:427:PRO:C	7:D:1239:HOH:O	2.59	0.40
1:D:575:GLU:HG2	1:D:580:VAL:HG11	2.03	0.40
1:D:782:ASP:OD2	2:E:360:ASN:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:954:GLU:HB2	1:D:955:GLU:OE1	2.22	0.40
2:E:70:TRP:HB3	2:E:96:LYS:HD2	2.02	0.40
3:F:91:ASP:OD1	3:F:123:LYS:HD3	2.20	0.40
1:A:49:VAL:HG22	3:C:75:LEU:CD1	2.52	0.40
1:A:122:LYS:HA	1:A:122:LYS:HD2	1.70	0.40
1:A:517:LEU:HD23	1:A:517:LEU:HA	1.87	0.40
2:B:4:LEU:HB2	2:B:6:LEU:HD13	1.99	0.40
1:D:27:LEU:O	1:D:31:VAL:HG23	2.22	0.40
1:A:109:LEU:O	1:A:113:THR:HG23	2.22	0.40
1:A:607:VAL:HG13	1:A:608:MET:HG2	2.02	0.40
1:A:703:GLY:C	1:A:705:PRO:HD2	2.42	0.40
1:A:989:LEU:HD11	1:A:1022:ILE:HG22	2.04	0.40
2:B:8:PRO:CA	2:B:10:GLU:OE1	2.70	0.40
1:D:262:ASN:OD1	1:D:318:PHE:HA	2.22	0.40
1:D:626:GLN:HB3	1:D:627:PRO:HD2	2.03	0.40
2:E:59:VAL:HA	2:E:195:PRO:HG2	2.02	0.40
3:F:146:TYR:CG	3:F:147:TYR:N	2.90	0.40
1:A:24:ASP:O	1:A:28:LEU:HB2	2.22	0.40
1:A:232:PHE:HD2	1:A:232:PHE:HA	1.78	0.40
1:A:922:ILE:O	1:A:926:ILE:HG12	2.21	0.40
2:B:359:GLU:HA	7:B:389:HOH:O	2.20	0.40
3:C:8:GLN:HE21	3:C:8:GLN:HB2	1.68	0.40
3:C:29:ARG:NE	3:C:154:ASN:HD21	2.19	0.40
3:C:101:VAL:N	3:C:102:PRO:CD	2.85	0.40
1:D:379:GLU:HG2	1:D:405:ARG:HH22	1.85	0.40
2:E:279:PRO:CB	2:E:294:PRO:HB2	2.51	0.40
2:E:280:TYR:CE1	2:E:281:MET:HG3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1034/1073 (96%)	931 (90%)	85 (8%)	18 (2%)	9	29
1	D	1034/1073 (96%)	933 (90%)	83 (8%)	18 (2%)	9	29
2	B	285/362 (79%)	251 (88%)	23 (8%)	11 (4%)	3	10
2	E	287/362 (79%)	249 (87%)	28 (10%)	10 (4%)	3	12
3	C	171/176 (97%)	157 (92%)	13 (8%)	1 (1%)	25	56
3	F	171/176 (97%)	154 (90%)	16 (9%)	1 (1%)	25	56
All	All	2982/3222 (93%)	2675 (90%)	248 (8%)	59 (2%)	7	24

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
1	A	963	ASN
2	B	216	GLU
1	D	123	GLU
1	D	963	ASN
2	E	216	GLU
2	E	290	VAL
2	E	292	ALA
1	A	54	LYS
1	A	64	ASP
1	A	122	LYS
1	A	484	VAL
1	A	486	GLY
1	A	1027	GLY
1	A	1029	ASP
2	B	33	SER
2	B	54	LYS
1	D	41	ALA
1	D	54	LYS
1	D	64	ASP
1	D	122	LYS
1	D	486	GLY
1	D	1027	GLY
1	D	1029	ASP
2	E	54	LYS
1	A	21	GLN
1	A	277	SER
1	A	961	PRO
1	A	1035	LEU
2	B	181	GLN

