Full wwPDB X-ray Structure Validation Report (i)

Jan 27, 2024 – 05:08 PM EST

PDB ID	:	1D2E
Title	:	CRYSTAL STRUCTURE OF MITOCHONDRIAL EF-TU IN COMPLEX WITH GDP
Authors	:	Andersen, G.R.; Thirup, S.; Spremulli, L.L.; Nyborg, J.
Deposited on	:	1999-09-23
Resolution	:	1.94 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:

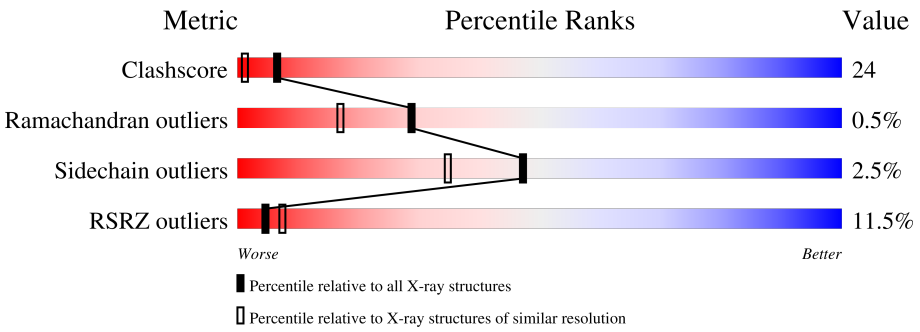
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.94 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))
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	397	3% 72% 26% •
1	B	397	11% 58% 41% •
1	C	397	7% 64% 35% •
1	D	397	25% 52% 46% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13597 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.

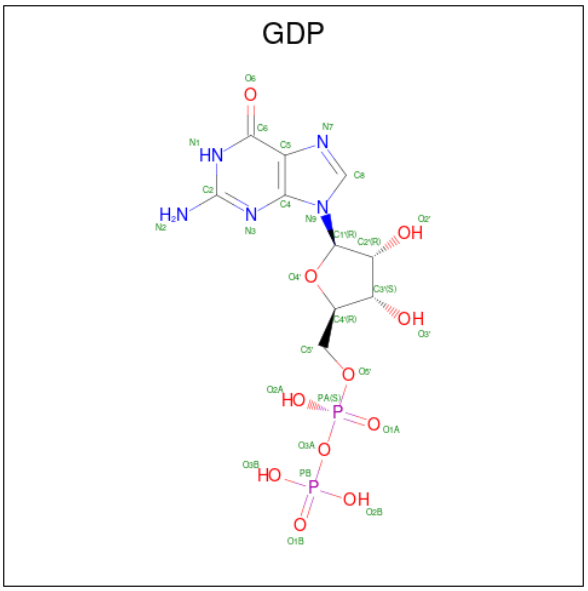
- Molecule 1 is a protein called ELONGATION FACTOR TU (EF-TU).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	397	3070	1938	539	577	16	0	0	0
1	B	397	3070	1938	539	577	16	0	0	0
1	C	397	3070	1938	539	577	16	0	0	0
1	D	397	3070	1938	539	577	16	0	0	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 4 is water.

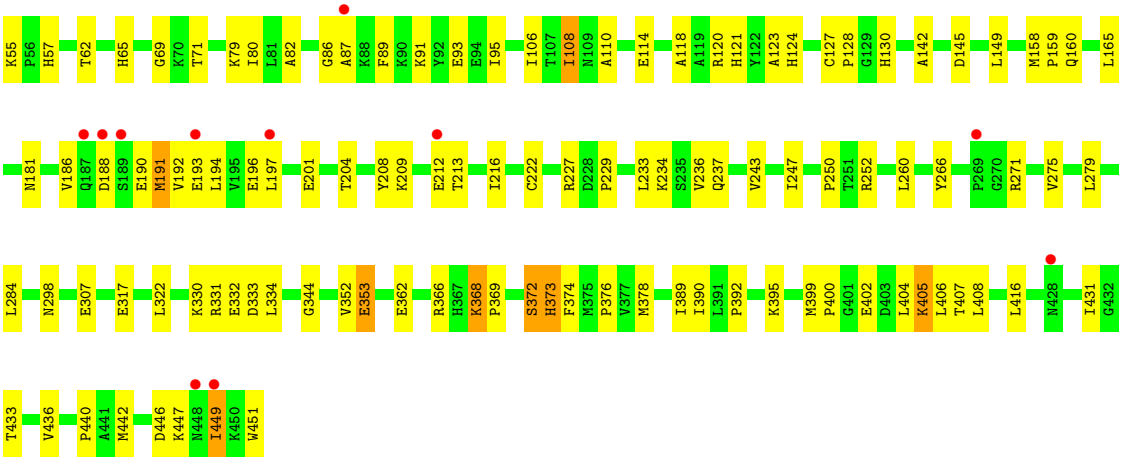
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	387	Total	O	0	0
			387	387		
4	B	274	Total	O	0	0
			274	274		
4	C	295	Total	O	0	0
			295	295		
4	D	245	Total	O	0	0
			245	245		

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.

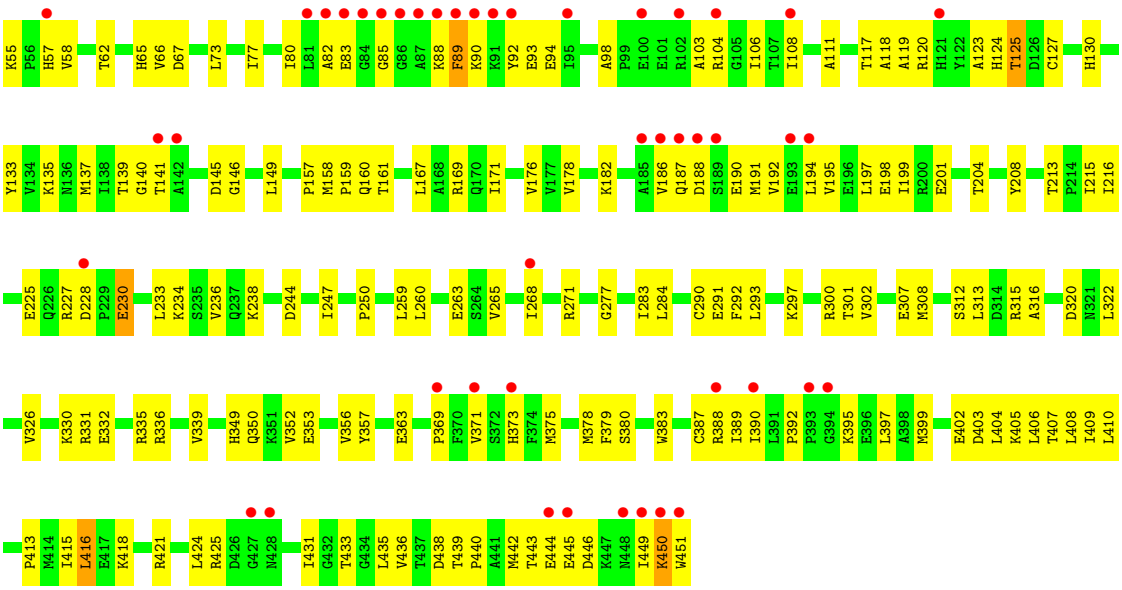
• Molecule 1: ELONGATION FACTOR TU (EF-TU)

Chain A:



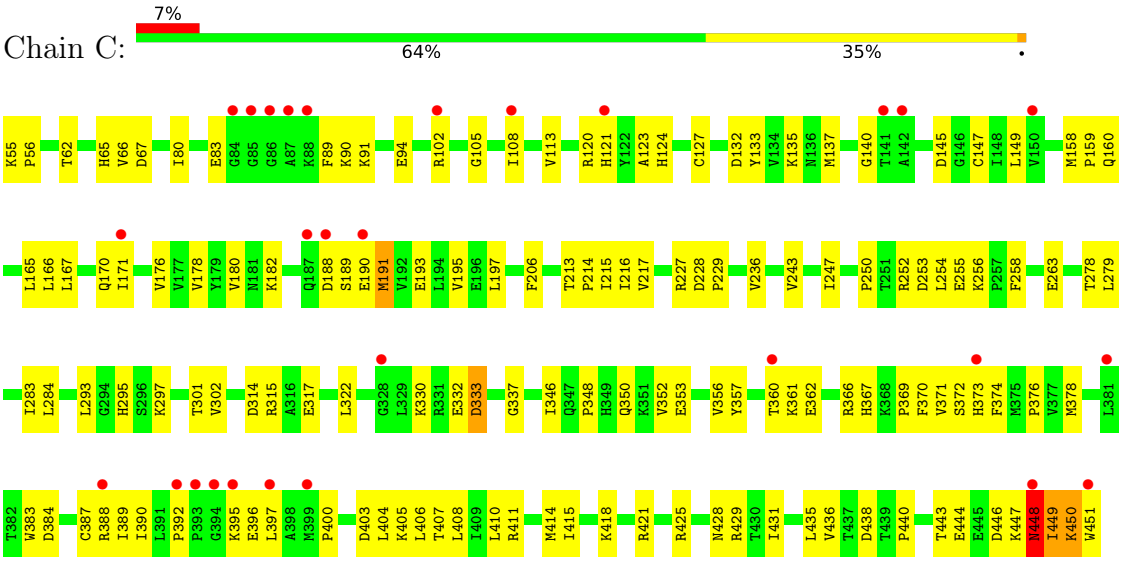
• Molecule 1: ELONGATION FACTOR TU (EF-TU)

Chain B:



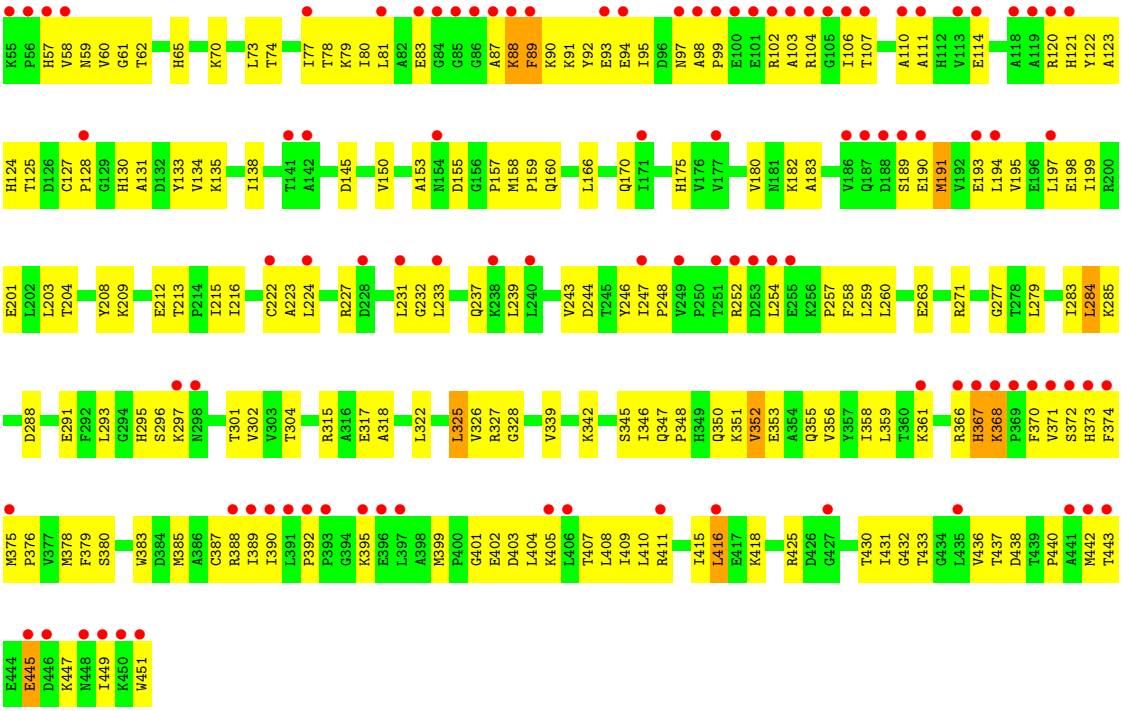
• Molecule 1: ELONGATION FACTOR TU (EF-TU)

Chain C:



• Molecule 1: ELONGATION FACTOR TU (EF-TU)

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.09Å 119.78Å 128.89Å 90.00° 96.97° 90.00°	Depositor
Resolution (Å)	34.70 – 1.94 33.87 – 1.94	Depositor EDS
% Data completeness (in resolution range)	98.0 (34.70-1.94) 98.1 (33.87-1.94)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 1.94Å)	Xtriage
Refinement program	CNS 0.3	Depositor
R, R_{free}	0.237 , 0.257 0.236 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	36.9	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13597	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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: GDP, 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	0.38	0/3127	0.73	1/4232 (0.0%)
1	B	0.32	0/3127	0.66	0/4232
1	C	0.33	0/3127	0.68	1/4232 (0.0%)
1	D	0.32	0/3127	0.67	0/4232
All	All	0.34	0/12508	0.69	2/16928 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	123	ALA	N-CA-C	-5.08	97.27	111.00
1	A	353	GLU	N-CA-C	-5.02	97.44	111.00

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	3070	0	3122	106	0
1	B	3070	0	3122	164	0
1	C	3070	0	3122	132	0
1	D	3070	0	3123	194	0
2	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	28	0	12	0	0
3	B	28	0	12	1	0
3	C	28	0	12	1	0
3	D	28	0	12	1	0
4	A	387	0	0	7	0
4	B	274	0	0	8	0
4	C	295	0	0	12	0
4	D	245	0	0	15	0
All	All	13597	0	12537	592	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 24.

