Full wwPDB X-ray Structure Validation Report (i)

Oct 16, 2021 – 10:42 PM EDT

PDB ID	:	1NEX
Title	:	Crystal Structure of ScSkp1-ScCdc4-CPD peptide complex
Authors	:	Orlicky, S.; Tang, X.; Willems, A.; Tyers, M.; Sicheri, F.
Deposited on	:	2002-12-12
Resolution	:	2.70 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 following versions of software and data (see references (i)) were used in the production of this report:

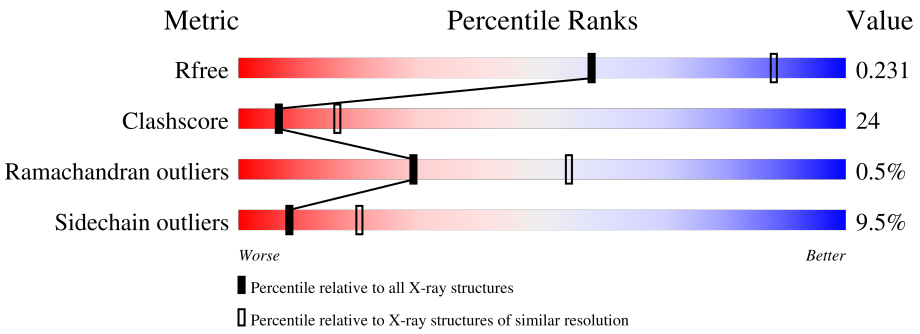
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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%

Mol	Chain	Length	Quality of chain
1	A	169	42% 28% 6% 24%
1	C	169	41% 30% 7% 23%
2	B	464	53% 37% 6% •
2	D	464	56% 34% 5% •
3	E	9	22% 11% 11% 56%
3	F	9	56% 22% 11% 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9435 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 Centromere DNA-binding protein complex CBF3 subunit D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	129	1047	666	182	195	1	3	0	0	0
1	C	130	1058	672	186	196	1	3	0	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	cloning artifact	UNP P52286
A	-1	ALA	-	cloning artifact	UNP P52286
A	0	HIS	-	cloning artifact	UNP P52286
A	1	MSE	MET	modified residue	UNP P52286
A	36	MSE	MET	modified residue	UNP P52286
A	?	-	HIS	deletion	UNP P52286
A	?	-	ASP	deletion	UNP P52286
A	?	-	SER	deletion	UNP P52286
A	?	-	ASN	deletion	UNP P52286
A	?	-	LEU	deletion	UNP P52286
A	?	-	GLN	deletion	UNP P52286
A	?	-	ASN	deletion	UNP P52286
A	?	-	ASN	deletion	UNP P52286
A	?	-	SER	deletion	UNP P52286
A	?	-	ASP	deletion	UNP P52286
A	?	-	SER	deletion	UNP P52286
A	?	-	GLU	deletion	UNP P52286
A	?	-	SER	deletion	UNP P52286
A	?	-	ASP	deletion	UNP P52286
A	?	-	SER	deletion	UNP P52286
A	?	-	ASP	deletion	UNP P52286
A	?	-	SER	deletion	UNP P52286
A	?	-	GLU	deletion	UNP P52286
A	?	-	THR	deletion	UNP P52286
A	?	-	ASN	deletion	UNP P52286

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	HIS	deletion	UNP P52286
A	?	-	LYS	deletion	UNP P52286
A	?	-	SER	deletion	UNP P52286
A	?	-	LYS	deletion	UNP P52286
A	?	-	ASP	deletion	UNP P52286
A	?	-	ASN	deletion	UNP P52286
A	?	-	ASN	deletion	UNP P52286
A	?	-	ASN	deletion	UNP P52286
A	77	MSE	MET	modified residue	UNP P52286
A	130	MSE	MET	modified residue	UNP P52286
A	157	MSE	MET	modified residue	UNP P52286
C	-2	GLY	-	cloning artifact	UNP P52286
C	-1	ALA	-	cloning artifact	UNP P52286
C	0	HIS	-	cloning artifact	UNP P52286
C	1	MSE	MET	modified residue	UNP P52286
C	36	MSE	MET	modified residue	UNP P52286
C	?	-	HIS	deletion	UNP P52286
C	?	-	ASP	deletion	UNP P52286
C	?	-	SER	deletion	UNP P52286
C	?	-	ASN	deletion	UNP P52286
C	?	-	LEU	deletion	UNP P52286
C	?	-	GLN	deletion	UNP P52286
C	?	-	ASN	deletion	UNP P52286
C	?	-	ASN	deletion	UNP P52286
C	?	-	SER	deletion	UNP P52286
C	?	-	ASP	deletion	UNP P52286
C	?	-	SER	deletion	UNP P52286
C	?	-	GLU	deletion	UNP P52286
C	?	-	SER	deletion	UNP P52286
C	?	-	ASP	deletion	UNP P52286
C	?	-	SER	deletion	UNP P52286
C	?	-	ASP	deletion	UNP P52286
C	?	-	SER	deletion	UNP P52286
C	?	-	GLU	deletion	UNP P52286
C	?	-	THR	deletion	UNP P52286
C	?	-	ASN	deletion	UNP P52286
C	?	-	HIS	deletion	UNP P52286
C	?	-	LYS	deletion	UNP P52286
C	?	-	SER	deletion	UNP P52286
C	?	-	LYS	deletion	UNP P52286
C	?	-	ASP	deletion	UNP P52286
C	?	-	ASN	deletion	UNP P52286

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ASN	deletion	UNP P52286
C	?	-	ASN	deletion	UNP P52286
C	77	MSE	MET	modified residue	UNP P52286
C	130	MSE	MET	modified residue	UNP P52286
C	157	MSE	MET	modified residue	UNP P52286

- Molecule 2 is a protein called CDC4 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	B	444	3582	2296	618	656	6	6	0	0	0
			Total	C	N	O	S	Se			
2	D	444	3582	2296	618	656	6	6	0	0	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	261	GLY	-	cloning artifact	UNP P07834
B	262	ALA	-	cloning artifact	UNP P07834
B	381	MSE	MET	modified residue	UNP P07834
B	403	MSE	MET	modified residue	UNP P07834
B	530	MSE	MET	modified residue	UNP P07834
B	560	MSE	MET	modified residue	UNP P07834
B	590	MSE	MET	modified residue	UNP P07834
B	?	-	ASN	deletion	UNP P07834
B	?	-	ILE	deletion	UNP P07834
B	?	-	TRP	deletion	UNP P07834
B	?	-	ASN	deletion	UNP P07834
B	608	LEU	CYS	engineered mutation	UNP P07834
B	?	-	SER	deletion	UNP P07834
B	?	-	TYR	deletion	UNP P07834
B	?	-	ALA	deletion	UNP P07834
B	?	-	THR	deletion	UNP P07834
B	?	-	ASN	deletion	UNP P07834
B	?	-	SER	deletion	UNP P07834
B	?	-	ALA	deletion	UNP P07834
B	?	-	SER	deletion	UNP P07834
B	?	-	PRO	deletion	UNP P07834
B	?	-	CYS	deletion	UNP P07834
B	?	-	ALA	deletion	UNP P07834
B	?	-	LYS	deletion	UNP P07834
B	?	-	ILE	deletion	UNP P07834