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Mol	Chain	Res	Type
2	B	291	PRO
1	D	1035	LEU
2	E	33	SER
2	E	166	ALA
2	E	181	GLN
1	A	259	MET
2	B	43	ARG
2	B	351	PRO
1	D	258	PRO
1	D	277	SER
1	D	427	PRO
1	A	258	PRO
1	A	427	PRO
2	B	16	GLN
3	C	76	ARG
1	D	51	THR
1	D	259	MET
1	D	468	ASP
1	D	484	VAL
3	F	76	ARG
1	A	114	SER
1	D	392	PRO
2	E	294	PRO
2	B	26	PRO
2	B	294	PRO
1	A	143	PRO
2	B	287	GLY
2	E	26	PRO
2	E	291	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	942/973 (97%)	869 (92%)	73 (8%)	13	35
1	D	942/973 (97%)	870 (92%)	72 (8%)	13	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	263/327 (80%)	236 (90%)	27 (10%)	7 21
2	E	265/327 (81%)	244 (92%)	21 (8%)	12 34
3	C	152/154 (99%)	136 (90%)	16 (10%)	7 20
3	F	152/154 (99%)	133 (88%)	19 (12%)	4 14
All	All	2716/2908 (93%)	2488 (92%)	228 (8%)	11 31

All (228) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	23	LEU
1	A	29	ASP
1	A	33	ASN
1	A	34	CYS
1	A	35	LEU
1	A	45	MET
1	A	47	GLN
1	A	50	LEU
1	A	63	VAL
1	A	65	THR
1	A	74	ASN
1	A	86	VAL
1	A	103	LYS
1	A	121	GLU
1	A	129	LYS
1	A	146	TRP
1	A	158	ARG
1	A	163	LEU
1	A	187	THR
1	A	192	LYS
1	A	204	GLN
1	A	217	GLN
1	A	229	LEU
1	A	257	VAL
1	A	288	THR
1	A	301	ASN
1	A	312	LYS
1	A	320	GLN
1	A	348	MET
1	A	387	SER
1	A	391	SER

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Mol	Chain	Res	Type
1	A	402	ILE
1	A	423	ARG
1	A	440	VAL
1	A	443	GLU
1	A	447	ASP
1	A	479	LYS
1	A	493	ASN
1	A	521	ILE
1	A	525	LEU
1	A	535	ASP
1	A	571	GLU
1	A	578	ASP
1	A	597	ARG
1	A	606	GLU
1	A	613	GLU
1	A	620	THR
1	A	647	GLN
1	A	659	LEU
1	A	719	ASN
1	A	749	ARG
1	A	781	LEU
1	A	799	GLU
1	A	804	MET
1	A	807	ILE
1	A	818	GLU
1	A	828	GLU
1	A	834	ILE
1	A	875	LEU
1	A	887	ARG
1	A	891	ASP
1	A	959	SER
1	A	962	LEU
1	A	969	ASN
1	A	970	ASN
1	A	976	ASP
1	A	1016	ARG
1	A	1028	GLU
1	A	1030	THR
1	A	1031	SER
1	A	1048	GLU
1	A	1050	HIS
2	B	4	LEU

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Mol	Chain	Res	Type
2	B	10	GLU
2	B	32	LYS
2	B	33	SER
2	B	34	LYS
2	B	38	LEU
2	B	92	LYS
2	B	111	VAL
2	B	120	ILE
2	B	128	LYS
2	B	129	ARG
2	B	138	SER
2	B	150	ASN
2	B	189	MET
2	B	223	LYS
2	B	234	ASN
2	B	235	PHE
2	B	240	GLU
2	B	264	THR
2	B	270	SER
2	B	274	VAL
2	B	282	VAL
2	B	295	LEU
2	B	352	ASP
2	B	353	HIS
2	B	356	CYS
2	B	357	LEU
3	C	8	GLN
3	C	27	VAL
3	C	29	ARG
3	C	38	LYS
3	C	40	VAL
3	C	43	LEU
3	C	51	VAL
3	C	55	ASN
3	C	70	GLU
3	C	75	LEU
3	C	76	ARG
3	C	77	ASP
3	C	140	ARG
3	C	141	LYS
3	C	143	ASN
3	C	156	ASN