All (592) 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)
1:A:368:LYS:HD3	1:A:368:LYS:H	1.08	1.08
1:A:352:VAL:HG11	1:A:416:LEU:HD12	1.30	1.06
1:A:352:VAL:HG11	1:A:416:LEU:CD1	1.92	0.99
1:B:388:ARG:HH12	1:B:450:LYS:HE2	1.30	0.97
1:D:405:LYS:NZ	1:D:437:THR:HG21	1.80	0.96
1:A:449:ILE:HD13	1:A:449:ILE:H	1.35	0.91
1:A:368:LYS:HD3	1:A:368:LYS:N	1.86	0.88
1:B:352:VAL:CG2	1:B:436:VAL:HG13	2.02	0.88
1:A:446:ASP:O	1:A:449:ILE:HG23	1.74	0.87
1:D:405:LYS:HZ1	1:D:437:THR:HG21	1.40	0.86
1:D:416:LEU:HD22	1:D:436:VAL:HG21	1.58	0.86
1:D:443:THR:HG22	1:D:445:GLU:H	1.42	0.84
1:A:332:GLU:HB3	1:C:229:PRO:HG3	1.60	0.84
1:D:81:LEU:HB2	4:D:1380:HOH:O	1.78	0.84
1:A:446:ASP:O	1:A:449:ILE:HD12	1.78	0.83
1:D:91:LYS:HD3	1:D:92:TYR:H	1.42	0.82
1:A:449:ILE:HG12	1:A:451:TRP:HE1	1.41	0.82
1:B:352:VAL:HG21	1:B:436:VAL:HG13	1.59	0.82
1:C:108:ILE:HD11	1:C:135:LYS:HB2	1.59	0.82
1:C:392:PRO:HG3	1:C:405:LYS:O	1.78	0.82
1:D:368:LYS:HD3	1:D:368:LYS:N	1.95	0.81
1:A:392:PRO:HG3	1:A:405:LYS:O	1.81	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:LEU:HD22	1:B:436:VAL:HG21	1.62	0.80
1:C:189:SER:O	1:C:193:GLU:HG3	1.82	0.80
1:D:78:THR:HB	1:D:89:PHE:HA	1.63	0.79
1:C:145:ASP:CG	1:C:250:PRO:HG3	2.02	0.79
1:C:361:LYS:HE2	1:C:367:HIS:O	1.82	0.79
1:A:108:ILE:HD11	1:A:110:ALA:HB2	1.66	0.78
1:D:73:LEU:O	1:D:77:ILE:HG13	1.83	0.78
1:A:416:LEU:CD1	1:A:436:VAL:HG21	2.13	0.78
1:D:304:THR:OG1	1:D:325:LEU:HD22	1.83	0.78
1:D:368:LYS:HD3	1:D:368:LYS:H	1.48	0.77
1:C:352:VAL:CG2	1:C:436:VAL:HG13	2.13	0.77
1:B:90:LYS:NZ	1:B:94:GLU:HG2	2.01	0.76
1:A:374:PHE:CE2	1:A:376:PRO:HG3	2.20	0.76
1:D:97:ASN:HB3	4:D:1533:HOH:O	1.86	0.76
1:A:193:GLU:O	1:A:197:LEU:HG	1.86	0.76
1:A:449:ILE:CG1	1:A:451:TRP:HE1	1.96	0.75
1:D:90:LYS:HG2	1:D:94:GLU:HG2	1.68	0.75
1:A:449:ILE:HG12	1:A:451:TRP:NE1	2.00	0.75
1:D:98:ALA:HB2	1:D:111:ALA:HB2	1.65	0.75
1:B:145:ASP:CG	1:B:250:PRO:HG3	2.07	0.75
1:B:353:GLU:HG3	1:B:440:PRO:HG2	1.67	0.75
1:B:98:ALA:HB2	1:B:111:ALA:HB2	1.66	0.75
1:D:375:MET:HE2	1:D:388:ARG:HD3	1.68	0.75
1:A:209:LYS:HB3	1:A:212:GLU:OE2	1.87	0.74
1:D:79:LYS:O	1:D:83:GLU:HG2	1.87	0.74
1:D:153:ALA:HB2	1:D:180:VAL:HG12	1.70	0.74
1:A:266:TYR:HA	1:A:331:ARG:HE	1.52	0.73
1:D:418:LYS:HE2	1:D:438:ASP:HA	1.70	0.73
1:B:228:ASP:HB3	1:B:230:GLU:OE2	1.89	0.72
1:B:58:VAL:HG21	1:B:120:ARG:HH21	1.55	0.72
1:C:243:VAL:HG13	1:C:247:ILE:HD12	1.72	0.71
1:D:392:PRO:HD2	1:D:395:LYS:HD2	1.73	0.70
1:D:375:MET:CE	1:D:388:ARG:HD3	2.21	0.70
1:D:405:LYS:NZ	1:D:437:THR:CG2	2.55	0.70
1:B:58:VAL:HG21	1:B:120:ARG:NH2	2.06	0.70
1:D:353:GLU:HG3	1:D:440:PRO:HG2	1.73	0.70
1:C:387:CYS:HB3	1:C:410:LEU:HD23	1.72	0.69
1:A:416:LEU:HD11	1:A:436:VAL:HG21	1.75	0.69
1:B:388:ARG:NH1	1:B:450:LYS:HE2	2.07	0.69
1:C:443:THR:HG22	1:C:446:ASP:OD2	1.93	0.68
1:C:352:VAL:HG21	1:C:436:VAL:HG13	1.73	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:ARG:HH21	1:D:254:LEU:HD11	1.57	0.68
1:D:301:THR:OG1	1:D:327:ARG:HG2	1.93	0.68
1:B:389:ILE:HG12	1:B:408:LEU:CD2	2.23	0.68
1:A:352:VAL:CG1	1:A:416:LEU:HD12	2.15	0.67
1:B:66:VAL:HG13	1:B:160:GLN:OE1	1.95	0.67
1:B:387:CYS:HB3	1:B:410:LEU:HD23	1.76	0.67
1:B:450:LYS:HD3	1:B:450:LYS:H	1.59	0.67
1:B:268:ILE:HG23	1:B:271:ARG:HB2	1.75	0.67
1:D:104:ARG:HG2	1:D:104:ARG:HH11	1.60	0.67
1:C:166:LEU:O	1:C:170:GLN:HG3	1.94	0.66
1:D:209:LYS:O	1:D:213:THR:HG23	1.94	0.66
1:A:145:ASP:CG	1:A:250:PRO:HG3	2.16	0.66
1:D:447:LYS:HB3	4:D:1522:HOH:O	1.95	0.66
1:B:291:GLU:OE2	1:B:293:LEU:HD21	1.95	0.66
1:B:332:GLU:H	1:B:332:GLU:CD	1.99	0.66
1:B:451:TRP:HB3	4:B:1451:HOH:O	1.96	0.66
1:D:65:HIS:HD2	1:D:160:GLN:H	1.44	0.66
1:A:368:LYS:H	1:A:368:LYS:CD	1.97	0.66
1:C:371:VAL:HG12	1:C:397:LEU:HD23	1.78	0.66
1:C:145:ASP:OD1	1:C:250:PRO:HG3	1.95	0.65
1:C:371:VAL:HG12	1:C:397:LEU:CD2	2.27	0.65
1:A:416:LEU:HD13	1:A:436:VAL:HG21	1.78	0.65
1:A:372:SER:O	1:A:373:HIS:HB2	1.97	0.65
1:B:331:ARG:HG3	1:B:331:ARG:HH11	1.61	0.65
1:A:93:GLU:CD	1:A:93:GLU:H	2.00	0.65
1:C:102:ARG:HE	1:C:105:GLY:HA2	1.61	0.65
1:A:298:ASN:HB2	4:A:1664:HOH:O	1.97	0.64
1:B:90:LYS:HZ1	1:B:94:GLU:HG2	1.60	0.64
1:A:449:ILE:H	1:A:449:ILE:CD1	2.08	0.64
1:A:416:LEU:HD11	1:A:436:VAL:CG2	2.27	0.64
1:A:344:GLY:O	1:D:418:LYS:NZ	2.31	0.63
1:B:352:VAL:HG23	1:B:438:ASP:O	1.98	0.63
1:C:102:ARG:HB2	4:C:1543:HOH:O	1.99	0.63
1:D:231:LEU:HD23	4:D:1351:HOH:O	1.98	0.63
1:D:252:ARG:NH2	1:D:254:LEU:HD21	2.14	0.63
1:A:229:PRO:O	1:A:234:LYS:HG2	1.98	0.63
1:C:140:GLY:HA3	1:C:421:ARG:NE	2.13	0.63
1:B:390:ILE:HB	1:B:407:THR:HB	1.81	0.62
1:B:268:ILE:HD13	1:B:271:ARG:HD3	1.81	0.62
1:B:65:HIS:HD2	1:B:160:GLN:H	1.46	0.62
1:D:246:TYR:O	1:D:248:PRO:HD3	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:ILE:CG2	1:B:271:ARG:HB2	2.29	0.62
1:B:409:ILE:HG23	1:B:442:MET:HE1	1.83	0.61
1:D:60:VAL:HG12	1:D:61:GLY:N	2.15	0.61
1:D:366:ARG:NH1	1:D:368:LYS:O	2.33	0.61
1:D:239:LEU:O	1:D:243:VAL:HG23	2.01	0.60
1:C:389:ILE:C	1:C:390:ILE:HD12	2.20	0.60
1:D:80:ILE:HD13	1:D:233:LEU:HD12	1.82	0.60
1:D:322:LEU:C	1:D:322:LEU:HD12	2.22	0.60
1:B:216:ILE:HD12	1:B:216:ILE:N	2.16	0.60
1:C:108:ILE:HD12	1:C:132:ASP:HA	1.83	0.60
1:D:431:ILE:HD12	1:D:432:GLY:N	2.16	0.60
1:D:353:GLU:HG3	1:D:440:PRO:CG	2.31	0.60
1:C:443:THR:HG22	1:C:446:ASP:CG	2.22	0.60
1:D:131:ALA:O	1:D:135:LYS:HG3	2.01	0.60
1:D:352:VAL:HG22	1:D:436:VAL:HG13	1.83	0.60
1:B:308:MET:HE2	1:B:313:LEU:HD12	1.84	0.60
1:D:350:GLN:HG3	1:D:410:LEU:O	2.02	0.59
1:C:65:HIS:HE1	4:C:1571:HOH:O	1.85	0.59
1:D:194:LEU:HD23	4:D:1541:HOH:O	2.01	0.59
1:D:405:LYS:HZ2	1:D:437:THR:CB	2.15	0.59
1:C:425:ARG:HD3	4:C:1546:HOH:O	2.01	0.59
1:A:330:LYS:HG2	1:A:333:ASP:OD1	2.03	0.59
1:C:293:LEU:HB3	1:C:348:PRO:HG3	1.83	0.59
1:C:171:ILE:HG22	1:C:435:LEU:HD22	1.83	0.59
1:B:265:VAL:HB	1:B:331:ARG:HH12	1.68	0.59
1:A:368:LYS:N	1:A:368:LYS:CD	2.63	0.59
1:B:192:VAL:O	1:B:195:VAL:HG12	2.02	0.58
1:C:279:LEU:HD23	1:C:317:GLU:C	2.23	0.58
1:D:433:THR:HG22	4:D:1362:HOH:O	2.03	0.58
1:A:65:HIS:HD2	1:A:160:GLN:H	1.51	0.58
1:C:390:ILE:HD12	1:C:390:ILE:N	2.17	0.58
1:C:449:ILE:C	1:C:449:ILE:HD12	2.23	0.58
1:D:374:PHE:CD2	1:D:376:PRO:HG3	2.39	0.58
1:B:373:HIS:HA	1:B:388:ARG:CG	2.33	0.58
1:C:137:MET:CE	1:C:167:LEU:HD23	2.33	0.58
1:D:385:MET:SD	1:D:411:ARG:HG3	2.44	0.58
1:C:360:THR:HG22	1:C:362:GLU:H	1.67	0.58
1:B:352:VAL:HG23	1:B:436:VAL:HG13	1.82	0.58
1:C:137:MET:HE3	1:C:167:LEU:HD23	1.85	0.57
1:B:146:GLY:HA3	1:B:247:ILE:HD12	1.85	0.57
1:C:278:THR:HG23	4:C:1367:HOH:O	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:361:LYS:HD3	1:D:367:HIS:CD2	2.38	0.57
1:A:307:GLU:HG2	4:A:1352:HOH:O	2.02	0.57