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLY	deletion	UNP P07834
B	?	-	ALA	deletion	UNP P07834
B	625	MSE	MET	modified residue	UNP P07834
D	261	GLY	-	cloning artifact	UNP P07834
D	262	ALA	-	cloning artifact	UNP P07834
D	381	MSE	MET	modified residue	UNP P07834
D	403	MSE	MET	modified residue	UNP P07834
D	530	MSE	MET	modified residue	UNP P07834
D	560	MSE	MET	modified residue	UNP P07834
D	590	MSE	MET	modified residue	UNP P07834
D	?	-	ASN	deletion	UNP P07834
D	?	-	ILE	deletion	UNP P07834
D	?	-	TRP	deletion	UNP P07834
D	?	-	ASN	deletion	UNP P07834
D	608	LEU	CYS	engineered mutation	UNP P07834
D	?	-	SER	deletion	UNP P07834
D	?	-	TYR	deletion	UNP P07834
D	?	-	ALA	deletion	UNP P07834
D	?	-	THR	deletion	UNP P07834
D	?	-	ASN	deletion	UNP P07834
D	?	-	SER	deletion	UNP P07834
D	?	-	ALA	deletion	UNP P07834
D	?	-	SER	deletion	UNP P07834
D	?	-	PRO	deletion	UNP P07834
D	?	-	CYS	deletion	UNP P07834
D	?	-	ALA	deletion	UNP P07834
D	?	-	LYS	deletion	UNP P07834
D	?	-	ILE	deletion	UNP P07834
D	?	-	GLY	deletion	UNP P07834
D	?	-	ALA	deletion	UNP P07834
D	625	MSE	MET	modified residue	UNP P07834

- Molecule 3 is a protein called GLL(TPO)PPQSG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	E	4	33	20	4	8	1	0	0	0
			Total	C	N	O	P			
3	F	8	61	36	9	15	1	0	0	0

- Molecule 4 is water.

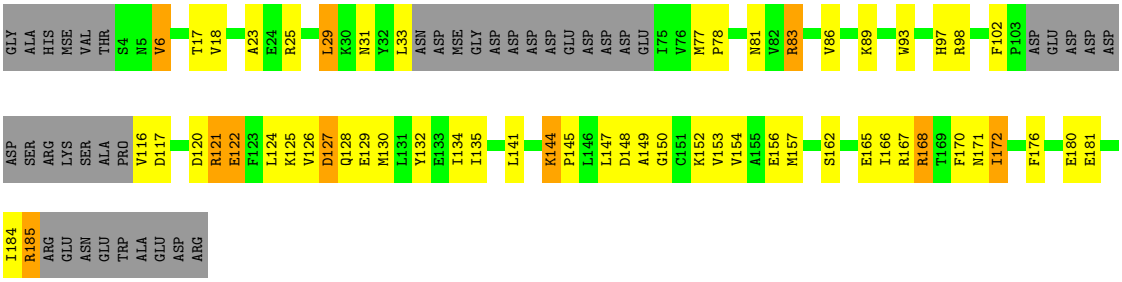
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	9	9	9	0	0
			Total	O		
4	B	25	25	25	0	0
			Total	O		
4	C	9	9	9	0	0
			Total	O		
4	D	27	27	27	0	0
			Total	O		
4	E	2	2	2	0	0

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. 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. 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.

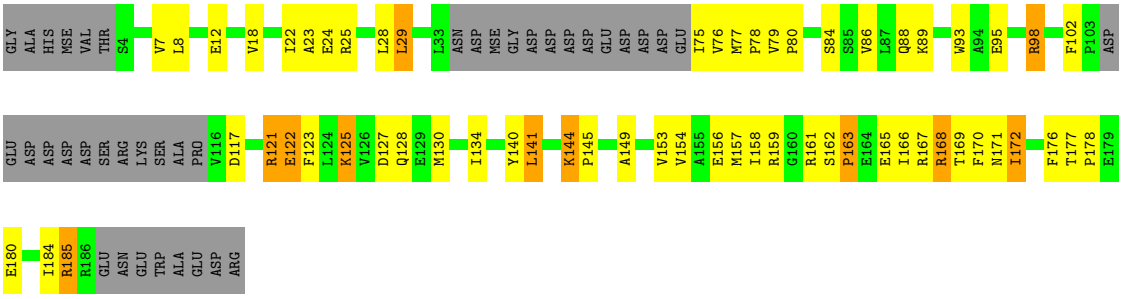
• Molecule 1: Centromere DNA-binding protein complex CBF3 subunit D

Chain A: 42% 28% 6% 24%



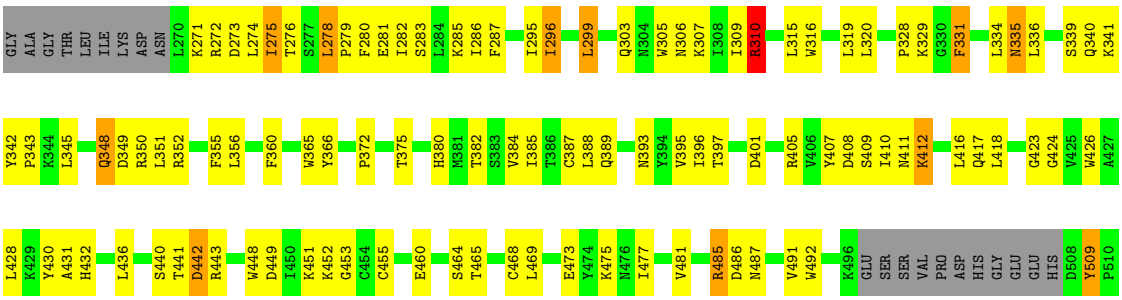
• Molecule 1: Centromere DNA-binding protein complex CBF3 subunit D

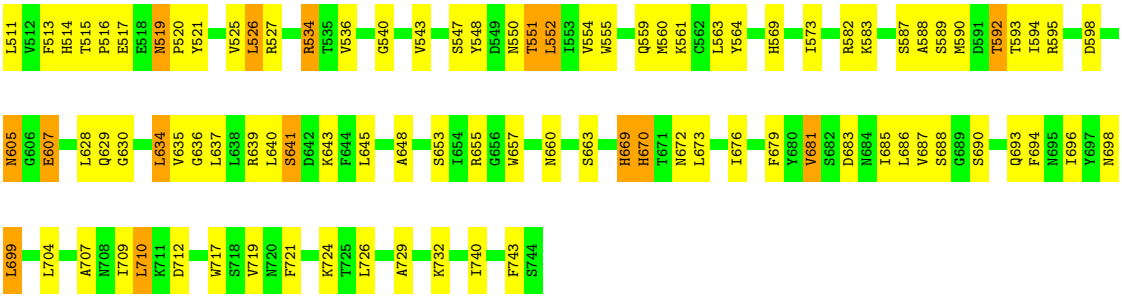
Chain C: 41% 30% 7% 23%



• Molecule 2: CDC4 protein

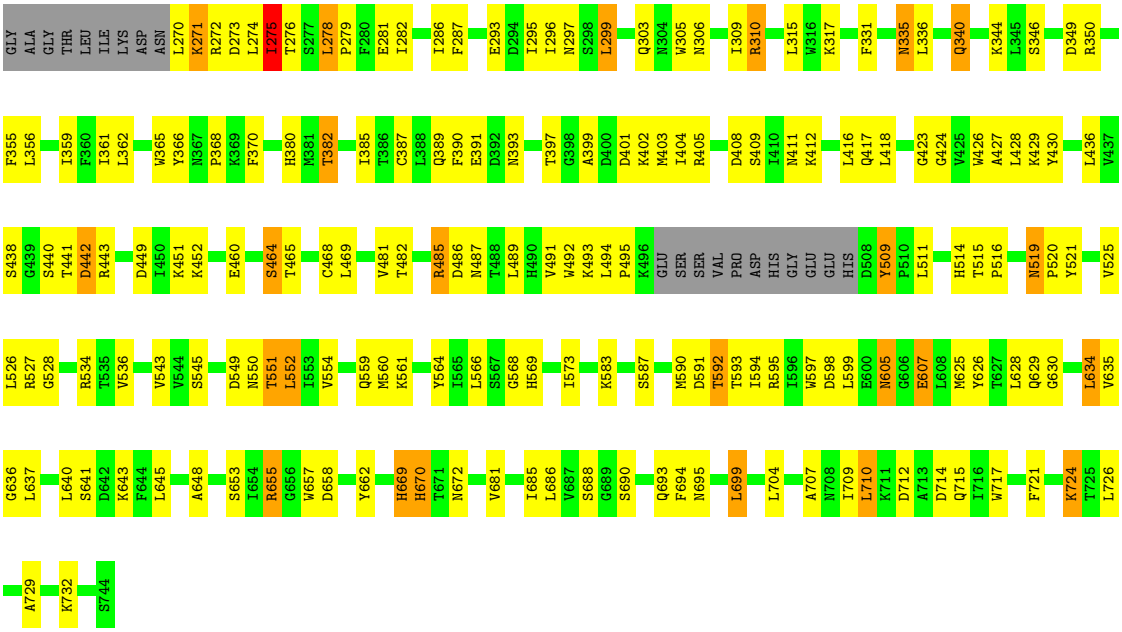
Chain B: 53% 37% 6% •





• Molecule 2: CDC4 protein

Chain D:



