



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:59 am GMT

PDB ID : 1JMU
Title : Crystal Structure of the Reovirus mu1/sigma3 Complex
Authors : Liemann, S.; Nibert, M.L.; Harrison, S.C.
Deposited on : 2001-07-20
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

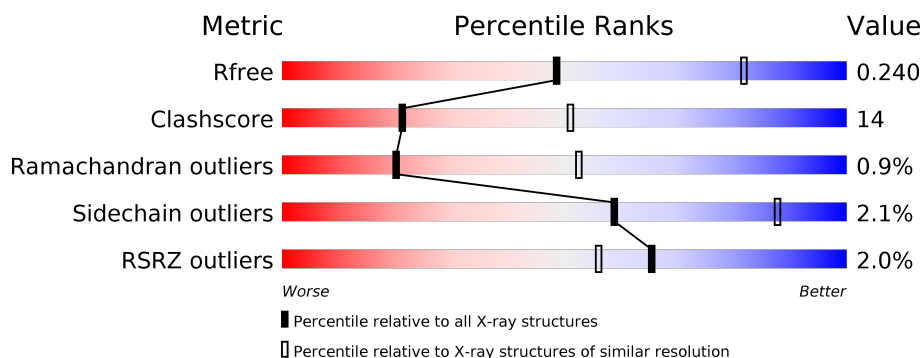
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. 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	41	<div> <div>2%</div> <div> <div></div> <div>49%</div> <div>32%</div> <div>20%</div> </div> </div>
1	C	41	<div> <div></div> <div>54%</div> <div>27%</div> <div>20%</div> </div>
1	E	41	<div> <div></div> <div>49%</div> <div>32%</div> <div>20%</div> </div>
2	B	666	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>26%</div> <div>9%</div> </div> </div>
2	D	666	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>26%</div> <div>9%</div> </div> </div>
2	F	666	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>26%</div> <div>9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	G	366	 77% 23%
3	H	366	 77% 22%
3	I	366	 78% 22%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BOG	B	709	-	-	-	X
4	BOG	D	709	-	-	-	X
4	BOG	F	709	-	-	-	X
7	CL	A	601	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 23657 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 PROTEIN MU-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	33	Total	C	N	O	S	0	0	0
			230	141	37	51	1			
1	C	33	Total	C	N	O	S	0	0	0
			230	141	37	51	1			
1	E	33	Total	C	N	O	S	0	0	0
			230	141	37	51	1			

- Molecule 2 is a protein called PROTEIN MU-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	608	Total	C	N	O	S	0	0	0
			4641	2950	770	903	18			
2	D	608	Total	C	N	O	S	0	0	0
			4641	2950	770	903	18			
2	F	608	Total	C	N	O	S	0	0	0
			4641	2950	770	903	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	272	PRO	LEU	SEE REMARK 999	UNP P11077
B	284	LYS	ARG	SEE REMARK 999	UNP P11077
B	344	LEU	PRO	SEE REMARK 999	UNP P11077
B	359	PHE	LEU	SEE REMARK 999	UNP P11077
D	272	PRO	LEU	SEE REMARK 999	UNP P11077
D	284	LYS	ARG	SEE REMARK 999	UNP P11077
D	344	LEU	PRO	SEE REMARK 999	UNP P11077
D	359	PHE	LEU	SEE REMARK 999	UNP P11077
F	272	PRO	LEU	SEE REMARK 999	UNP P11077
F	284	LYS	ARG	SEE REMARK 999	UNP P11077
F	344	LEU	PRO	SEE REMARK 999	UNP P11077
F	359	PHE	LEU	SEE REMARK 999	UNP P11077