1:D:89:PHE:CD1	1:D:89:PHE:C	2.78	0.57
1:D:166:LEU:O	1:D:170:GLN:HG3	2.05	0.57
1:D:315:ARG:HG2	4:D:1394:HOH:O	2.05	0.57
1:D:385:MET:SD	1:D:411:ARG:CG	2.92	0.57
1:C:428:ASN:HA	4:C:1546:HOH:O	2.04	0.57
1:D:368:LYS:N	1:D:368:LYS:CD	2.66	0.57
1:A:197:LEU:O	1:A:201:GLU:HG3	2.04	0.57
1:C:372:SER:O	1:C:373:HIS:HB2	2.04	0.57
1:A:449:ILE:CG1	1:A:451:TRP:NE1	2.61	0.57
1:C:145:ASP:OD2	1:C:250:PRO:HG3	2.04	0.57
1:B:395:LYS:HE2	1:B:404:LEU:HD13	1.86	0.56
1:A:449:ILE:HD13	1:A:449:ILE:N	2.15	0.56
1:B:135:LYS:HE2	1:B:357:TYR:CZ	2.40	0.56
1:B:395:LYS:HE2	1:B:404:LEU:CD1	2.36	0.56
1:D:366:ARG:HD3	1:D:370:PHE:HD2	1.71	0.56
1:A:120:ARG:NH1	1:A:247:ILE:O	2.37	0.56
1:B:127:CYS:HB2	1:B:133:TYR:CE1	2.40	0.56
1:C:62:THR:HG23	1:C:124:HIS:CE1	2.40	0.56
1:D:197:LEU:O	1:D:201:GLU:HG2	2.05	0.56
1:D:295:HIS:O	1:D:297:LYS:HG3	2.05	0.56
1:D:258:PHE:HB2	1:D:279:LEU:HD11	1.88	0.56
1:B:83:GLU:C	1:B:85:GLY:H	2.09	0.56
1:C:188:ASP:HB2	1:C:190:GLU:OE1	2.06	0.56
1:B:93:GLU:CD	1:B:93:GLU:H	2.08	0.56
1:B:57:HIS:HB2	4:B:1431:HOH:O	2.05	0.55
1:B:335:ARG:NH2	4:B:1309:HOH:O	2.39	0.55
1:C:429:ARG:HH11	1:C:429:ARG:HB2	1.71	0.55
1:B:392:PRO:HG3	1:B:405:LYS:O	2.07	0.55
1:D:222:CYS:HB3	1:D:227:ARG:O	2.07	0.55
1:A:216:ILE:N	1:A:216:ILE:HD12	2.22	0.55
1:B:65:HIS:CD2	1:B:160:GLN:HB2	2.42	0.55
1:D:390:ILE:HB	1:D:407:THR:HB	1.86	0.55
1:B:433:THR:HG22	4:B:1357:HOH:O	2.06	0.55
1:B:330:LYS:HB3	1:B:332:GLU:OE2	2.07	0.55
1:C:121:HIS:HB2	4:C:1471:HOH:O	2.07	0.55
1:C:65:HIS:HD2	1:C:160:GLN:H	1.53	0.55
1:D:57:HIS:CE1	1:D:123:ALA:HB2	2.41	0.55
1:D:431:ILE:HD12	1:D:431:ILE:C	2.27	0.55
1:C:102:ARG:NE	1:C:105:GLY:HA2	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:LYS:HD2	1:D:91:LYS:NZ	2.22	0.55
1:D:191:MET:O	1:D:195:VAL:HG23	2.07	0.54
1:D:58:VAL:HB	1:D:122:TYR:CE1	2.41	0.54
1:D:263:GLU:HG3	4:D:1384:HOH:O	2.06	0.54
1:A:390:ILE:N	1:A:390:ILE:HD12	2.22	0.54
1:B:438:ASP:C	1:B:440:PRO:HD3	2.28	0.54
1:D:351:LYS:HB2	1:D:442:MET:SD	2.47	0.54
1:A:209:LYS:O	1:A:213:THR:HG23	2.08	0.54
1:A:404:LEU:HD23	1:A:404:LEU:N	2.22	0.54
1:B:312:SER:O	1:B:313:LEU:HD23	2.08	0.54
1:B:353:GLU:HG3	1:B:440:PRO:CG	2.37	0.54
1:C:378:MET:CE	1:C:408:LEU:HD22	2.38	0.54
1:A:243:VAL:HG13	1:A:247:ILE:HD12	1.88	0.54
1:D:233:LEU:O	1:D:237:GLN:HG3	2.08	0.54
1:C:135:LYS:HE2	1:C:357:TYR:CZ	2.42	0.54
1:B:416:LEU:HD22	1:B:436:VAL:CG2	2.35	0.53
1:D:60:VAL:CG1	1:D:61:GLY:N	2.71	0.53
1:B:139:THR:O	1:B:139:THR:HG22	2.08	0.53
1:C:322:LEU:HD12	1:C:322:LEU:C	2.28	0.53
1:B:106:ILE:HG23	1:B:363:GLU:OE2	2.08	0.53
1:C:353:GLU:OE2	1:C:440:PRO:HG2	2.08	0.53
1:A:352:VAL:HG11	1:A:416:LEU:HD11	1.87	0.53
1:C:252:ARG:HH21	1:C:254:LEU:HD11	1.73	0.53
1:B:62:THR:HG23	1:B:124:HIS:CE1	2.44	0.53
1:B:140:GLY:HA3	1:B:421:ARG:NE	2.24	0.53
1:D:104:ARG:HG2	1:D:104:ARG:NH1	2.23	0.53
1:C:360:THR:CG2	1:C:362:GLU:HG2	2.38	0.53
1:C:360:THR:HG22	1:C:361:LYS:N	2.23	0.53
1:A:392:PRO:HD2	1:A:395:LYS:CB	2.39	0.53
1:B:450:LYS:HD2	4:B:1457:HOH:O	2.09	0.53
1:C:366:ARG:NH1	1:C:370:PHE:HB3	2.23	0.52
1:B:120:ARG:HH11	1:B:244:ASP:HA	1.73	0.52
1:D:378:MET:CE	1:D:408:LEU:HD13	2.39	0.52
1:D:443:THR:CG2	1:D:445:GLU:HB3	2.38	0.52
1:A:65:HIS:CD2	1:A:160:GLN:HB2	2.44	0.52
1:B:65:HIS:CE1	1:B:66:VAL:HG22	2.45	0.52
1:A:82:ALA:HA	1:A:87:ALA:O	2.09	0.52
1:B:178:VAL:HB	1:B:215:ILE:HG12	1.91	0.52
1:B:119:ALA:C	1:B:120:ARG:HG3	2.30	0.52
1:C:411:ARG:HA	1:C:451:TRP:CZ2	2.45	0.52
1:D:257:PRO:CB	1:D:345:SER:HB2	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:387:CYS:HB3	1:D:410:LEU:HD23	1.91	0.52
1:A:89:PHE:CE2	1:A:91:LYS:HG2	2.45	0.52
1:A:158:MET:HB3	1:A:159:PRO:CD	2.39	0.52
1:A:260:LEU:HD13	1:A:260:LEU:C	2.30	0.52
1:C:448:ASN:ND2	1:C:448:ASN:O	2.43	0.52
1:D:375:MET:HA	1:D:387:CYS:O	2.09	0.52
1:D:62:THR:O	1:D:133:TYR:CE2	2.63	0.52
1:D:243:VAL:HG13	1:D:247:ILE:HD12	1.90	0.52
1:D:404:LEU:N	1:D:404:LEU:HD23	2.25	0.52
1:B:58:VAL:CG2	1:B:120:ARG:HH21	2.22	0.51
1:B:316:ALA:CB	1:B:322:LEU:HD22	2.41	0.51
1:D:352:VAL:CG2	1:D:436:VAL:HG13	2.40	0.51
1:B:118:ALA:HB3	4:B:1561:HOH:O	2.09	0.51
1:B:187:GLN:HA	4:B:1458:HOH:O	2.11	0.51
1:D:213:THR:HG22	4:D:1500:HOH:O	2.11	0.51
1:D:346:ILE:CD1	1:D:415:ILE:HG23	2.41	0.51
1:B:352:VAL:HG22	1:B:353:GLU:N	2.26	0.51
1:B:389:ILE:HG12	1:B:408:LEU:HD21	1.91	0.51
1:B:409:ILE:HG23	1:B:442:MET:CE	2.40	0.51
1:A:374:PHE:CD2	1:A:376:PRO:HG3	2.45	0.51
1:B:57:HIS:CE1	1:B:123:ALA:HB2	2.45	0.51
1:B:449:ILE:HG12	1:B:450:LYS:N	2.26	0.51
1:A:322:LEU:HD12	1:A:322:LEU:C	2.31	0.51
1:B:188:ASP:HB3	1:B:190:GLU:OE1	2.11	0.51
1:B:349:HIS:ND1	1:B:439:THR:HG21	2.25	0.51
1:D:98:ALA:HB1	1:D:110:ALA:C	2.31	0.51
1:D:271:ARG:HG2	1:D:325:LEU:HD11	1.92	0.51
1:B:350:GLN:HG2	1:B:442:MET:HE2	1.93	0.51
1:B:443:THR:CG2	1:B:445:GLU:HG2	2.40	0.51
1:B:399:MET:O	1:B:402:GLU:HB3	2.11	0.51
1:D:65:HIS:HA	1:D:160:GLN:HB2	1.92	0.51
1:B:350:GLN:HG2	1:B:442:MET:CE	2.41	0.51
1:D:284:LEU:HD23	1:D:285:LYS:N	2.26	0.51
1:C:55:LYS:HB2	1:C:56:PRO:CD	2.40	0.50
1:A:332:GLU:CB	1:C:229:PRO:HG3	2.39	0.50
1:C:147:CYS:O	1:C:176:VAL:HG13	2.11	0.50
1:C:369:PRO:HG3	1:C:400:PRO:CG	2.42	0.50
1:D:106:ILE:HD11	1:D:433:THR:OG1	2.11	0.50
1:D:399:MET:HB2	1:D:402:GLU:CD	2.32	0.50
1:B:167:LEU:O	1:B:171:ILE:HG23	2.11	0.50
1:D:104:ARG:NH2	1:D:430:THR:OG1	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:LYS:O	1:B:238:LYS:HG3	2.11	0.50
1:D:74:THR:HG22	1:D:95:ILE:HD13	1.92	0.50
1:A:252:ARG:HD3	4:A:1418:HOH:O	2.12	0.50
1:B:283:ILE:HD13	1:B:315:ARG:NH2	2.27	0.50
1:C:451:TRP:HB2	4:C:1523:HOH:O	2.12	0.50
1:D:98:ALA:CB	1:D:111:ALA:HB2	2.36	0.50
1:B:378:MET:CE	1:B:408:LEU:HD13	2.42	0.50
1:C:443:THR:HG23	1:C:446:ASP:H	1.77	0.50
1:D:283:ILE:HD12	1:D:315:ARG:NH2	2.27	0.50
1:D:389:ILE:HG12	1:D:408:LEU:CD2	2.42	0.50
1:B:58:VAL:HG21	1:B:120:ARG:CZ	2.42	0.50
1:B:265:VAL:HB	1:B:331:ARG:NH1	2.26	0.50
1:C:91:LYS:HD3	1:C:94:GLU:OE2	2.12	0.50
1:D:259:LEU:HD11	1:D:339:VAL:HG11	1.93	0.50
1:D:285:LYS:N	1:D:288:ASP:OD2	2.44	0.49
1:B:443:THR:HG22	1:B:445:GLU:H	1.76	0.49
1:D:216:ILE:N	1:D:216:ILE:HD12	2.26	0.49
1:A:57:HIS:CE1	1:A:123:ALA:HB2	2.47	0.49
1:B:369:PRO:CG	1:B:399:MET:SD	3.00	0.49
1:B:446:ASP:O	1:B:449:ILE:HG22	2.13	0.49
1:A:86:GLY:O	1:A:87:ALA:HB2	2.12	0.49
1:B:308:MET:CE	1:B:313:LEU:HD12	2.41	0.49
1:B:418:LYS:HA	1:B:436:VAL:HG12	1.95	0.49
1:C:450:LYS:HD3	1:C:450:LYS:N	2.28	0.49
1:D:285:LYS:HB2	1:D:285:LYS:NZ	2.28	0.49
1:D:418:LYS:HA	1:D:436:VAL:HG12	1.95	0.49
1:C:89:PHE:CZ	1:C:91:LYS:HE3	2.48	0.49
1:D:62:THR:HG23	1:D:124:HIS:NE2	2.28	0.49
1:D:158:MET:HB3	1:D:159:PRO:CD	2.43	0.49
1:C:188:ASP:OD2	1:C:191:MET:HB2	2.13	0.49