• Molecule 3: GLL(TPO)PPQSG

Chain E:

• Molecule 3: GLL(TPO)PPQSG

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	107.67Å 107.67Å 168.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.99 – 2.70 19.99 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.7 (19.99-2.70) 98.2 (19.99-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 2.71Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.273 0.233 , 0.231	Depositor DCC
R_{free} test set	9884 reflections (8.51%)	wwPDB-VP
Wilson B-factor (Å^2)	41.6	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 18.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.244 for -h,-k,l 0.085 for h,-h-k,-l 0.078 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9435	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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: TPO

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	0.46	0/1061	0.65	0/1428
1	C	0.46	0/1072	0.63	0/1442
2	B	0.45	0/3657	0.69	3/4939 (0.1%)
2	D	0.45	0/3657	0.70	3/4939 (0.1%)
3	E	0.47	0/22	0.81	0/28
3	F	0.47	0/50	0.73	0/64
All	All	0.45	0/9519	0.68	6/12840 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	310	ARG	NE-CZ-NH1	7.12	123.86	120.30
2	B	310	ARG	NE-CZ-NH1	6.22	123.41	120.30
2	D	275	ILE	CG1-CB-CG2	5.58	123.67	111.40
2	B	310	ARG	NE-CZ-NH2	-5.58	117.51	120.30
2	B	645	LEU	N-CA-C	-5.36	96.53	111.00
2	D	310	ARG	NE-CZ-NH2	-5.14	117.73	120.30