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Mol	Chain	Res	Type
1	D	23	LEU
1	D	27	LEU
1	D	29	ASP
1	D	33	ASN
1	D	34	CYS
1	D	35	LEU
1	D	45	MET
1	D	47	GLN
1	D	58	ASP
1	D	63	VAL
1	D	65	THR
1	D	74	ASN
1	D	86	VAL
1	D	103	LYS
1	D	113	THR
1	D	118	THR
1	D	129	LYS
1	D	136	GLN
1	D	146	TRP
1	D	158	ARG
1	D	187	THR
1	D	204	GLN
1	D	229	LEU
1	D	257	VAL
1	D	288	THR
1	D	301	ASN
1	D	312	LYS
1	D	320	GLN
1	D	348	MET
1	D	361	GLU
1	D	387	SER
1	D	389	SER
1	D	401	ASP
1	D	402	ILE
1	D	423	ARG
1	D	436	ASP
1	D	447	ASP
1	D	451	ILE
1	D	479	LYS
1	D	493	ASN
1	D	521	ILE
1	D	525	LEU

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Mol	Chain	Res	Type
1	D	535	ASP
1	D	571	GLU
1	D	597	ARG
1	D	606	GLU
1	D	613	GLU
1	D	620	THR
1	D	647	GLN
1	D	659	LEU
1	D	719	ASN
1	D	749	ARG
1	D	781	LEU
1	D	799	GLU
1	D	804	MET
1	D	807	ILE
1	D	818	GLU
1	D	828	GLU
1	D	829	CYS
1	D	834	ILE
1	D	875	LEU
1	D	891	ASP
1	D	916	GLN
1	D	963	ASN
1	D	970	ASN
1	D	976	ASP
1	D	1016	ARG
1	D	1030	THR
1	D	1031	SER
1	D	1047	GLU
1	D	1048	GLU
1	D	1052	LEU
2	E	4	LEU
2	E	15	SER
2	E	32	LYS
2	E	33	SER
2	E	34	LYS
2	E	38	LEU
2	E	111	VAL
2	E	120	ILE
2	E	138	SER
2	E	150	ASN
2	E	161	ARG
2	E	189	MET

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Mol	Chain	Res	Type
2	E	234	ASN
2	E	235	PHE
2	E	240	GLU
2	E	264	THR
2	E	270	SER
2	E	274	VAL
2	E	282	VAL
2	E	352	ASP
2	E	357	LEU
3	F	8	GLN
3	F	9	VAL
3	F	27	VAL
3	F	29	ARG
3	F	38	LYS
3	F	40	VAL
3	F	43	LEU
3	F	51	VAL
3	F	55	ASN
3	F	70	GLU
3	F	71	LYS
3	F	75	LEU
3	F	76	ARG
3	F	77	ASP
3	F	113	GLU
3	F	140	ARG
3	F	141	LYS
3	F	143	ASN
3	F	156	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (126) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	43	GLN
1	A	47	GLN
1	A	74	ASN
1	A	97	ASN
1	A	131	ASN
1	A	165	GLN
1	A	167	ASN
1	A	185	GLN
1	A	200	ASN

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Mol	Chain	Res	Type
1	A	301	ASN
1	A	317	ASN
1	A	320	GLN
1	A	321	ASN
1	A	483	GLN
1	A	493	ASN
1	A	495	ASN
1	A	536	ASN
1	A	629	GLN
1	A	662	ASN
1	A	663	GLN
1	A	671	GLN
1	A	675	ASN
1	A	704	HIS
1	A	709	GLN
1	A	719	ASN
1	A	733	GLN
1	A	767	ASN
1	A	821	GLN
1	A	853	GLN
1	A	856	ASN
1	A	858	HIS
1	A	903	ASN
1	A	916	GLN
1	A	924	GLN
1	A	942	HIS
1	A	951	ASN
1	A	963	ASN
1	A	970	ASN
1	A	990	GLN
1	A	1006	GLN
1	A	1021	GLN
1	A	1046	GLN
2	B	19	ASN
2	B	25	HIS
2	B	40	GLN
2	B	61	HIS
2	B	101	GLN
2	B	117	GLN
2	B	150	ASN
2	B	160	ASN
2	B	163	ASN