1:B:186:VAL:HG12	1:B:188:ASP:H	1.78	0.49
1:D:120:ARG:HD2	1:D:122:TYR:OH	2.12	0.49
1:C:127:CYS:HB2	1:C:133:TYR:CE1	2.48	0.49
1:C:216:ILE:N	1:C:216:ILE:HD12	2.28	0.49
1:A:192:VAL:HG12	1:A:196:GLU:OE2	2.12	0.48
1:A:204:THR:HA	1:A:208:TYR:O	2.12	0.48
1:B:149:LEU:HD11	1:B:161:THR:HG23	1.94	0.48
1:B:350:GLN:HB2	1:B:413:PRO:HG3	1.95	0.48
1:C:65:HIS:HA	1:C:160:GLN:HB2	1.95	0.48
1:D:223:ALA:HB2	1:D:232:GLY:C	2.33	0.48
1:D:346:ILE:HD11	1:D:415:ILE:HG23	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:355:GLN:OE1	1:D:405:LYS:HE2	2.14	0.48
1:B:190:GLU:H	1:B:190:GLU:CD	2.17	0.48
1:C:418:LYS:HA	1:C:436:VAL:HG12	1.94	0.48
1:D:366:ARG:C	1:D:368:LYS:H	2.16	0.48
1:B:227:ARG:O	1:B:228:ASP:C	2.51	0.48
1:C:373:HIS:CD2	1:C:388:ARG:NE	2.81	0.48
1:A:369:PRO:CG	1:A:399:MET:SD	3.01	0.48
1:B:380:SER:HB3	1:B:383:TRP:CZ2	2.49	0.48
1:B:443:THR:HB	1:B:446:ASP:OD2	2.12	0.48
1:C:279:LEU:HD23	1:C:317:GLU:CA	2.42	0.48
1:D:371:VAL:HG23	1:D:373:HIS:H	1.78	0.48
1:B:88:LYS:HD3	1:B:89:PHE:N	2.28	0.48
1:B:404:LEU:HD11	1:B:406:LEU:HD21	1.95	0.48
1:C:137:MET:HE3	1:C:167:LEU:HB3	1.96	0.48
1:C:295:HIS:O	1:C:297:LYS:HG3	2.13	0.48
1:A:188:ASP:OD2	1:A:190:GLU:HG2	2.14	0.48
1:B:67:ASP:OD1	1:B:67:ASP:O	2.31	0.48
1:B:373:HIS:HA	1:B:388:ARG:HG2	1.94	0.48
1:A:442:MET:HE3	1:A:446:ASP:HB3	1.96	0.48
1:B:225:GLU:HB2	1:B:227:ARG:HD3	1.96	0.48
1:A:142:ALA:HB2	4:A:1496:HOH:O	2.14	0.48
1:B:204:THR:HA	1:B:208:TYR:O	2.14	0.47
1:B:418:LYS:HE2	1:B:439:THR:H	1.79	0.47
1:C:102:ARG:HE	1:C:105:GLY:CA	2.26	0.47
1:C:350:GLN:HG3	1:C:410:LEU:O	2.14	0.47
1:B:73:LEU:O	1:B:77:ILE:HG13	2.14	0.47
1:D:283:ILE:HD12	1:D:315:ARG:CZ	2.44	0.47
1:D:443:THR:C	1:D:445:GLU:N	2.66	0.47
1:A:62:THR:HG23	1:A:124:HIS:CE1	2.50	0.47
1:A:279:LEU:HD23	1:A:317:GLU:C	2.35	0.47
1:B:145:ASP:OD1	1:B:250:PRO:HG3	2.13	0.47
1:D:79:LYS:HD3	1:D:224:LEU:HD12	1.96	0.47
1:D:342:LYS:HE3	4:D:1451:HOH:O	2.13	0.47
1:D:358:ILE:O	1:D:401:GLY:N	2.38	0.47
1:C:252:ARG:NH2	1:C:317:GLU:OE2	2.48	0.47
1:D:405:LYS:NZ	1:D:437:THR:OG1	2.43	0.47
1:B:89:PHE:CD1	1:B:89:PHE:C	2.88	0.47
1:B:190:GLU:O	1:B:194:LEU:HG	2.15	0.47
1:B:225:GLU:O	1:B:227:ARG:HG3	2.14	0.47
1:C:374:PHE:HE2	1:C:431:ILE:CD1	2.27	0.47
1:B:371:VAL:HG12	1:B:397:LEU:HD23	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:VAL:HG21	1:B:120:ARG:NE	2.30	0.47
1:C:451:TRP:CD1	1:C:451:TRP:N	2.83	0.47
1:D:130:HIS:ND1	1:D:160:GLN:HG2	2.30	0.47
1:C:158:MET:HB3	1:C:159:PRO:CD	2.45	0.46
1:C:346:ILE:HD12	1:C:415:ILE:HD12	1.97	0.46
1:A:79:LYS:HB2	1:A:89:PHE:CE1	2.51	0.46
1:A:80:ILE:HD12	1:A:236:VAL:HG11	1.96	0.46
1:C:188:ASP:C	1:C:190:GLU:N	2.69	0.46
1:D:252:ARG:NH2	1:D:317:GLU:OE2	2.35	0.46
1:D:385:MET:SD	1:D:411:ARG:NE	2.80	0.46
1:D:405:LYS:HB3	4:D:1478:HOH:O	2.15	0.46
1:B:82:ALA:HA	4:B:1330:HOH:O	2.15	0.46
1:B:260:LEU:C	1:B:260:LEU:HD13	2.36	0.46
1:C:421:ARG:HG2	1:C:421:ARG:HH11	1.79	0.46
1:A:114:GLU:OE1	1:A:121:HIS:NE2	2.46	0.46
1:B:404:LEU:N	1:B:404:LEU:HD23	2.30	0.46
1:C:90:LYS:HD2	1:C:113:VAL:HG12	1.96	0.46
1:D:366:ARG:HG3	1:D:368:LYS:O	2.16	0.46
1:B:263:GLU:HG2	1:B:277:GLY:HA2	1.97	0.46
1:D:57:HIS:HE1	1:D:123:ALA:HB2	1.81	0.46
1:D:283:ILE:HG22	4:D:1450:HOH:O	2.16	0.46
1:B:331:ARG:HG3	1:B:331:ARG:NH1	2.28	0.46
1:B:443:THR:HG22	1:B:445:GLU:HG2	1.98	0.46
1:C:253:ASP:HB3	1:C:256:LYS:HD2	1.97	0.46
1:D:195:VAL:O	1:D:199:ILE:HG13	2.15	0.46
1:D:252:ARG:NH2	1:D:254:LEU:HD11	2.27	0.46
1:D:260:LEU:HD11	1:D:277:GLY:HA3	1.98	0.46
1:B:225:GLU:OE1	1:B:227:ARG:NH1	2.46	0.46
1:C:376:PRO:HG3	1:C:389:ILE:HD11	1.97	0.46
1:D:79:LYS:HD2	1:D:91:LYS:HZ3	1.81	0.46
1:D:91:LYS:HD3	1:D:92:TYR:N	2.20	0.46
1:D:190:GLU:O	1:D:194:LEU:HG	2.16	0.46
1:D:366:ARG:HD3	1:D:370:PHE:CD2	2.49	0.46
1:D:373:HIS:HB3	1:D:388:ARG:NH2	2.30	0.46
1:D:134:VAL:O	1:D:138:ILE:HG13	2.16	0.46
1:B:442:MET:SD	1:B:446:ASP:HB3	2.56	0.46
1:C:254:LEU:HD22	1:C:317:GLU:HB2	1.98	0.46
1:A:392:PRO:HD2	1:A:395:LYS:HB2	1.98	0.45
1:B:292:PHE:HZ	1:B:326:VAL:HG11	1.81	0.45
1:B:297:LYS:HE2	1:B:297:LYS:HB3	1.77	0.45
1:A:222:CYS:HB3	1:A:227:ARG:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ALA:O	1:B:104:ARG:HB2	2.16	0.45
1:B:158:MET:HB3	1:B:159:PRO:CD	2.46	0.45
1:D:366:ARG:O	1:D:368:LYS:N	2.49	0.45
1:D:392:PRO:HG2	1:D:405:LYS:O	2.16	0.45
1:D:409:ILE:O	1:D:451:TRP:HH2	1.99	0.45
1:A:108:ILE:CD1	1:A:110:ALA:HB2	2.40	0.45
1:A:188:ASP:OD2	1:A:190:GLU:HB2	2.17	0.45
1:B:356:VAL:O	1:B:403:ASP:HA	2.17	0.45
1:D:157:PRO:HD2	1:D:198:GLU:OE2	2.16	0.45
1:B:418:LYS:HE2	1:B:438:ASP:HA	1.98	0.45
1:C:182:LYS:HG2	3:C:1303:GDP:C6	2.52	0.45
1:C:366:ARG:HH11	1:C:370:PHE:HB3	1.80	0.45
1:D:60:VAL:O	1:D:124:HIS:HA	2.16	0.45
1:D:65:HIS:CD2	1:D:160:GLN:HB2	2.51	0.45
1:D:90:LYS:HE2	1:D:94:GLU:HG2	1.98	0.45
1:D:93:GLU:CD	1:D:93:GLU:H	2.20	0.45
1:D:120:ARG:NH1	1:D:247:ILE:O	2.44	0.45
1:D:449:ILE:HG22	4:D:1508:HOH:O	2.15	0.45
1:C:252:ARG:NH2	1:C:254:LEU:HD11	2.30	0.45
1:D:170:GLN:HE22	1:D:405:LYS:HZ1	1.64	0.45
1:D:271:ARG:NH2	4:D:1448:HOH:O	2.49	0.45
1:A:404:LEU:HD11	1:A:406:LEU:HD21	1.99	0.45
1:C:383:TRP:CG	1:C:414:MET:HE2	2.51	0.45
1:C:404:LEU:HD11	1:C:406:LEU:HD21	1.99	0.45
1:B:195:VAL:O	1:B:199:ILE:HG13	2.17	0.45
1:D:91:LYS:HG3	1:D:93:GLU:OE1	2.15	0.45
1:A:106:ILE:HD13	1:A:433:THR:HG21	1.98	0.45
1:B:55:LYS:NZ	1:B:117:THR:O	2.48	0.45
1:B:388:ARG:NH2	1:B:449:ILE:HG13	2.32	0.45
1:D:356:VAL:O	1:D:403:ASP:HA	2.17	0.45
1:C:149:LEU:HD22	1:C:165:LEU:HD21	1.98	0.45
1:D:353:GLU:HB2	1:D:438:ASP:HB2	1.98	0.45
1:D:158:MET:HB3	1:D:159:PRO:HD2	1.99	0.45
1:B:108:ILE:HD11	1:B:135:LYS:HB3	1.98	0.44
1:D:62:THR:O	1:D:133:TYR:HE2	1.99	0.44
1:D:366:ARG:H	1:D:431:ILE:HG22	1.82	0.44
1:A:190:GLU:O	1:A:194:LEU:HG	2.17	0.44
1:A:362:GLU:OE1	1:A:362:GLU:N	2.41	0.44
1:A:431:ILE:C	1:A:431:ILE:HD12	2.38	0.44
1:A:449:ILE:HG13	1:A:451:TRP:HE1	1.80	0.44
1:C:283:ILE:HD13	1:C:315:ARG:NH2	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:HIS:HA	4:D:1336:HOH:O	2.16	0.44
1:A:188:ASP:HA	4:A:1477:HOH:O	2.17	0.44
1:B:182:LYS:HG2	3:B:1302:GDP:C6	2.52	0.44
1:D:291:GLU:CD	1:D:293:LEU:HD21	2.37	0.44
1:A:57:HIS:HE1	1:A:123:ALA:HB2	1.83	0.44
1:C:378:MET:O	1:C:384:ASP:HA	2.17	0.44
1:C:102:ARG:HD3	4:C:1508:HOH:O	2.17	0.44
1:C:337:GLY:CA	1:C:383:TRP:HB3	2.48	0.44
1:C:443:THR:CG2	1:C:446:ASP:H	2.30	0.44
1:D:209:LYS:CB	1:D:212:GLU:HG2	2.46	0.44
1:A:212:GLU:OE2	1:A:212:GLU:N	2.49	0.44
1:D:62:THR:HG23	1:D:124:HIS:CE1	2.52	0.44
1:A:390:ILE:HB	1:A:407:THR:HB	2.00	0.44
1:D:405:LYS:NZ	1:D:437:THR:CB	2.81	0.44
1:A:366:ARG:NH2	1:A:368:LYS:HG2	2.33	0.44
1:B:140:GLY:HA3	1:B:421:ARG:CZ	2.48	0.44