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	1047	0	1055	60	0
1	C	1058	0	1068	65	0
2	B	3582	0	3581	181	0
2	D	3582	0	3581	157	0
3	E	33	0	29	5	0
3	F	61	0	56	6	0
4	A	9	0	0	3	0
4	B	25	0	0	5	0
4	C	9	0	0	1	0
4	D	27	0	0	1	0
4	E	2	0	0	0	0
All	All	9435	0	9370	442	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 (442) 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:167:ARG:HG2	1:A:172:ILE:HG22	1.30	1.12
2:D:491:VAL:HB	2:D:560:MSE:HE1	1.34	1.07
2:D:275:ILE:HG21	2:D:305:TRP:NE1	1.72	1.04
2:D:270:LEU:HD23	2:D:271:LYS:H	1.24	1.03
1:C:171:ASN:HD22	2:D:271:LYS:HD2	1.19	1.02
1:C:86:VAL:HG22	1:C:130:MSE:HE1	1.39	1.01
1:C:130:MSE:HE2	1:C:134:ILE:HG13	1.45	0.98
2:B:348:GLN:HE21	2:B:348:GLN:H	0.98	0.98
2:B:491:VAL:HB	2:B:560:MSE:HE1	1.46	0.97
1:A:130:MSE:HE2	1:A:134:ILE:HG13	1.44	0.96
1:A:168:ARG:HE	1:A:168:ARG:HA	1.30	0.94
2:B:275:ILE:HG21	2:B:305:TRP:NE1	1.83	0.94
2:B:348:GLN:H	2:B:348:GLN:NE2	1.66	0.92
2:D:355:PHE:CE2	2:D:359:ILE:HD11	2.03	0.92
1:A:86:VAL:HG22	1:A:130:MSE:HE1	1.51	0.92
2:D:275:ILE:HG21	2:D:305:TRP:CE2	2.05	0.91
2:D:389:GLN:HE21	2:D:430:TYR:H	1.03	0.91
1:A:167:ARG:HG2	1:A:172:ILE:CG2	2.01	0.90
1:A:122:GLU:OE2	1:A:122:GLU:HA	1.72	0.89
2:B:485:ARG:HH12	3:E:4:TPO:HG22	1.37	0.89
1:C:122:GLU:OE2	1:C:122:GLU:HA	1.70	0.89
2:B:275:ILE:HD11	2:B:287:PHE:CE2	2.07	0.88
1:C:171:ASN:ND2	2:D:271:LYS:HD2	1.88	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:273:ASP:OD1	2:D:275:ILE:HG22	1.74	0.87
2:B:275:ILE:HD11	2:B:287:PHE:CZ	2.09	0.87
2:B:275:ILE:HG21	2:B:305:TRP:CE2	2.10	0.87
2:D:424:GLY:O	2:D:440:SER:HB2	1.76	0.86
2:B:273:ASP:OD1	2:B:275:ILE:HG22	1.75	0.86
2:D:485:ARG:HH12	3:F:4:TPO:HG22	1.39	0.86
2:B:296:ILE:HD11	2:B:356:LEU:HD21	1.59	0.84
2:B:389:GLN:HE21	2:B:430:TYR:H	1.23	0.83
1:C:168:ARG:HE	1:C:168:ARG:HA	1.43	0.83
2:D:270:LEU:CD2	2:D:271:LYS:H	1.92	0.82
1:C:86:VAL:HG22	1:C:130:MSE:CE	2.10	0.81
2:D:355:PHE:CD2	2:D:359:ILE:HD11	2.16	0.81
2:D:426:TRP:CD2	3:F:5:PRO:HG3	2.16	0.80
1:A:184:ILE:O	1:A:185:ARG:HB2	1.79	0.80
2:D:440:SER:OG	2:D:442:ASP:HB3	1.81	0.80
2:B:348:GLN:HE21	2:B:348:GLN:N	1.78	0.80
2:B:426:TRP:CD2	3:E:5:PRO:HG3	2.16	0.79
2:D:275:ILE:CG2	2:D:305:TRP:NE1	2.46	0.79
2:D:275:ILE:HD11	2:D:287:PHE:CE2	2.18	0.79
2:D:491:VAL:CB	2:D:560:MSE:HE1	2.12	0.76
2:D:361:ILE:HD13	2:D:724:LYS:HB3	1.67	0.76
2:D:709:ILE:HG22	2:D:710:LEU:HD13	1.65	0.76
1:C:180:GLU:O	1:C:184:ILE:HG13	1.85	0.75
1:A:162:SER:OG	1:A:165:GLU:HG3	1.86	0.75
2:B:336:LEU:O	2:B:340:GLN:HG3	1.86	0.75
2:D:468:CYS:SG	2:D:536:VAL:HG23	2.26	0.75
2:D:449:ASP:OD2	2:D:452:LYS:HG3	1.86	0.75
2:B:424:GLY:O	2:B:440:SER:HB2	1.85	0.74
2:B:590:MSE:HA	2:B:634:LEU:HD23	1.70	0.74
1:C:130:MSE:HE2	1:C:134:ILE:CG1	2.17	0.73
2:B:380:HIS:CE1	2:B:405:ARG:HG3	2.24	0.73
2:D:389:GLN:NE2	2:D:430:TYR:H	1.83	0.73
1:A:86:VAL:HG22	1:A:130:MSE:CE	2.18	0.72
1:C:154:VAL:HG11	2:D:286:ILE:HD13	1.70	0.72
2:D:591:ASP:O	2:D:592:THR:HB	1.88	0.72
2:B:440:SER:OG	2:B:442:ASP:HB3	1.88	0.72
1:C:78:PRO:O	1:C:80:PRO:HD3	1.90	0.72
1:A:144:LYS:HB3	1:A:145:PRO:HD3	1.72	0.71
2:B:559:GLN:O	2:B:561:LYS:HG3	1.90	0.71
2:D:423:GLY:N	2:D:442:ASP:HB2	2.06	0.71
2:D:559:GLN:O	2:D:561:LYS:HG3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:275:ILE:HD11	2:D:287:PHE:CZ	2.27	0.69
1:A:130:MSE:HE2	1:A:134:ILE:CG1	2.20	0.69
2:B:299:LEU:HD23	2:B:306:ASN:OD1	1.93	0.68
2:B:329:LYS:HG2	4:B:7:HOH:O	1.94	0.68
2:D:670:HIS:HD2	2:D:690:SER:OG	1.75	0.68
2:D:525:VAL:HG23	2:D:527:ARG:HG3	1.74	0.68
2:B:634:LEU:HD22	2:B:635:VAL:N	2.09	0.67
2:B:380:HIS:HE1	2:B:397:THR:OG1	1.76	0.67
1:C:78:PRO:C	1:C:80:PRO:HD3	2.14	0.67
2:D:630:GLY:O	2:D:655:ARG:HD2	1.95	0.66
1:C:184:ILE:O	1:C:184:ILE:HG22	1.95	0.66
2:B:519:ASN:HD22	2:B:519:ASN:C	1.98	0.66
2:B:275:ILE:CG2	2:B:305:TRP:NE1	2.58	0.66
2:B:385:ILE:HG13	2:B:729:ALA:HB1	1.78	0.66
1:A:176:PHE:HE1	2:B:303:GLN:HE21	1.38	0.65
2:B:316:TRP:CZ2	2:B:352:ARG:HD3	2.31	0.65
2:D:356:LEU:HA	2:D:359:ILE:HD12	1.77	0.65
1:C:171:ASN:HD22	2:D:271:LYS:CD	2.05	0.65
2:B:475:LYS:O	2:B:477:ILE:HG13	1.97	0.65
2:B:630:GLY:O	2:B:655:ARG:HD2	1.97	0.65
1:C:176:PHE:HE1	2:D:303:GLN:HE21	1.45	0.65
2:D:441:THR:HA	2:D:465:THR:HG23	1.78	0.64
1:A:89:LYS:HG2	1:A:134:ILE:HD11	1.80	0.64
2:B:491:VAL:CB	2:B:560:MSE:HE1	2.24	0.63
2:D:569:HIS:HE1	2:D:587:SER:OG	1.82	0.63
1:C:163:PRO:O	1:C:167:ARG:HG3	1.99	0.63
2:D:270:LEU:HD23	2:D:271:LYS:N	2.06	0.63
2:B:341:LYS:HD3	2:B:342:TYR:CE2	2.33	0.63
2:B:389:GLN:HG2	2:B:428:LEU:HD12	1.80	0.63
2:B:598:ASP:HB3	2:B:607:GLU:OE1	1.99	0.62
2:D:634:LEU:HD22	2:D:635:VAL:N	2.13	0.62
2:B:336:LEU:HD21	1:C:98:ARG:NE	2.14	0.62
2:D:317:LYS:HD2	2:D:331:PHE:CZ	2.35	0.62
2:D:590:MSE:HA	2:D:634:LEU:HD23	1.80	0.62
1:C:170:PHE:HE1	2:D:274:LEU:HD12	1.65	0.61
2:B:569:HIS:HE1	2:B:587:SER:OG	1.84	0.61
1:C:159:ARG:NH2	4:C:200:HOH:O	2.33	0.61
2:D:365:TRP:CE3	2:D:685:ILE:HD13	2.35	0.61
2:D:389:GLN:HG2	2:D:428:LEU:HD12	1.81	0.61
2:B:519:ASN:ND2	2:B:521:TYR:H	1.99	0.61
1:C:149:ALA:O	1:C:153:VAL:HG23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:465:THR:HB	2:D:485:ARG:HG3	1.83	0.60