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Mol	Chain	Res	Type
2	B	200	GLN
2	B	234	ASN
2	B	261	HIS
3	C	8	GLN
3	C	30	HIS
3	C	55	ASN
3	C	82	GLN
3	C	100	ASN
3	C	105	HIS
3	C	145	GLN
3	C	154	ASN
3	C	156	ASN
1	D	11	HIS
1	D	15	GLN
1	D	42	GLN
1	D	43	GLN
1	D	47	GLN
1	D	74	ASN
1	D	165	GLN
1	D	166	ASN
1	D	167	ASN
1	D	200	ASN
1	D	293	GLN
1	D	301	ASN
1	D	317	ASN
1	D	320	GLN
1	D	321	ASN
1	D	352	HIS
1	D	483	GLN
1	D	493	ASN
1	D	536	ASN
1	D	558	HIS
1	D	598	HIS
1	D	629	GLN
1	D	663	GLN
1	D	671	GLN
1	D	675	ASN
1	D	704	HIS
1	D	733	GLN
1	D	735	ASN
1	D	767	ASN
1	D	821	GLN

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Mol	Chain	Res	Type
1	D	856	ASN
1	D	858	HIS
1	D	895	GLN
1	D	903	ASN
1	D	916	GLN
1	D	924	GLN
1	D	942	HIS
1	D	951	ASN
1	D	970	ASN
1	D	990	GLN
1	D	1006	GLN
1	D	1050	HIS
2	E	16	GLN
2	E	19	ASN
2	E	40	GLN
2	E	51	GLN
2	E	61	HIS
2	E	101	GLN
2	E	117	GLN
2	E	150	ASN
2	E	160	ASN
2	E	163	ASN
2	E	200	GLN
2	E	261	HIS
3	F	30	HIS
3	F	55	ASN
3	F	82	GLN
3	F	100	ASN
3	F	105	HIS
3	F	145	GLN
3	F	154	ASN
3	F	156	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GTP	F	217	5	26,34,34	1.12	1 (3%)	32,54,54	1.53	5 (15%)
4	GTP	C	217	5	26,34,34	1.16	2 (7%)	32,54,54	1.57	6 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	F	217	5	-	7/18/38/38	0/3/3/3
4	GTP	C	217	5	-	3/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	217	GTP	C5-C6	-3.73	1.39	1.47
4	F	217	GTP	C5-C6	-3.70	1.39	1.47
4	C	217	GTP	O4'-C4'	-2.03	1.40	1.45

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	217	GTP	PB-O3B-PG	-4.55	117.22	132.83
4	F	217	GTP	PA-O3A-PB	-4.08	118.84	132.83
4	F	217	GTP	PB-O3B-PG	-3.20	121.83	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	217	GTP	C8-N7-C5	3.16	109.02	102.99
4	C	217	GTP	C5-C6-N1	3.07	119.37	113.95
4	F	217	GTP	C8-N7-C5	3.00	108.71	102.99
4	F	217	GTP	C5-C6-N1	2.98	119.21	113.95
4	F	217	GTP	C2-N1-C6	-2.72	120.09	125.10
4	C	217	GTP	PA-O3A-PB	-2.68	123.61	132.83
4	C	217	GTP	C2-N1-C6	-2.45	120.59	125.10
4	C	217	GTP	N1-C2-N3	-2.00	119.58	123.32

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	217	GTP	PB-O3B-PG-O3G
4	F	217	GTP	PB-O3B-PG-O2G
4	F	217	GTP	C5'-O5'-PA-O3A
4	F	217	GTP	O4'-C4'-C5'-O5'
4	F	217	GTP	C3'-C4'-C5'-O5'
4	F	217	GTP	C5'-O5'-PA-O1A
4	F	217	GTP	C5'-O5'-PA-O2A
4	F	217	GTP	PG-O3B-PB-O1B
4	C	217	GTP	PB-O3B-PG-O1G
4	C	217	GTP	O4'-C4'-C5'-O5'

There are no ring outliers.