1:C:180:VAL:HB	1:C:217:VAL:HG22	2.00	0.44
1:D:102:ARG:NH1	1:D:102:ARG:HG3	2.32	0.44
1:D:103:ALA:O	1:D:104:ARG:HB3	2.18	0.44
1:D:291:GLU:HG2	1:D:293:LEU:HD21	2.00	0.44
1:A:353:GLU:HG3	1:A:440:PRO:HG2	1.99	0.44
1:C:263:GLU:HG3	4:C:1514:HOH:O	2.18	0.44
1:D:98:ALA:HA	1:D:99:PRO:HD3	1.80	0.44
1:D:380:SER:HB3	1:D:383:TRP:CZ2	2.53	0.44
1:D:130:HIS:O	1:D:134:VAL:HG23	2.18	0.43
1:D:252:ARG:CZ	1:D:254:LEU:HD21	2.47	0.43
1:A:378:MET:CE	1:A:408:LEU:HD22	2.48	0.43
1:B:301:THR:OG1	1:B:302:VAL:N	2.48	0.43
1:B:349:HIS:CE1	1:B:439:THR:HG21	2.53	0.43
1:D:87:ALA:O	1:D:88:LYS:C	2.56	0.43
1:B:111:ALA:O	1:B:125:THR:HA	2.18	0.43
1:B:373:HIS:O	1:B:375:MET:HG3	2.19	0.43
1:B:388:ARG:HH12	1:B:450:LYS:CE	2.15	0.43
1:D:153:ALA:HB2	1:D:180:VAL:CG1	2.42	0.43
1:D:203:LEU:HD13	1:D:213:THR:OG1	2.18	0.43
1:D:347:GLN:HA	1:D:348:PRO:HD3	1.82	0.43
1:D:411:ARG:HA	1:D:451:TRP:CZ2	2.54	0.43
1:B:157:PRO:HD2	1:B:198:GLU:OE1	2.18	0.43
1:B:188:ASP:O	1:B:191:MET:HB3	2.19	0.43
1:B:431:ILE:C	1:B:431:ILE:HD12	2.39	0.43
1:C:171:ILE:HA	1:C:435:LEU:HD21	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:LYS:HA	1:D:150:VAL:HG21	2.00	0.43
1:D:170:GLN:NE2	1:D:405:LYS:HZ1	2.17	0.43
1:A:233:LEU:O	1:A:237:GLN:HG3	2.19	0.43
1:B:171:ILE:HG22	1:B:435:LEU:HD22	2.00	0.43
1:B:290:CYS:SG	1:B:301:THR:HG23	2.59	0.43
1:C:374:PHE:HE2	1:C:431:ILE:HD11	1.83	0.43
1:C:55:LYS:HB2	1:C:56:PRO:HD2	1.99	0.43
1:A:130:HIS:ND1	1:A:160:GLN:HG2	2.34	0.43
1:C:356:VAL:O	1:C:403:ASP:HA	2.19	0.43
1:D:114:GLU:HB3	1:D:121:HIS:HE1	1.83	0.43
1:A:106:ILE:CD1	1:A:433:THR:HG21	2.49	0.43
1:C:330:LYS:HB3	1:C:333:ASP:OD1	2.18	0.43
1:C:444:GLU:HA	1:C:447:LYS:HD3	2.01	0.43
1:B:216:ILE:N	1:B:216:ILE:CD1	2.81	0.42
1:B:353:GLU:CG	1:B:440:PRO:HG2	2.44	0.42
1:C:373:HIS:HD2	1:C:388:ARG:NE	2.17	0.42
1:C:396:GLU:O	1:C:397:LEU:HD23	2.18	0.42
1:B:395:LYS:HE3	1:B:395:LYS:HB3	1.88	0.42
1:C:360:THR:HG21	1:C:362:GLU:HG2	2.01	0.42
1:D:79:LYS:CD	1:D:224:LEU:HD12	2.49	0.42
1:D:183:ALA:HB3	1:D:231:LEU:HD22	2.01	0.42
1:C:176:VAL:O	1:C:213:THR:HG23	2.19	0.42
1:C:258:PHE:HB2	1:C:279:LEU:HD11	2.02	0.42
1:D:372:SER:O	1:D:389:ILE:O	2.38	0.42
1:A:69:GLY:HA3	1:A:181:ASN:ND2	2.35	0.42
1:B:335:ARG:HG3	1:B:336:ARG:N	2.34	0.42
1:D:107:THR:O	1:D:135:LYS:NZ	2.45	0.42
1:D:189:SER:O	1:D:193:GLU:HG3	2.20	0.42
1:A:266:TYR:HB2	1:A:331:ARG:HH21	1.84	0.42
1:A:399:MET:O	1:A:402:GLU:HB3	2.20	0.42
1:B:58:VAL:HG21	1:B:120:ARG:HE	1.83	0.42
1:B:133:TYR:HB3	1:B:137:MET:HE1	2.01	0.42
1:C:332:GLU:CD	1:C:332:GLU:N	2.72	0.42
1:C:392:PRO:HD2	1:C:395:LYS:HB2	2.02	0.42
1:D:209:LYS:HB2	1:D:212:GLU:HG2	2.00	0.42
1:D:379:PHE:CE1	1:D:425:ARG:HD3	2.54	0.42
1:A:389:ILE:C	1:A:390:ILE:HD12	2.39	0.42
1:B:169:ARG:HA	1:B:169:ARG:HD2	1.91	0.42
1:C:390:ILE:HB	1:C:407:THR:HB	2.01	0.42
1:C:425:ARG:CD	4:C:1546:HOH:O	2.65	0.42
1:D:127:CYS:HB2	1:D:133:TYR:CE1	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:LYS:HB2	1:D:288:ASP:OD2	2.20	0.42
1:A:372:SER:O	1:A:373:HIS:CB	2.67	0.42
1:B:204:THR:HG23	1:C:255:GLU:HB3	2.01	0.42
1:B:379:PHE:CE1	1:B:425:ARG:HD2	2.54	0.42
1:C:56:PRO:HB2	1:C:120:ARG:HG2	2.02	0.42
1:C:197:LEU:HD23	4:C:1405:HOH:O	2.20	0.42
1:D:260:LEU:HD13	1:D:260:LEU:C	2.39	0.42
1:A:71:THR:HG23	1:A:95:ILE:HG22	2.02	0.42
1:A:79:LYS:HE3	1:A:89:PHE:CD1	2.55	0.42
1:B:80:ILE:HD13	1:B:233:LEU:HD12	2.02	0.42
1:C:191:MET:O	1:C:195:VAL:HG23	2.20	0.42
1:D:90:LYS:CG	1:D:94:GLU:HG2	2.45	0.42
1:D:215:ILE:C	1:D:216:ILE:HD12	2.39	0.42
1:D:301:THR:OG1	1:D:302:VAL:N	2.49	0.42
1:D:405:LYS:HD3	1:D:405:LYS:HA	1.85	0.42
1:C:91:LYS:N	1:C:91:LYS:HD2	2.35	0.42
1:C:404:LEU:N	1:C:404:LEU:HD23	2.35	0.42
1:C:438:ASP:C	1:C:440:PRO:HD3	2.41	0.42
1:A:400:PRO:HD2	4:A:1631:HOH:O	2.20	0.41
1:A:447:LYS:O	1:A:449:ILE:HD13	2.20	0.41
1:B:190:GLU:CD	1:B:190:GLU:N	2.73	0.41
1:A:55:LYS:HE2	1:A:118:ALA:O	2.19	0.41
1:A:127:CYS:HA	1:A:128:PRO:HD3	1.89	0.41
1:A:404:LEU:HD23	1:A:404:LEU:H	1.85	0.41
1:B:145:ASP:OD2	1:B:250:PRO:HG3	2.21	0.41
1:B:176:VAL:O	1:B:213:THR:HG23	2.21	0.41
1:C:80:ILE:HD12	1:C:236:VAL:HG11	2.02	0.41
1:C:135:LYS:HE2	1:C:357:TYR:CE1	2.55	0.41
1:A:408:LEU:HD12	1:A:408:LEU:N	2.34	0.41
1:B:339:VAL:HB	1:B:415:ILE:HG13	2.02	0.41
1:C:411:ARG:HG2	1:C:411:ARG:HH11	1.85	0.41
1:D:204:THR:HA	1:D:208:TYR:O	2.21	0.41
1:D:252:ARG:NH1	1:D:318:ALA:O	2.53	0.41
1:B:308:MET:SD	1:B:320:ASP:HB3	2.60	0.41
1:A:158:MET:HB3	1:A:159:PRO:HD2	2.02	0.41
1:C:158:MET:HB3	1:C:159:PRO:HD2	2.03	0.41
1:D:352:VAL:HG22	1:D:438:ASP:O	2.20	0.41
1:B:135:LYS:HE2	1:B:357:TYR:OH	2.20	0.41
1:C:166:LEU:HB2	1:C:206:PHE:CE2	2.56	0.41
1:D:325:LEU:HD23	1:D:326:VAL:N	2.35	0.41
1:A:93:GLU:CD	1:A:93:GLU:N	2.71	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:VAL:CG1	1:A:191:MET:HB3	2.51	0.41
1:B:215:ILE:C	1:B:216:ILE:HD12	2.41	0.41
1:B:291:GLU:OE1	1:B:300:ARG:HD3	2.21	0.41
1:B:352:VAL:CG2	1:B:353:GLU:N	2.84	0.41
1:C:227:ARG:O	1:C:228:ASP:C	2.58	0.41
1:D:104:ARG:CZ	1:D:430:THR:OG1	2.68	0.41
1:D:122:TYR:OH	1:D:244:ASP:HA	2.20	0.41
1:D:180:VAL:N	1:D:216:ILE:O	2.51	0.41
1:D:182:LYS:HG2	3:D:1304:GDP:C6	2.55	0.41
1:A:275:VAL:CG1	1:A:334:LEU:HD13	2.51	0.41
1:B:124:HIS:CD2	1:B:124:HIS:C	2.94	0.41
1:C:55:LYS:N	4:C:1510:HOH:O	2.54	0.41
1:B:389:ILE:HD11	1:B:424:LEU:HD13	2.03	0.41
1:B:443:THR:HG22	1:B:444:GLU:N	2.35	0.41
1:C:66:VAL:O	1:C:67:ASP:HB2	2.21	0.41
1:C:374:PHE:CD2	1:C:376:PRO:HD3	2.56	0.41
1:D:74:THR:O	1:D:77:ILE:HB	2.20	0.41
1:D:359:LEU:N	1:D:359:LEU:HD12	2.35	0.41
1:D:361:LYS:HD3	1:D:367:HIS:NE2	2.35	0.41
1:D:416:LEU:HD22	1:D:436:VAL:CG2	2.38	0.41
1:A:149:LEU:HD22	1:A:165:LEU:HD21	2.01	0.41
1:B:80:ILE:HD12	1:B:236:VAL:HG11	2.03	0.41
1:C:213:THR:HA	1:C:214:PRO:HD3	1.95	0.41
1:C:421:ARG:HG2	1:C:421:ARG:NH1	2.36	0.41
1:B:268:ILE:HG23	1:B:268:ILE:O	2.21	0.40
1:C:228:ASP:N	1:C:229:PRO:HD3	2.35	0.40
1:A:271:ARG:HD2	4:A:1684:HOH:O	2.21	0.40
1:B:259:LEU:C	1:B:259:LEU:HD23	2.42	0.40
1:C:178:VAL:HB	1:C:215:ILE:HG12	2.02	0.40
1:C:188:ASP:O	1:C:191:MET:HB3	2.20	0.40
1:C:301:THR:OG1	1:C:302:VAL:N	2.51	0.40
1:D:175:HIS:CD2	1:D:248:PRO:HD2	2.56	0.40
1:B:130:HIS:HB2	1:B:160:GLN:OE1	2.21	0.40
1:B:197:LEU:O	1:B:201:GLU:HG3	2.22	0.40
1:D:59:ASN:N	1:D:145:ASP:OD2	2.41	0.40
1:D:89:PHE:CE1	1:D:91:LYS:HE2	2.57	0.40
1:D:293:LEU:CD1	1:D:346:ILE:HG23	2.51	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	395/397 (100%)	381 (96%)	14 (4%)	0	100	100
1	B	395/397 (100%)	376 (95%)	18 (5%)	1 (0%)	41	32
1	C	395/397 (100%)	381 (96%)	12 (3%)	2 (0%)	29	17
1	D	395/397 (100%)	361 (91%)	29 (7%)	5 (1%)	12	4
All	All	1580/1588 (100%)	1499 (95%)	73 (5%)	8 (0%)	29	17