1:C:170:PHE:CE1	2:D:274:LEU:HD12	2.36	0.60
2:D:287:PHE:CZ	2:D:309:ILE:HD11	2.37	0.60
2:D:566:LEU:HD13	2:D:597:TRP:CG	2.36	0.60
1:C:28:LEU:HD22	1:C:140:TYR:O	2.02	0.60
2:D:554:VAL:HG21	2:D:599:LEU:HD22	1.84	0.60
2:B:375:THR:HG21	2:B:412:LYS:HB3	1.83	0.60
2:D:380:HIS:HE1	2:D:397:THR:OG1	1.85	0.60
1:A:162:SER:O	1:A:166:ILE:HG13	2.03	0.59
1:A:172:ILE:HD11	2:B:273:ASP:OD2	2.02	0.59
2:B:275:ILE:HD11	2:B:287:PHE:HE2	1.64	0.59
2:D:382:THR:HG22	2:D:401:ASP:HB3	1.84	0.59
2:B:336:LEU:HD21	1:C:98:ARG:HE	1.68	0.59
2:D:293:GLU:O	2:D:297:ASN:ND2	2.32	0.58
2:B:388:LEU:C	2:B:388:LEU:HD23	2.24	0.58
2:B:468:CYS:SG	2:B:536:VAL:HG23	2.43	0.58
1:C:25:ARG:NH2	1:C:102:PHE:CD1	2.71	0.58
2:D:605:ASN:OD1	2:D:607:GLU:OE1	2.21	0.58
1:A:171:ASN:HB2	2:B:271:LYS:HG3	1.85	0.58
2:B:561:LYS:NZ	2:B:561:LYS:HB3	2.18	0.58
1:A:83:ARG:HD2	4:A:196:HOH:O	2.04	0.58
1:A:184:ILE:O	1:A:184:ILE:HG22	2.04	0.58
2:B:593:THR:HG22	2:B:629:GLN:HE22	1.68	0.58
2:D:670:HIS:CD2	2:D:690:SER:OG	2.56	0.58
2:B:275:ILE:HD11	2:B:287:PHE:HZ	1.66	0.58
2:D:389:GLN:HE21	2:D:430:TYR:N	1.87	0.58
1:A:170:PHE:HE1	2:B:274:LEU:HD12	1.69	0.58
2:D:672:ASN:OD1	2:D:693:GLN:NE2	2.37	0.58
2:B:452:LYS:HD3	2:B:509:TYR:HE1	1.68	0.58
2:B:382:THR:HG22	2:B:401:ASP:HB3	1.86	0.57
2:D:380:HIS:HB3	2:D:401:ASP:OD2	2.03	0.57
2:B:592:THR:HG23	2:B:592:THR:O	2.03	0.57
2:B:670:HIS:HE1	2:B:688:SER:OG	1.87	0.57
2:B:525:VAL:HG21	2:B:527:ARG:CZ	2.35	0.57
2:B:460:GLU:OE1	2:B:514:HIS:HA	2.04	0.57
1:C:171:ASN:HB3	2:D:271:LYS:HB2	1.86	0.56
2:D:275:ILE:CG2	2:D:276:THR:N	2.68	0.56
1:C:122:GLU:OE2	1:C:122:GLU:CA	2.51	0.56
1:A:180:GLU:O	1:A:184:ILE:HG13	2.05	0.56
1:C:89:LYS:HG3	1:C:123:PHE:CE1	2.41	0.56
1:A:130:MSE:CE	1:A:134:ILE:HG13	2.29	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:443:ARG:HD2	2:D:464:SER:HA	1.87	0.56
2:D:605:ASN:ND2	2:D:607:GLU:CD	2.59	0.56
2:D:403:MSE:HG2	2:D:417:GLN:NE2	2.21	0.56
2:D:426:TRP:CE2	3:F:5:PRO:HG3	2.40	0.56
2:B:449:ASP:OD2	2:B:451:LYS:HB2	2.07	0.56
1:A:168:ARG:HE	1:A:168:ARG:CA	2.10	0.55
2:D:346:SER:O	2:D:350:ARG:HG3	2.05	0.55
1:C:25:ARG:NH2	1:C:102:PHE:CE1	2.75	0.55
2:D:429:LYS:HB3	2:D:469:LEU:HD11	1.88	0.55
1:A:167:ARG:CG	1:A:172:ILE:HG22	2.22	0.55
1:A:170:PHE:CE1	2:B:274:LEU:HD12	2.42	0.55
2:B:681:VAL:HG13	2:B:686:LEU:HD13	1.89	0.55
2:B:712:ASP:OD2	2:B:732:LYS:HD2	2.06	0.55
2:D:485:ARG:NH2	3:F:7:GLN:HB2	2.22	0.55
2:D:598:ASP:HB3	2:D:607:GLU:OE1	2.06	0.55
2:B:416:LEU:C	2:B:416:LEU:HD12	2.26	0.55
2:D:516:PRO:HD2	4:D:56:HOH:O	2.06	0.55
1:C:167:ARG:HG2	1:C:172:ILE:HG22	1.88	0.55
1:A:149:ALA:O	1:A:153:VAL:HG23	2.07	0.55
2:D:460:GLU:OE1	2:D:514:HIS:HA	2.07	0.54
2:D:385:ILE:HG13	2:D:729:ALA:HB1	1.90	0.54
2:B:275:ILE:CG2	2:B:276:THR:N	2.70	0.54
1:C:25:ARG:HH21	1:C:102:PHE:HD1	1.54	0.54
2:B:681:VAL:HG13	2:B:686:LEU:CD1	2.38	0.54
2:D:694:PHE:CE2	2:D:710:LEU:HD22	2.43	0.54
1:C:86:VAL:CG2	1:C:130:MSE:HE1	2.25	0.54
2:B:513:PHE:CE2	2:B:520:PRO:HD2	2.43	0.53
1:C:79:VAL:HG13	1:C:141:LEU:HD21	1.90	0.53
2:D:362:LEU:HD11	2:D:366:TYR:CZ	2.43	0.53
2:B:343:PRO:HG2	1:C:88:GLN:OE1	2.08	0.53
2:D:482:THR:O	2:D:489:LEU:HA	2.09	0.53
1:A:25:ARG:HH21	1:A:102:PHE:HE1	1.55	0.53
2:B:509:TYR:O	2:B:511:LEU:N	2.40	0.53
1:C:154:VAL:CG1	2:D:286:ILE:HD13	2.38	0.53
2:D:634:LEU:HD22	2:D:634:LEU:C	2.29	0.53
2:B:331:PHE:O	2:B:334:LEU:HB3	2.09	0.53
1:A:122:GLU:OE2	1:A:122:GLU:CA	2.52	0.53
2:B:306:ASN:O	2:B:310:ARG:HG3	2.09	0.52
2:B:721:PHE:HB3	2:B:726:LEU:CD1	2.40	0.52
1:C:75:ILE:HG23	1:C:76:VAL:N	2.25	0.52
2:B:551:THR:HG23	2:B:552:LEU:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:670:HIS:HD2	2:B:690:SER:OG	1.93	0.52
1:A:116:VAL:HG23	1:A:152:LYS:HD3	1.90	0.52
1:C:128:GLN:NE2	1:C:170:PHE:CD1	2.78	0.52
1:C:185:ARG:NH1	1:C:185:ARG:HB2	2.24	0.52
2:B:356:LEU:O	2:B:360:PHE:HD2	1.93	0.52
2:D:370:PHE:CD1	2:D:370:PHE:C	2.83	0.51
1:C:18:VAL:CG2	1:C:23:ALA:HB2	2.41	0.51
1:A:117:ASP:HB3	1:A:120:ASP:HB2	1.93	0.51
2:D:645:LEU:O	2:D:657:TRP:HD1	1.93	0.51
2:B:372:PRO:HG3	2:B:743:PHE:CE2	2.46	0.51
2:B:605:ASN:ND2	2:B:607:GLU:CD	2.64	0.51
2:D:593:THR:HG22	2:D:629:GLN:NE2	2.25	0.51
1:A:124:LEU:CD1	1:A:153:VAL:HG21	2.41	0.51
2:B:452:LYS:HD3	2:B:509:TYR:CE1	2.46	0.51
2:B:513:PHE:HE2	2:B:520:PRO:HD2	1.75	0.51
2:B:694:PHE:HB3	4:B:60:HOH:O	2.10	0.51
2:D:704:LEU:HD21	2:D:707:ALA:HB2	1.92	0.51
2:D:390:PHE:C	2:D:391:GLU:HG2	2.31	0.50
2:D:568:GLY:HA3	2:D:595:ARG:NH1	2.26	0.50
2:B:436:LEU:HD12	2:B:436:LEU:C	2.31	0.50
2:B:721:PHE:HB3	2:B:726:LEU:HD13	1.93	0.50
2:B:319:LEU:HB3	2:B:355:PHE:CE2	2.46	0.50
1:C:172:ILE:HD11	2:D:273:ASP:OD2	2.11	0.50
1:A:31:ASN:O	1:A:33:LEU:HG	2.11	0.50
2:B:393:ASN:HA	2:B:409:SER:OG	2.12	0.50
2:B:704:LEU:HD21	2:B:707:ALA:HB2	1.93	0.50
2:B:534:ARG:HB2	2:B:548:TYR:CE1	2.46	0.50
2:D:275:ILE:HG21	2:D:305:TRP:CD1	2.45	0.50
1:A:6:VAL:HG11	1:A:29:LEU:HD21	1.94	0.50
2:D:443:ARG:HD2	2:D:464:SER:CA	2.42	0.50
2:B:365:TRP:HB3	2:B:685:ILE:HD11	1.92	0.50
2:B:526:LEU:HG	2:B:555:TRP:CE3	2.47	0.50
2:B:309:ILE:HG23	2:B:315:LEU:CD2	2.42	0.49