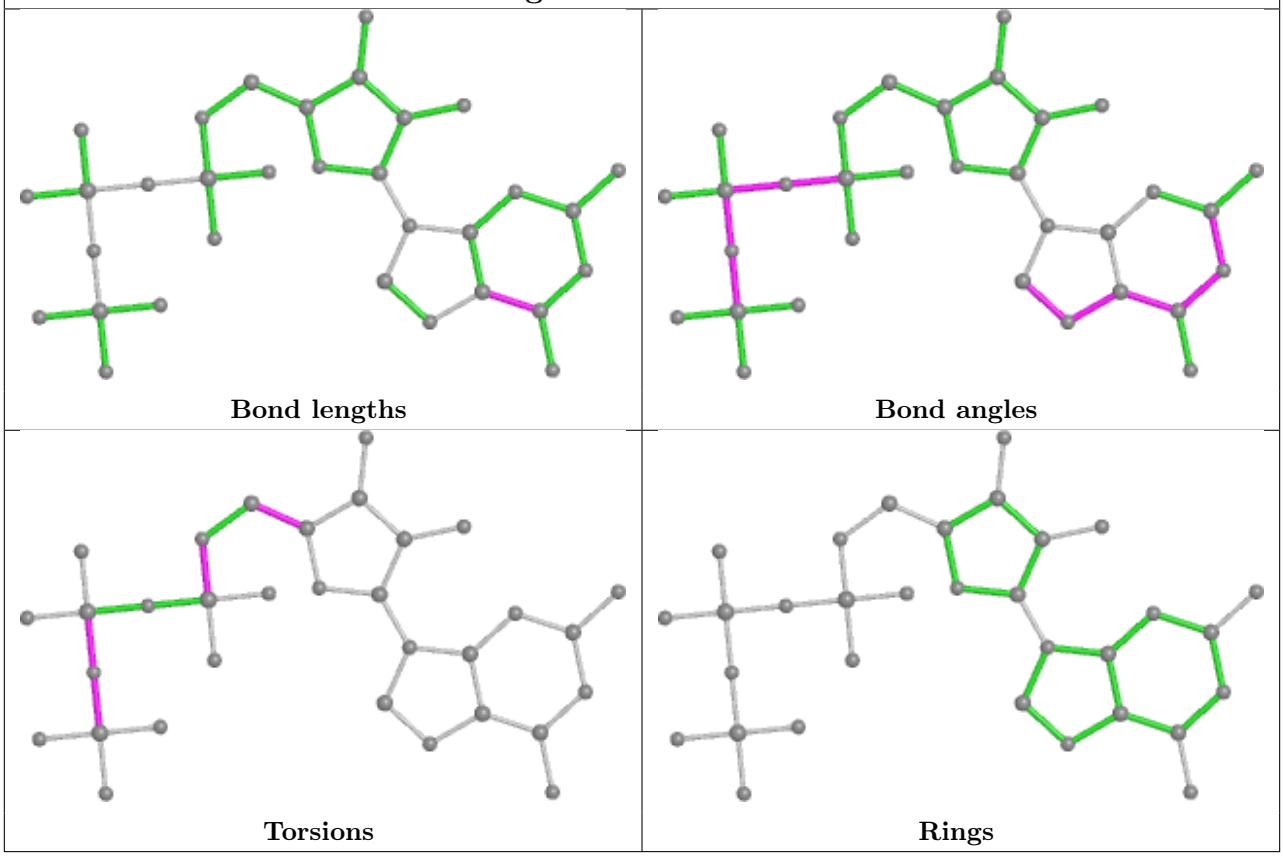
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	217	GTP	2	0
4	C	217	GTP	4	0