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	83	GLU
1	D	88	LYS
1	D	367	HIS
1	C	448	ASN
1	D	128	PRO
1	D	328	GLY
1	B	92	TYR
1	D	296	SER

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	332/332 (100%)	324 (98%)	8 (2%)	49	36
1	B	332/332 (100%)	324 (98%)	8 (2%)	49	36

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	332/332 (100%)	325 (98%)	7 (2%)	53	41
1	D	332/332 (100%)	322 (97%)	10 (3%)	41	27
All	All	1328/1328 (100%)	1295 (98%)	33 (2%)	47	35

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ILE
1	A	191	MET
1	A	284	LEU
1	A	368	LYS
1	A	372	SER
1	A	373	HIS
1	A	405	LYS
1	A	449	ILE
1	B	89	PHE
1	B	125	THR
1	B	141	THR
1	B	230	GLU
1	B	284	LEU
1	B	307	GLU
1	B	416	LEU
1	B	450	LYS
1	C	191	MET
1	C	284	LEU
1	C	314	ASP
1	C	333	ASP
1	C	448	ASN
1	C	449	ILE
1	C	450	LYS
1	D	89	PHE
1	D	125	THR
1	D	155	ASP
1	D	191	MET
1	D	284	LEU
1	D	325	LEU
1	D	352	VAL
1	D	368	LYS
1	D	416	LEU
1	D	445	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	HIS
1	A	175	HIS
1	A	347	GLN
1	A	367	HIS
1	A	448	ASN
1	B	65	HIS
1	B	97	ASN
1	B	170	GLN
1	B	355	GLN
1	C	65	HIS
1	C	347	GLN
1	C	349	HIS
1	C	373	HIS
1	C	428	ASN
1	C	448	ASN
1	D	65	HIS
1	D	170	GLN
1	D	175	HIS
1	D	367	HIS
1	D	412	GLN
1	D	448	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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
3	GDP	A	1301	2	24,30,30	1.17	2 (8%)	30,47,47	0.98	2 (6%)
3	GDP	B	1302	2	24,30,30	1.19	3 (12%)	30,47,47	1.01	3 (10%)
3	GDP	D	1304	2	24,30,30	1.11	2 (8%)	30,47,47	1.03	4 (13%)
3	GDP	C	1303	2	24,30,30	1.17	2 (8%)	30,47,47	0.98	3 (10%)

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
3	GDP	A	1301	2	-	2/12/32/32	0/3/3/3
3	GDP	B	1302	2	-	2/12/32/32	0/3/3/3
3	GDP	D	1304	2	-	2/12/32/32	0/3/3/3
3	GDP	C	1303	2	-	2/12/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1303	GDP	C5-C6	-2.77	1.41	1.47
3	B	1302	GDP	C5-C6	-2.68	1.42	1.47
3	A	1301	GDP	C5-C6	-2.40	1.42	1.47
3	C	1303	GDP	PB-O2B	-2.29	1.46	1.54
3	B	1302	GDP	O4'-C1'	2.26	1.44	1.41
3	D	1304	GDP	C5-C6	-2.25	1.42	1.47
3	B	1302	GDP	PB-O2B	-2.23	1.46	1.54
3	A	1301	GDP	PB-O3B	-2.10	1.46	1.54
3	D	1304	GDP	PB-O2B	-2.04	1.47	1.54

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1303	GDP	O3'-C3'-C4'	-2.36	104.22	111.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1304	GDP	O3'-C3'-C4'	-2.31	104.36	111.05
3	B	1302	GDP	O3'-C3'-C4'	-2.27	104.48	111.05
3	D	1304	GDP	O6-C6-N1	-2.25	117.99	120.65
3	D	1304	GDP	C3'-C2'-C1'	2.23	104.33	100.98
3	A	1301	GDP	O3'-C3'-C4'	-2.22	104.64	111.05
3	B	1302	GDP	O6-C6-N1	-2.19	118.06	120.65
3	A	1301	GDP	O4'-C1'-C2'	-2.16	103.77	106.93
3	C	1303	GDP	O6-C6-N1	-2.14	118.12	120.65
3	C	1303	GDP	O6-C6-C5	2.10	128.47	124.37
3	D	1304	GDP	O6-C6-C5	2.09	128.45	124.37
3	B	1302	GDP	O6-C6-C5	2.06	128.39	124.37

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1301	GDP	PA-O3A-PB-O2B
3	B	1302	GDP	PA-O3A-PB-O2B
3	C	1303	GDP	PA-O3A-PB-O2B
3	D	1304	GDP	PA-O3A-PB-O2B
3	D	1304	GDP	PA-O3A-PB-O1B
3	A	1301	GDP	PA-O3A-PB-O1B
3	C	1303	GDP	PA-O3A-PB-O1B
3	B	1302	GDP	PA-O3A-PB-O1B

There are no ring outliers.

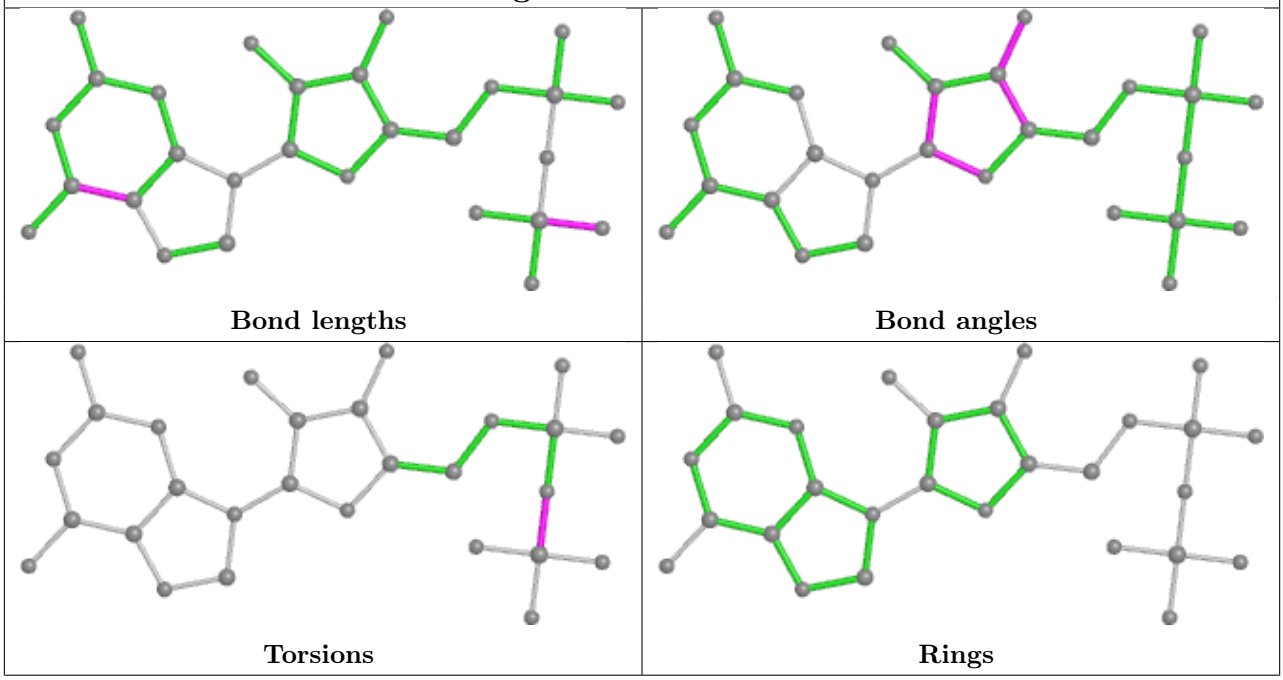
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1302	GDP	1	0
3	D	1304	GDP	1	0
3	C	1303	GDP	1	0