2:D:336:LEU:HD13	2:D:340:GLN:NE2	2.27	0.49
2:D:712:ASP:OD2	2:D:732:LYS:HD2	2.12	0.49
2:D:519:ASN:HD22	2:D:520:PRO:CD	2.25	0.49
2:B:275:ILE:HG21	2:B:305:TRP:CD1	2.46	0.49
2:D:509:TYR:O	2:D:511:LEU:N	2.46	0.49
2:D:561:LYS:NZ	2:D:561:LYS:HB3	2.27	0.49
2:B:320:LEU:CD1	2:B:351:LEU:HD22	2.42	0.49
2:B:365:TRP:CE3	2:B:685:ILE:HD13	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:VAL:HG22	1:C:23:ALA:HB2	1.95	0.49
1:A:156:GLU:HG3	4:A:202:HOH:O	2.12	0.49
2:D:299:LEU:HD21	2:D:310:ARG:HD3	1.95	0.49
2:B:396:ILE:HD12	2:B:396:ILE:N	2.28	0.48
2:B:679:PHE:HA	2:B:687:VAL:O	2.13	0.48
1:C:8:LEU:HD21	1:C:29:LEU:HD23	1.94	0.48
1:A:128:GLN:OE1	2:B:271:LYS:HA	2.12	0.48
1:C:125:LYS:NZ	1:C:125:LYS:HB3	2.28	0.48
2:D:591:ASP:O	2:D:592:THR:CB	2.58	0.48
1:C:168:ARG:HA	1:C:168:ARG:NE	2.16	0.48
2:D:605:ASN:ND2	2:D:607:GLU:OE2	2.45	0.48
2:B:525:VAL:HG23	2:B:527:ARG:HG3	1.96	0.48
2:B:679:PHE:CD1	2:B:679:PHE:C	2.86	0.48
2:D:449:ASP:OD2	2:D:451:LYS:HB2	2.13	0.48
1:A:25:ARG:NH2	1:A:102:PHE:CE1	2.77	0.48
1:A:168:ARG:HA	1:A:168:ARG:NE	2.12	0.48
2:B:554:VAL:O	2:B:563:LEU:HB2	2.14	0.48
2:B:687:VAL:CG1	2:B:719:VAL:HG21	2.44	0.48
1:C:130:MSE:CE	1:C:134:ILE:HG13	2.30	0.48
2:B:356:LEU:O	2:B:360:PHE:CD2	2.67	0.47
2:B:328:PRO:HB2	4:B:7:HOH:O	2.14	0.47
2:D:331:PHE:CE2	2:D:335:ASN:ND2	2.82	0.47
2:D:416:LEU:HD12	2:D:416:LEU:C	2.34	0.47
2:D:486:ASP:O	2:D:487:ASN:HB2	2.14	0.47
2:B:335:ASN:HD22	2:B:335:ASN:HA	1.50	0.47
2:B:341:LYS:HE2	2:B:342:TYR:OH	2.14	0.47
2:B:339:SER:HB2	2:B:350:ARG:NH1	2.30	0.47
2:B:349:ASP:OD1	2:B:352:ARG:NH2	2.46	0.47
2:B:593:THR:HG22	2:B:629:GLN:NE2	2.28	0.47
1:C:7:VAL:N	1:C:75:ILE:O	2.42	0.47
2:D:287:PHE:CE1	2:D:309:ILE:HD11	2.49	0.47
2:D:481:VAL:HG21	2:D:543:VAL:HG21	1.97	0.47
2:D:573:ILE:N	2:D:573:ILE:HD12	2.30	0.47
2:D:636:GLY:O	2:D:637:LEU:HD23	2.14	0.47
1:C:162:SER:OG	1:C:165:GLU:HG3	2.14	0.47
1:A:77:MSE:HA	1:A:78:PRO:HD3	1.80	0.47
1:A:93:TRP:HH2	1:A:145:PRO:HB2	1.78	0.47
2:B:569:HIS:NE2	2:B:595:ARG:HG3	2.30	0.47
1:C:144:LYS:HB3	1:C:145:PRO:HD3	1.97	0.47
2:D:275:ILE:HG23	2:D:276:THR:N	2.30	0.47
2:D:436:LEU:C	2:D:436:LEU:HD12	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:GLN:NE2	1:A:170:PHE:CD1	2.82	0.47
2:B:634:LEU:HD22	2:B:634:LEU:C	2.35	0.47
1:C:185:ARG:HB2	1:C:185:ARG:HH11	1.79	0.47
2:D:441:THR:CG2	3:F:5:PRO:HB3	2.45	0.47
2:D:275:ILE:CG2	2:D:305:TRP:HE1	2.28	0.47
1:C:121:ARG:HE	1:C:121:ARG:HB3	1.38	0.47
1:C:185:ARG:HH11	1:C:185:ARG:CB	2.28	0.47
2:D:549:ASP:O	2:D:550:ASN:HB2	2.15	0.47
2:D:653:SER:HB3	2:D:669:HIS:CE1	2.50	0.47
2:D:427:ALA:O	2:D:438:SER:HA	2.15	0.46
1:A:148:ASP:OD1	2:B:285:LYS:NZ	2.44	0.46
2:D:299:LEU:HD23	2:D:306:ASN:OD1	2.15	0.46
1:A:83:ARG:HB2	4:A:199:HOH:O	2.15	0.46
1:A:86:VAL:HA	1:A:130:MSE:HE1	1.97	0.46
2:B:275:ILE:CD1	2:B:287:PHE:HZ	2.27	0.46
2:B:519:ASN:HD22	2:B:520:PRO:N	2.14	0.46
1:C:22:ILE:HG21	1:C:95:GLU:HA	1.97	0.46
1:A:121:ARG:HE	1:A:121:ARG:HB3	1.43	0.46
2:B:519:ASN:C	2:B:519:ASN:ND2	2.64	0.46
2:B:548:TYR:C	2:B:550:ASN:H	2.18	0.46
2:D:275:ILE:CD1	2:D:287:PHE:CZ	2.97	0.46
1:A:150:GLY:O	1:A:154:VAL:HG23	2.15	0.46
2:D:452:LYS:HD3	2:D:509:TYR:HE1	1.81	0.46
2:D:625:MSE:HE2	2:D:626:TYR:CE2	2.50	0.46
1:A:86:VAL:CG2	1:A:130:MSE:HE1	2.34	0.46
2:D:551:THR:HG23	2:D:552:LEU:N	2.31	0.46
2:D:594:ILE:HB	2:D:628:LEU:HB2	1.97	0.46
2:D:694:PHE:CD2	2:D:710:LEU:HD22	2.51	0.46
2:B:486:ASP:O	2:B:487:ASN:HB2	2.16	0.46
2:B:412:LYS:HG3	2:B:740:ILE:HG21	1.97	0.45
2:B:481:VAL:HG21	2:B:543:VAL:HG21	1.97	0.45
2:B:515:THR:HA	2:B:516:PRO:HD3	1.77	0.45
2:D:564:TYR:OH	2:D:605:ASN:HA	2.16	0.45
2:B:657:TRP:CD1	2:B:657:TRP:N	2.84	0.45
2:B:696:ILE:HD12	2:B:709:ILE:HD12	1.98	0.45
2:D:361:ILE:CD1	2:D:724:LYS:HB3	2.41	0.45
2:B:387:CYS:SG	2:B:428:LEU:HG	2.56	0.45
2:B:408:ASP:OD2	2:B:411:ASN:HB2	2.16	0.45
2:B:426:TRP:CE3	3:E:5:PRO:HG3	2.52	0.45
2:B:441:THR:HA	2:B:465:THR:HG23	1.99	0.45
2:B:443:ARG:HD2	2:B:464:SER:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:494:LEU:HD12	2:D:495:PRO:HD2	1.97	0.45
2:B:592:THR:O	2:B:592:THR:CG2	2.64	0.45
2:B:685:ILE:CG2	2:B:686:LEU:N	2.79	0.45
2:D:340:GLN:H	2:D:340:GLN:HG2	1.49	0.45
2:D:519:ASN:HD22	2:D:520:PRO:N	2.15	0.45
2:D:714:ASP:C	2:D:715:GLN:HG2	2.36	0.45
1:A:135:ILE:HG23	1:A:147:LEU:CD1	2.47	0.45
2:B:279:PRO:HD2	2:B:282:ILE:HD13	1.98	0.45
2:D:423:GLY:H	2:D:442:ASP:HB2	1.80	0.45
2:B:348:GLN:NE2	2:B:348:GLN:N	2.48	0.44
2:D:404:ILE:HB	2:D:418:LEU:HB2	1.99	0.44
2:D:429:LYS:CB	2:D:469:LEU:HD11	2.47	0.44
2:D:712:ASP:O	2:D:732:LYS:HG2	2.16	0.44
2:B:548:TYR:OH	3:E:4:TPO:O3P	2.33	0.44
2:B:641:SER:OG	2:B:683:ASP:OD1	2.35	0.44
2:B:423:GLY:N	2:B:442:ASP:HB2	2.31	0.44
2:D:515:THR:HA	2:D:516:PRO:HD3	1.81	0.44
2:B:283:SER:O	2:B:286:ILE:HB	2.17	0.44
2:B:588:ALA:HB1	2:B:635:VAL:O	2.18	0.44
1:A:127:ASP:OD1	1:A:127:ASP:C	2.55	0.44
2:D:545:SER:O	2:D:552:LEU:HA	2.18	0.44
2:D:672:ASN:H	2:D:693:GLN:HE22	1.65	0.44
2:B:449:ASP:O	2:B:453:GLY:N	2.50	0.44
2:B:547:SER:OG	2:B:548:TYR:N	2.51	0.44
2:B:634:LEU:HD13	2:B:634:LEU:O	2.18	0.44