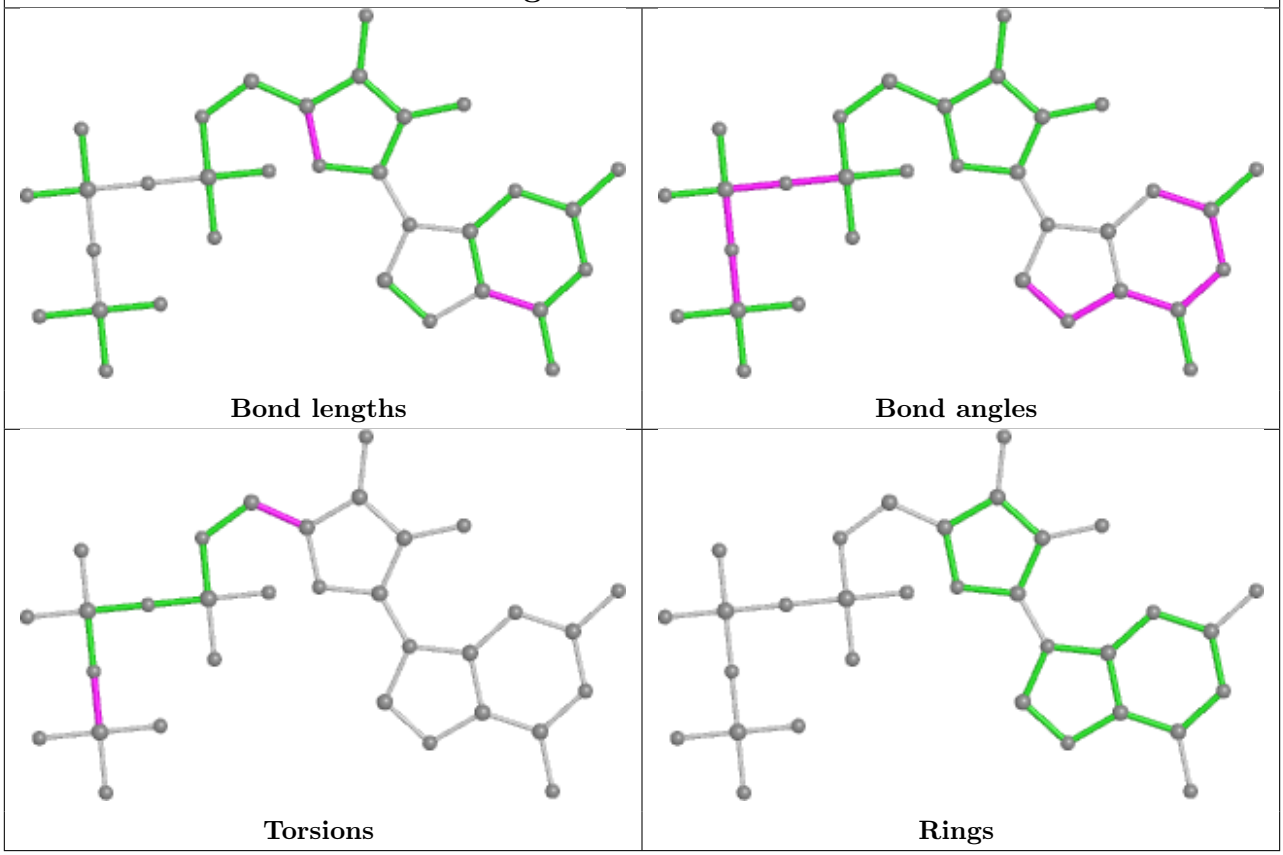
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.

Ligand GTP F 217



Ligand GTP C 217



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1038/1073 (96%)	-0.21	14 (1%)	77	72	14, 47, 107, 152	0
1	D	1038/1073 (96%)	-0.17	15 (1%)	75	70	14, 47, 103, 176	0
2	B	291/362 (80%)	-0.12	8 (2%)	54	44	15, 44, 116, 167	0
2	E	293/362 (80%)	-0.13	7 (2%)	59	49	15, 45, 123, 167	0
3	C	173/176 (98%)	-0.32	1 (0%)	89	86	21, 39, 79, 132	0
3	F	173/176 (98%)	-0.29	1 (0%)	89	86	20, 39, 79, 106	0
All	All	3006/3222 (93%)	-0.19	46 (1%)	73	68	14, 45, 106, 176	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	966	ASN	6.6
1	A	967	PRO	5.9
2	B	32	LYS	5.8
1	D	1028	GLU	4.8
2	E	360	ASN	4.7
1	A	119	CYS	4.5
2	B	288	VAL	4.4
1	A	1027	GLY	4.1
1	A	391	SER	4.0
2	B	33	SER	3.8
2	B	164	SER	3.6
1	D	276	VAL	3.5
1	A	16	LEU	3.5
3	F	180	PRO	3.5
1	D	19	PHE	3.4
1	D	60	TRP	3.4
2	B	350	SER	3.3
1	D	964	PRO	3.3
2	E	358	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	967	PRO	3.2
1	D	397	SER	3.1
2	E	31	TYR	3.1
1	D	37	HIS	3.0
2	E	32	LYS	3.0
1	A	19	PHE	3.0
1	A	1028	GLU	2.7
1	A	393	LEU	2.6
2	B	35	TYR	2.6
1	A	435	ASN	2.6
1	A	397	SER	2.5
1	A	1029	ASP	2.5
1	D	22	LYS	2.5
2	E	165	THR	2.4
1	D	398	GLN	2.4
2	E	90	THR	2.4
3	C	75	LEU	2.3
1	D	966	ASN	2.3
2	B	31	TYR	2.3
1	A	1032	ASP	2.2
2	B	347	SER	2.2
2	E	29	SER	2.1
1	D	118	THR	2.1
1	D	441	VAL	2.1
1	D	119	CYS	2.0
1	D	117	PRO	2.0
1	A	968	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