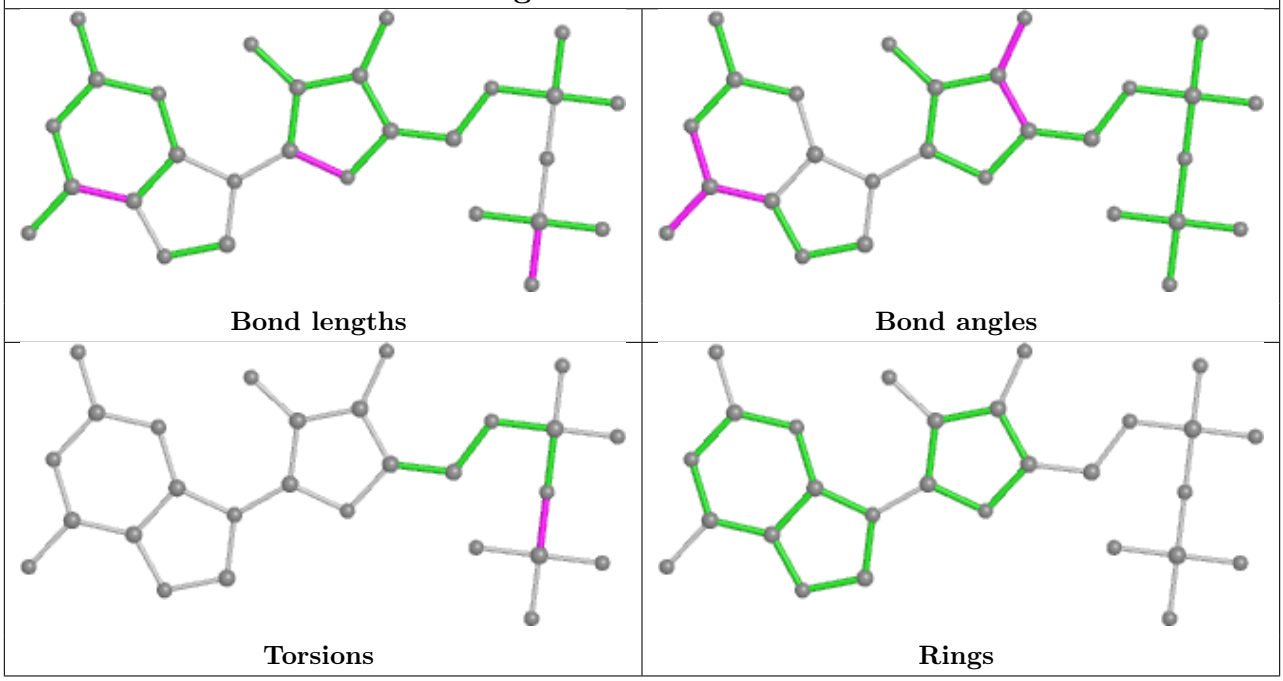
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