2:D:380:HIS:CD2	2:D:399:ALA:HB3	2.53	0.44
2:B:639:ARG:HG3	2:B:679:PHE:CE1	2.52	0.44
1:C:93:TRP:HH2	1:C:145:PRO:HB2	1.82	0.44
1:C:158:ILE:HG23	1:C:166:ILE:HD13	1.98	0.44
2:D:389:GLN:HG2	2:D:428:LEU:CD1	2.47	0.44
2:D:721:PHE:HB3	2:D:726:LEU:HD13	1.99	0.44
2:B:339:SER:HA	2:B:350:ARG:CZ	2.48	0.44
2:B:628:LEU:HD13	2:B:657:TRP:CD2	2.53	0.44
2:D:366:TYR:O	2:D:368:PRO:HD3	2.18	0.44
2:B:564:TYR:OH	2:B:605:ASN:HA	2.17	0.43
1:A:23:ALA:C	1:A:25:ARG:H	2.21	0.43
2:B:310:ARG:HD2	2:B:349:ASP:OD1	2.18	0.43
2:B:709:ILE:HG22	2:B:710:LEU:HD13	2.00	0.43
2:B:628:LEU:HD13	2:B:657:TRP:CE3	2.53	0.43
2:D:393:ASN:HA	2:D:409:SER:OG	2.18	0.43
2:B:491:VAL:CG2	2:B:560:MSE:HE1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:LEU:HD21	1:C:29:LEU:CD2	2.49	0.43
2:D:658:ASP:O	2:D:662:TYR:HA	2.18	0.43
2:B:342:TYR:CB	2:B:345:LEU:HD12	2.48	0.43
2:B:384:VAL:HG22	2:B:717:TRP:CZ2	2.54	0.43
1:C:157:MSE:HE2	1:C:169:THR:CG2	2.48	0.43
2:B:517:GLU:OE1	2:B:517:GLU:HA	2.18	0.43
2:D:426:TRP:CG	3:F:5:PRO:HG3	2.54	0.43
2:D:593:THR:HG22	2:D:629:GLN:HE22	1.84	0.43
2:D:695:ASN:HB3	2:D:704:LEU:HD11	2.01	0.43
2:D:401:ASP:O	2:D:402:LYS:HG2	2.19	0.43
2:D:408:ASP:OD2	2:D:411:ASN:HB2	2.19	0.43
2:D:519:ASN:ND2	2:D:521:TYR:H	2.17	0.43
1:A:132:TYR:HB2	2:B:274:LEU:CD2	2.48	0.42
2:B:393:ASN:CG	2:B:410:ILE:HD11	2.39	0.42
2:B:513:PHE:HD2	2:B:519:ASN:HA	1.84	0.42
2:B:605:ASN:HD21	2:B:607:GLU:CD	2.23	0.42
2:D:279:PRO:HD2	2:D:282:ILE:HD13	2.01	0.42
3:E:4:TPO:HA	3:E:5:PRO:HD3	1.78	0.42
1:A:126:VAL:HG21	1:A:130:MSE:CG	2.49	0.42
2:B:342:TYR:HB3	2:B:345:LEU:HD12	2.00	0.42
1:A:184:ILE:O	1:A:185:ARG:CB	2.59	0.42
2:D:317:LYS:HD2	2:D:331:PHE:CE1	2.54	0.42
2:D:605:ASN:CG	2:D:607:GLU:CD	2.77	0.42
2:B:448:TRP:CZ3	2:B:455:CYS:HB2	2.54	0.42
2:B:561:LYS:NZ	4:B:17:HOH:O	2.44	0.42
2:B:405:ARG:CD	2:B:417:GLN:HE21	2.32	0.42
2:B:431:ALA:O	2:B:432:HIS:C	2.58	0.42
1:C:161:ARG:CZ	1:C:165:GLU:HB3	2.50	0.42
1:A:129:GLU:OE2	2:B:272:ARG:HD2	2.19	0.42
2:B:380:HIS:HB3	2:B:401:ASP:OD2	2.19	0.42
2:B:648:ALA:HB1	2:B:676:ILE:HG21	2.02	0.42
1:A:153:VAL:O	1:A:157:MSE:HG3	2.20	0.42
2:B:594:ILE:HB	2:B:628:LEU:HB2	2.01	0.42
2:D:509:TYR:O	2:D:511:LEU:HG	2.20	0.42
2:D:699:LEU:HD12	2:D:699:LEU:HA	1.85	0.42
2:B:582:ARG:HD3	2:B:660:ASN:ND2	2.34	0.42
1:C:12:GLU:OE2	1:C:84:SER:N	2.48	0.42
1:C:177:THR:O	1:C:178:PRO:C	2.58	0.42
1:A:124:LEU:HD13	1:A:153:VAL:HG21	2.01	0.42
2:B:630:GLY:HA3	2:B:655:ARG:HD2	2.02	0.42
1:C:23:ALA:C	1:C:25:ARG:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:380:HIS:CE1	2:D:405:ARG:HG3	2.55	0.41
2:D:566:LEU:HD13	2:D:597:TRP:CD2	2.55	0.41
1:A:18:VAL:HG22	1:A:23:ALA:HB2	2.01	0.41
1:A:31:ASN:C	1:A:33:LEU:N	2.72	0.41
2:B:278:LEU:HD13	2:B:278:LEU:HA	1.82	0.41
2:B:687:VAL:HG12	2:B:719:VAL:HG21	2.02	0.41
2:D:306:ASN:O	2:D:310:ARG:HG3	2.19	0.41
2:D:315:LEU:C	2:D:315:LEU:HD23	2.41	0.41
2:D:401:ASP:C	2:D:402:LYS:HG2	2.40	0.41
2:D:428:LEU:HD12	2:D:428:LEU:O	2.19	0.41
2:B:487:ASN:N	2:B:487:ASN:HD22	2.18	0.41
2:B:589:SER:OG	2:B:590:MSE:N	2.53	0.41
2:B:607:GLU:OE1	2:B:607:GLU:N	2.48	0.41
2:B:636:GLY:O	2:B:637:LEU:HD23	2.21	0.41
2:B:582:ARG:HD3	2:B:660:ASN:HD22	1.85	0.41
2:B:663:SER:HB3	4:B:27:HOH:O	2.20	0.41
2:B:672:ASN:H	2:B:693:GLN:HE22	1.66	0.41
1:A:97:HIS:HE1	1:A:120:ASP:OD1	2.03	0.41
2:B:418:LEU:HB3	2:B:448:TRP:CZ3	2.56	0.41
2:B:469:LEU:HA	2:B:481:VAL:O	2.21	0.41
2:B:561:LYS:HB3	2:B:561:LYS:HZ2	1.86	0.41
2:B:395:VAL:HB	2:B:407:TYR:HB2	2.03	0.41
2:B:653:SER:HB3	2:B:669:HIS:CE1	2.56	0.41
1:A:176:PHE:CB	1:A:181:GLU:HG3	2.51	0.41
2:B:342:TYR:CG	2:B:345:LEU:HD12	2.56	0.41
1:C:127:ASP:OD1	1:C:127:ASP:C	2.59	0.41
1:C:167:ARG:HG2	1:C:172:ILE:CG2	2.51	0.41
2:D:493:LYS:HG2	2:D:521:TYR:O	2.21	0.41
2:D:648:ALA:HA	2:D:653:SER:O	2.21	0.41
1:C:7:VAL:HB	1:C:76:VAL:HG22	2.03	0.41
2:B:630:GLY:HA3	2:B:655:ARG:CD	2.51	0.40
2:D:519:ASN:HD22	2:D:520:PRO:HD2	1.86	0.40
2:D:685:ILE:CG2	2:D:686:LEU:N	2.83	0.40
2:B:519:ASN:HD22	2:B:521:TYR:H	1.68	0.40
1:C:158:ILE:HG23	1:C:166:ILE:CD1	2.51	0.40
1:C:184:ILE:O	1:C:184:ILE:CG2	2.66	0.40
1:A:17:THR:C	1:A:18:VAL:HG12	2.41	0.40
2:B:279:PRO:O	2:B:280:PHE:C	2.59	0.40
2:B:384:VAL:HA	2:B:717:TRP:NE1	2.36	0.40
2:B:699:LEU:HD12	2:B:699:LEU:HA	1.85	0.40
1:C:77:MSE:HA	1:C:78:PRO:HD3	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:670:HIS:HE1	2:D:688:SER:OG	2.04	0.40
2:D:717:TRP:HA	2:D:717:TRP:CE3	2.57	0.40
1:A:144:LYS:HB3	1:A:145:PRO:CD	2.47	0.40
2:B:366:TYR:CD1	2:B:698:ASN:ND2	2.90	0.40
2:B:465:THR:HB	2:B:485:ARG:HG3	2.03	0.40
2:B:473:GLU:O	2:B:540:GLY:HA2	2.20	0.40
2:B:573:ILE:N	2:B:573:ILE:HD12	2.36	0.40
2:D:274:LEU:O	2:D:278:LEU:CD2	2.70	0.40
2:D:274:LEU:O	2:D:278:LEU:HD23	2.22	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	123/169 (73%)	114 (93%)	9 (7%)	0	100	100
1	C	124/169 (73%)	115 (93%)	8 (6%)	1 (1%)	19	43
2	B	440/464 (95%)	406 (92%)	31 (7%)	3 (1%)	22	46
2	D	440/464 (95%)	423 (96%)	15 (3%)	2 (0%)	29	54
3	E	1/9 (11%)	1 (100%)	0	0	100	100
3	F	5/9 (56%)	3 (60%)	2 (40%)	0	100	100
All	All	1133/1284 (88%)	1062 (94%)	65 (6%)	6 (0%)	29	54