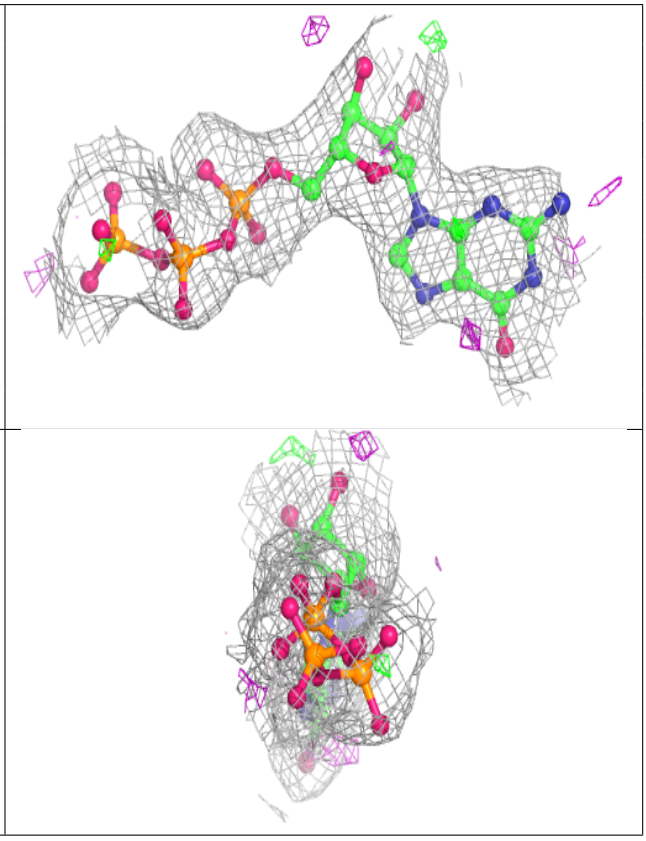
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NA	D	1072	1/1	0.85	0.19	52,52,52,52	0
6	NA	C	1	1/1	0.93	0.20	42,42,42,42	0
5	MG	F	218	1/1	0.95	0.17	26,26,26,26	0
4	GTP	C	217	32/32	0.97	0.15	12,29,37,71	0
4	GTP	F	217	32/32	0.97	0.16	16,34,50,56	0
5	MG	C	218	1/1	0.97	0.13	14,14,14,14	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

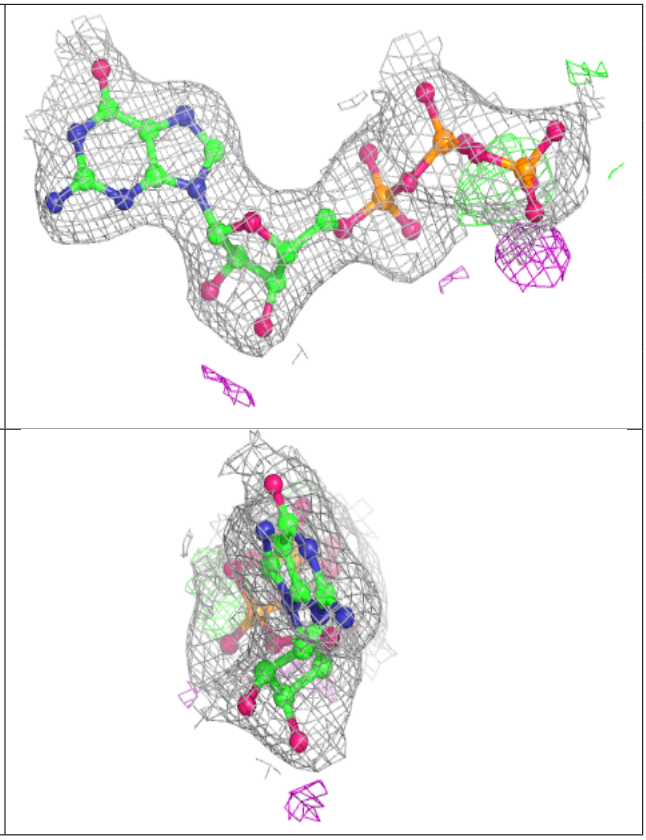
Electron density around GTP C 217:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



Electron density around GTP F 217:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.