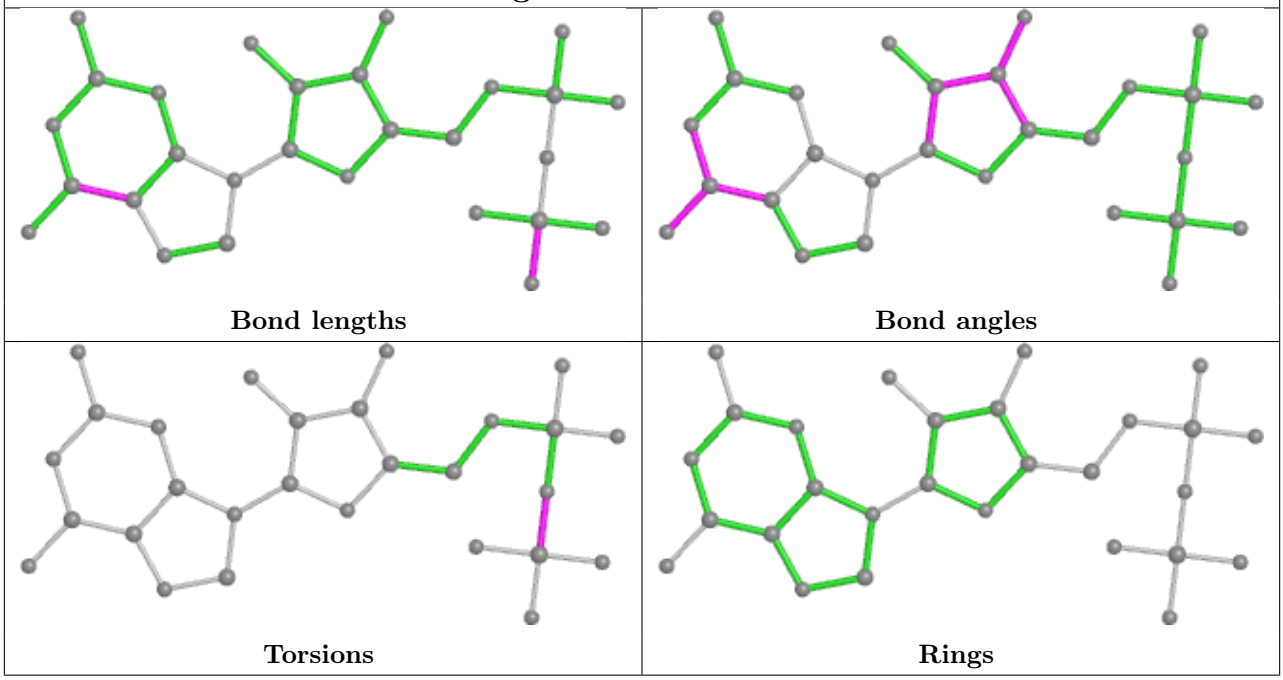
Ligand GDP A 1301



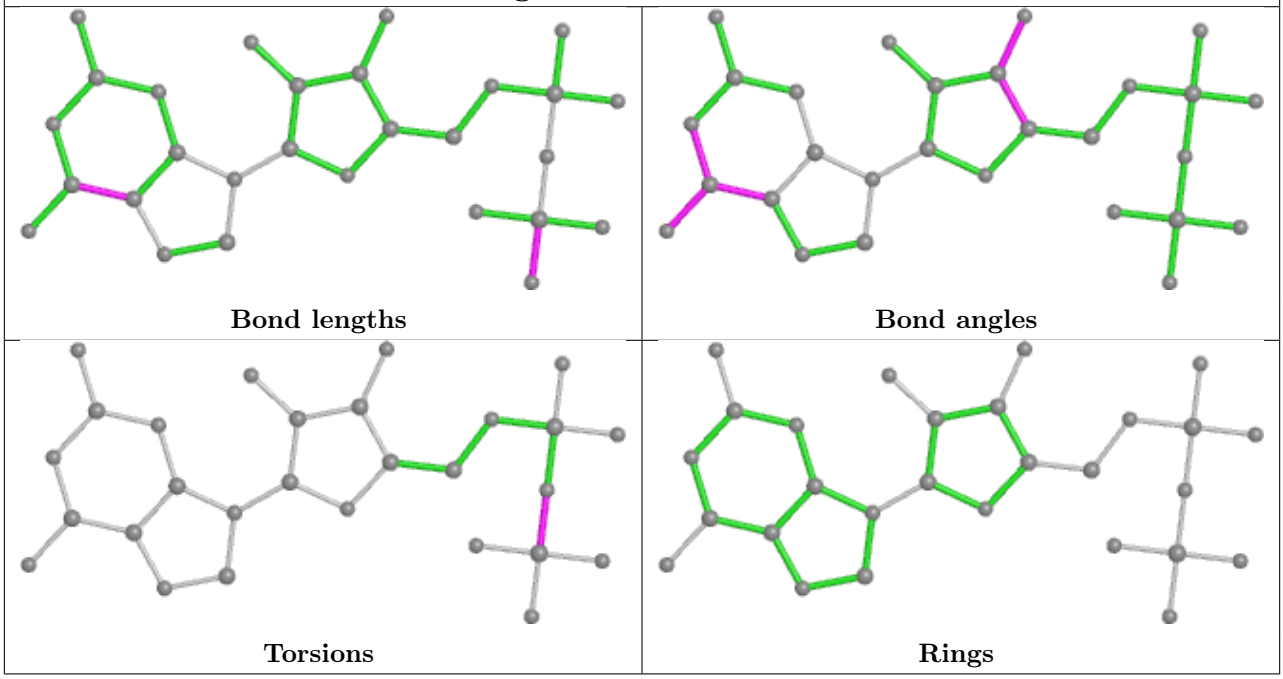
Ligand GDP B 1302



Ligand GDP D 1304



Ligand GDP C 1303



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	397/397 (100%)	0.45	11 (2%)	53	60	19, 35, 58, 69	0
1	B	397/397 (100%)	0.80	45 (11%)	5	8	33, 47, 66, 71	0
1	C	397/397 (100%)	0.65	28 (7%)	16	22	28, 44, 63, 71	0
1	D	397/397 (100%)	1.42	99 (24%)	0	0	27, 53, 67, 71	0
All	All	1588/1588 (100%)	0.83	183 (11%)	4	7	19, 45, 65, 71	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	85	GLY	11.4
1	B	87	ALA	9.0
1	B	141	THR	8.6
1	C	86	GLY	8.3
1	D	373	HIS	8.2
1	B	86	GLY	6.9
1	D	99	PRO	6.6
1	B	89	PHE	6.5
1	D	397	LEU	6.5
1	B	142	ALA	6.3
1	C	393	PRO	6.2
1	D	389	ILE	6.1
1	D	86	GLY	6.1
1	B	188	ASP	6.0
1	A	187	GLN	6.0
1	D	374	PHE	5.8
1	B	451	TRP	5.7
1	B	84	GLY	5.4
1	D	371	VAL	5.2
1	D	367	HIS	5.2
1	D	81	LEU	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	88	LYS	5.2
1	D	370	PHE	5.1
1	D	451	TRP	4.9
1	D	393	PRO	4.9
1	D	89	PHE	4.8
1	D	392	PRO	4.8
1	D	233	LEU	4.5
1	D	450	LYS	4.5
1	D	448	ASN	4.5
1	B	394	GLY	4.5
1	D	94	GLU	4.4
1	B	85	GLY	4.4
1	D	187	GLN	4.3
1	D	118	ALA	4.3
1	D	87	ALA	4.2
1	B	187	GLN	4.2
1	C	448	ASN	4.2
1	D	97	ASN	4.2
1	D	186	VAL	4.2
1	B	393	PRO	4.1
1	D	119	ALA	4.1
1	D	98	ALA	4.0
1	D	88	LYS	3.9
1	D	188	ASP	3.9
1	C	84	GLY	3.9
1	B	450	LYS	3.8
1	D	194	LEU	3.8
1	B	427	GLY	3.7
1	D	249	VAL	3.7
1	D	441	ALA	3.7
1	D	103	ALA	3.7
1	D	84	GLY	3.7
1	D	369	PRO	3.6
1	D	55	LYS	3.6
1	D	390	ILE	3.6
1	C	451	TRP	3.6
1	B	449	ILE	3.6
1	C	87	ALA	3.5
1	D	391	LEU	3.5
1	D	190	GLU	3.5
1	D	85	GLY	3.5
1	D	406	LEU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	252	ARG	3.4
1	D	251	THR	3.4
1	D	253	ASP	3.4
1	A	188	ASP	3.4
1	C	88	LYS	3.3
1	B	185	ALA	3.3
1	D	93	GLU	3.3
1	B	102	ARG	3.3
1	D	57	HIS	3.3
1	A	449	ILE	3.2
1	D	110	ALA	3.2
1	A	448	ASN	3.2
1	B	121	HIS	3.2
1	D	449	ILE	3.2
1	B	92	TYR	3.2
1	D	396	GLU	3.2
1	D	111	ALA	3.1
1	C	397	LEU	3.1
1	D	101	GLU	3.1
1	D	372	SER	3.1
1	B	371	VAL	3.1
1	C	141	THR	3.1
1	C	328	GLY	3.0
1	C	187	GLN	3.0
1	D	58	VAL	3.0
1	D	120	ARG	3.0
1	B	83	GLU	2.9
1	B	104	ARG	2.9
1	D	113	VAL	2.9
1	B	90	LYS	2.9
1	D	121	HIS	2.9
1	D	128	PRO	2.9
1	C	102	ARG	2.9
1	D	388	ARG	2.9
1	D	141	THR	2.8
1	D	443	THR	2.8
1	B	95	ILE	2.8
1	D	77	ILE	2.8
1	A	189	SER	2.8
1	D	100	GLU	2.8
1	B	428	ASN	2.8
1	D	154	ASN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	368	LYS	2.7
1	B	194	LEU	2.7
1	A	197	LEU	2.7
1	C	399	MET	2.7
1	C	373	HIS	2.7
1	D	105	GLY	2.7
1	D	231	LEU	2.7
1	B	91	LYS	2.6
1	A	428	ASN	2.6
1	D	189	SER	2.6
1	C	142	ALA	2.6
1	C	388	ARG	2.6
1	C	108	ILE	2.6
1	D	106	ILE	2.6
1	D	193	GLU	2.6
1	C	188	ASP	2.5
1	D	254	LEU	2.5
1	A	212	GLU	2.5
1	C	394	GLY	2.5
1	D	446	ASP	2.5
1	C	190	GLU	2.5
1	D	83	GLU	2.5
1	D	102	ARG	2.5
1	C	392	PRO	2.4
1	C	395	LYS	2.4
1	D	228	ASP	2.4
1	B	100	GLU	2.4
1	D	224	LEU	2.4
1	D	56	PRO	2.4
1	B	228	ASP	2.4
1	D	416	LEU	2.4
1	D	405	LYS	2.4
1	B	373	HIS	2.4
1	D	427	GLY	2.4
1	D	298	ASN	2.4
1	D	361	LYS	2.4
1	B	444	GLU	2.4
1	D	114	GLU	2.4
1	B	448	ASN	2.4
1	D	297	LYS	2.4
1	B	369	PRO	2.3
1	B	186	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	171	ILE	2.3
1	C	360	THR	2.3
1	B	268	ILE	2.3
1	D	238	LYS	2.3
1	B	82	ALA	2.3
1	D	366	ARG	2.3
1	D	107	THR	2.2
1	D	445	GLU	2.2
1	B	108	ILE	2.2
1	B	388	ARG	2.2
1	D	240	LEU	2.2
1	D	222	CYS	2.2
1	B	193	GLU	2.2
1	D	411	ARG	2.2
1	C	150	VAL	2.2
1	B	445	GLU	2.2
1	D	435	LEU	2.2
1	D	197	LEU	2.2
1	C	121	HIS	2.2
1	D	142	ALA	2.2
1	C	171	ILE	2.1
1	D	247	ILE	2.1
1	A	193	GLU	2.1
1	D	442	MET	2.1
1	B	390	ILE	2.1
1	C	381	LEU	2.1
1	D	177	VAL	2.1
1	B	81	LEU	2.1
1	D	255	GLU	2.1
1	D	375	MET	2.1
1	D	104	ARG	2.1
1	A	87	ALA	2.1
1	B	57	HIS	2.1
1	A	269	PRO	2.0
1	D	395	LYS	2.0
1	B	189	SER	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)

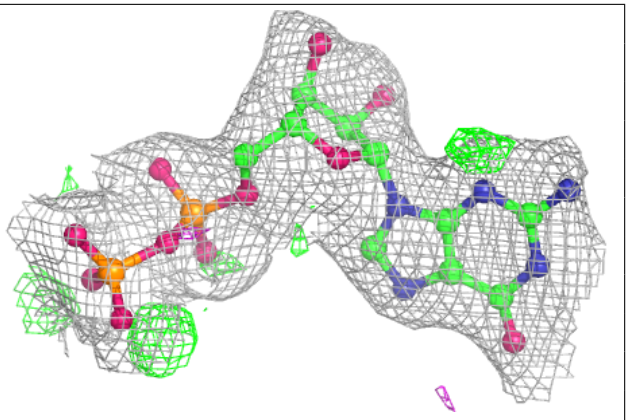
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

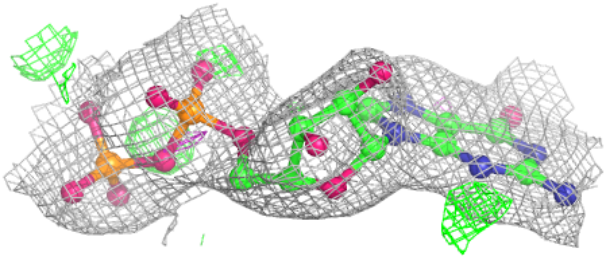
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	D	504	1/1	0.87	0.13	52,52,52,52	0
3	GDP	D	1304	28/28	0.90	0.12	50,54,58,58	0
2	MG	B	502	1/1	0.93	0.11	49,49,49,49	0
3	GDP	B	1302	28/28	0.96	0.09	44,51,53,55	0
2	MG	A	501	1/1	0.97	0.06	26,26,26,26	0
3	GDP	C	1303	28/28	0.97	0.11	31,34,37,39	0
3	GDP	A	1301	28/28	0.97	0.13	18,29,31,32	0
2	MG	C	503	1/1	0.99	0.08	35,35,35,35	0

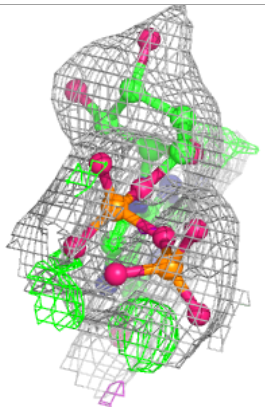
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP D 1304:

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

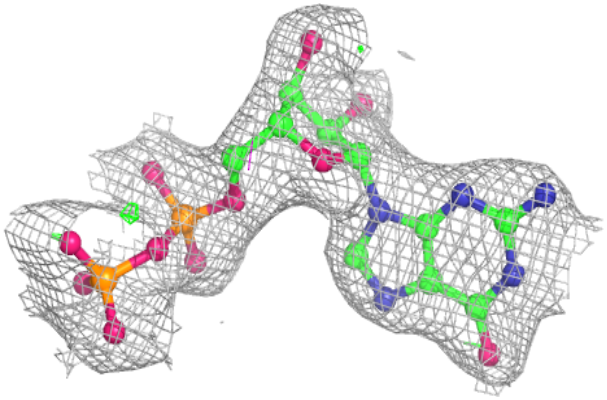


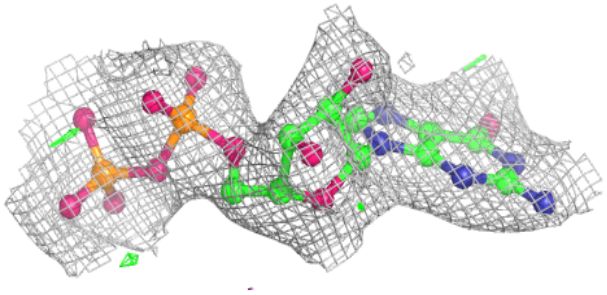


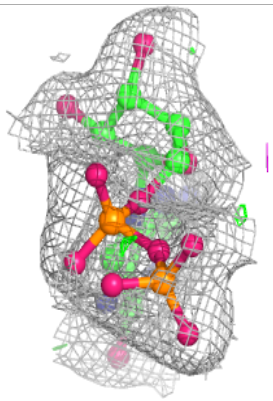


Electron density around GDP B 1302:

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

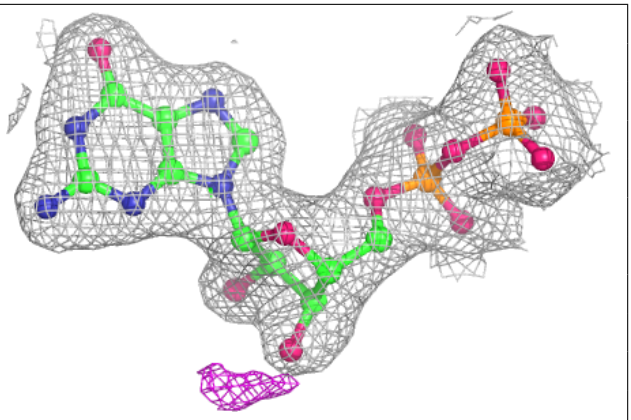


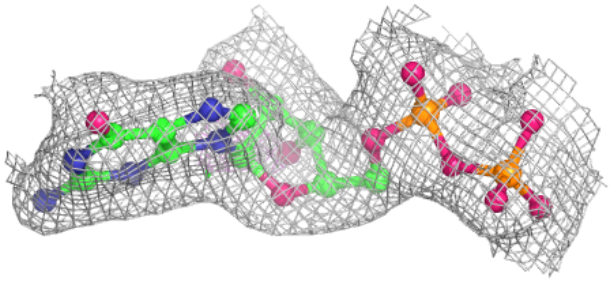


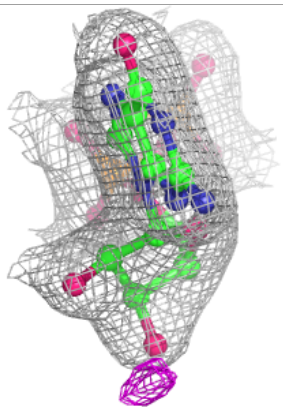


Electron density around GDP C 1303:

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

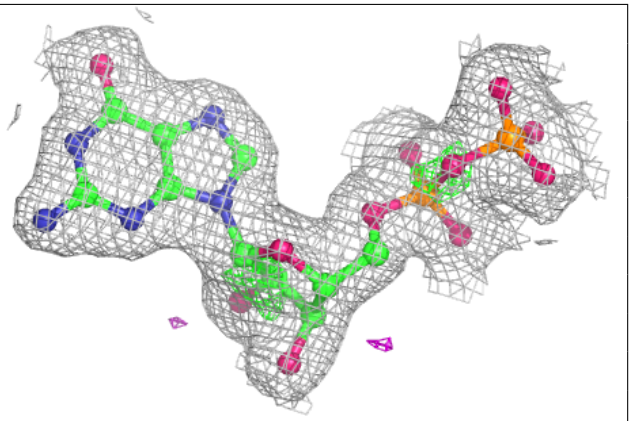


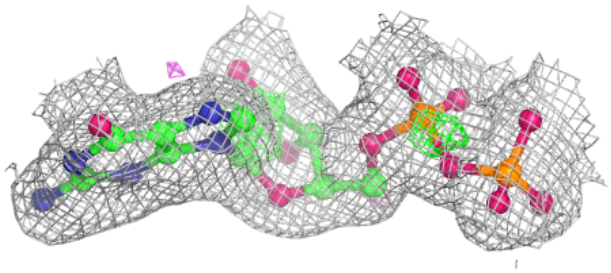


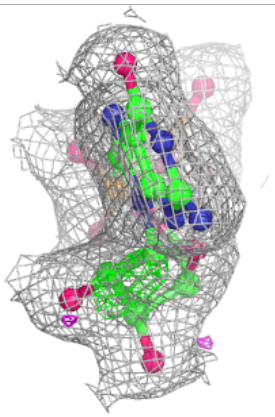


Electron density around GDP A 1301:

$2mF_o$-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.