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	605	ASN
2	D	605	ASN
2	B	673	LEU

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Mol	Chain	Res	Type
2	B	331	PHE
1	C	24	GLU
2	D	528	GLY

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	117/147 (80%)	103 (88%)	14 (12%)	5 11
1	C	118/147 (80%)	105 (89%)	13 (11%)	6 14
2	B	400/410 (98%)	367 (92%)	33 (8%)	11 25
2	D	400/410 (98%)	361 (90%)	39 (10%)	8 18
3	E	3/6 (50%)	3 (100%)	0	100 100
3	F	6/6 (100%)	6 (100%)	0	100 100
All	All	1044/1126 (93%)	945 (90%)	99 (10%)	8 20

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	29	LEU
1	A	81	ASN
1	A	83	ARG
1	A	98	ARG
1	A	121	ARG
1	A	122	GLU
1	A	125	LYS
1	A	127	ASP
1	A	141	LEU
1	A	144	LYS
1	A	168	ARG
1	A	172	ILE
1	A	185	ARG
2	B	275	ILE

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Mol	Chain	Res	Type
2	B	278	LEU
2	B	281	GLU
2	B	295	ILE
2	B	296	ILE
2	B	299	LEU
2	B	307	LYS
2	B	310	ARG
2	B	335	ASN
2	B	348	GLN
2	B	412	LYS
2	B	442	ASP
2	B	485	ARG
2	B	492	TRP
2	B	509	TYR
2	B	519	ASN
2	B	526	LEU
2	B	534	ARG
2	B	551	THR
2	B	552	LEU
2	B	583	LYS
2	B	592	THR
2	B	607	GLU
2	B	634	LEU
2	B	640	LEU
2	B	641	SER
2	B	643	LYS
2	B	669	HIS
2	B	670	HIS
2	B	681	VAL
2	B	699	LEU
2	B	710	LEU
2	B	724	LYS
1	C	29	LEU
1	C	98	ARG
1	C	117	ASP
1	C	121	ARG
1	C	122	GLU
1	C	125	LYS
1	C	141	LEU
1	C	144	LYS
1	C	156	GLU
1	C	163	PRO

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Mol	Chain	Res	Type
1	C	168	ARG
1	C	172	ILE
1	C	185	ARG
2	D	271	LYS
2	D	272	ARG
2	D	275	ILE
2	D	278	LEU
2	D	281	GLU
2	D	295	ILE
2	D	296	ILE
2	D	299	LEU
2	D	335	ASN
2	D	340	GLN
2	D	344	LYS
2	D	349	ASP
2	D	382	THR
2	D	387	CYS
2	D	412	LYS
2	D	442	ASP
2	D	464	SER
2	D	485	ARG
2	D	492	TRP
2	D	509	TYR
2	D	519	ASN
2	D	526	LEU
2	D	534	ARG
2	D	551	THR
2	D	552	LEU
2	D	583	LYS
2	D	592	THR
2	D	607	GLU
2	D	634	LEU
2	D	640	LEU
2	D	641	SER
2	D	643	LYS
2	D	655	ARG
2	D	669	HIS
2	D	670	HIS
2	D	681	VAL
2	D	699	LEU
2	D	710	LEU
2	D	724	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	88	GLN
1	A	97	HIS
2	B	348	GLN
2	B	358	ASN
2	B	364	ASN
2	B	380	HIS
2	B	389	GLN
2	B	417	GLN
2	B	463	ASN
2	B	487	ASN
2	B	519	ASN
2	B	569	HIS
2	B	660	ASN
2	B	669	HIS
2	B	670	HIS
2	B	692	ASN
2	B	693	GLN
2	B	695	ASN
1	C	31	ASN
1	C	97	HIS
1	C	128	GLN
1	C	171	ASN
2	D	340	GLN
2	D	364	ASN
2	D	380	HIS
2	D	389	GLN
2	D	417	GLN
2	D	457	HIS
2	D	463	ASN
2	D	487	ASN
2	D	519	ASN
2	D	569	HIS
2	D	670	HIS
2	D	692	ASN
2	D	693	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	TPO	F	4	3	8,10,11	1.94	2 (25%)	10,14,16	0.85	0
3	TPO	E	4	3	8,10,11	2.21	3 (37%)	10,14,16	0.77	0

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	TPO	F	4	3	-	2/9/11/13	-
3	TPO	E	4	3	-	2/9/11/13	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4	TPO	P-OG1	3.99	1.66	1.59
3	E	4	TPO	O-C	3.49	1.33	1.19
3	F	4	TPO	O-C	3.38	1.33	1.19
3	F	4	TPO	P-OG1	3.27	1.65	1.59
3	E	4	TPO	P-O1P	2.25	1.57	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	4	TPO	O-C-CA-CB
3	E	4	TPO	CG2-CB-OG1-P
3	F	4	TPO	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
3	F	4	TPO	CG2-CB-OG1-P

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	4	TPO	1	0
3	E	4	TPO	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.