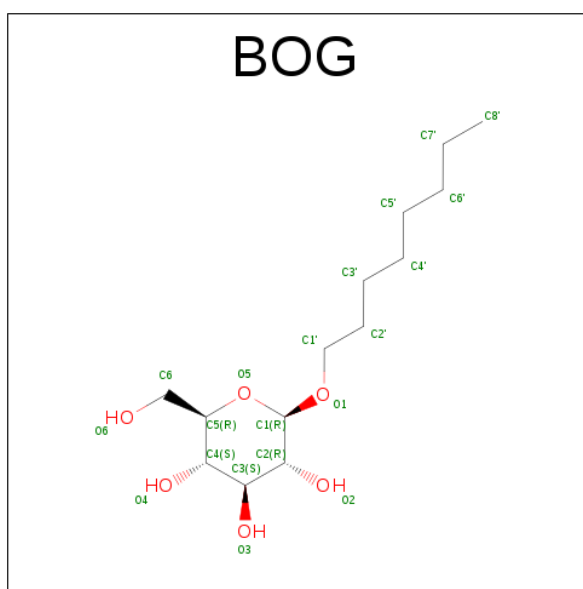
- Molecule 3 is a protein called SIGMA 3 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	366	Total	C	N	O	S	0	0	0
			2888	1820	508	532	28			
3	H	366	Total	C	N	O	S	0	0	0
			2888	1820	508	532	28			
3	I	366	Total	C	N	O	S	0	0	0
			2888	1820	508	532	28			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	104	CYS	ALA	ENGINEERED	UNP Q86292
G	325	ASN	ASP	SEE REMARK 999	UNP Q86292
H	104	CYS	ALA	ENGINEERED	UNP Q86292
H	325	ASN	ASP	SEE REMARK 999	UNP Q86292
I	104	CYS	ALA	ENGINEERED	UNP Q86292
I	325	ASN	ASP	SEE REMARK 999	UNP Q86292

- Molecule 4 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).

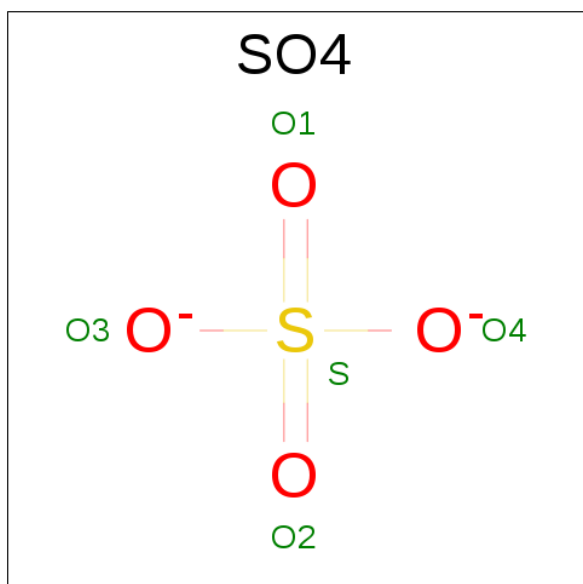


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			20	14	6		
4	D	1	Total	C	O	0	0
			20	14	6		
4	F	1	Total	C	O	0	0
			20	14	6		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	Zn	0	0
			1	1		
5	G	1	Total	Zn	0	0
			1	1		
5	I	1	Total	Zn	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		
6	I	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	I	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		

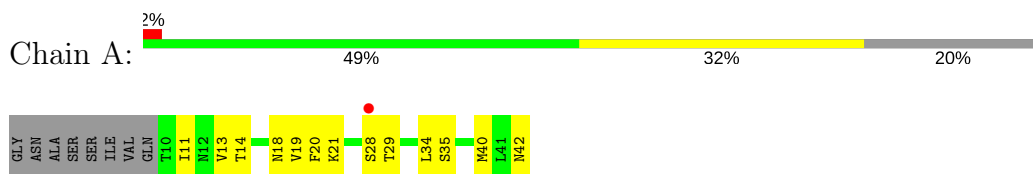
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	5	Total	O	0	0
			5	5		
8	B	42	Total	O	0	0
			42	42		
8	C	2	Total	O	0	0
			2	2		
8	D	46	Total	O	0	0
			46	46		
8	E	1	Total	O	0	0
			1	1		
8	F	56	Total	O	0	0
			56	56		
8	G	41	Total	O	0	0
			41	41		
8	H	45	Total	O	0	0
			45	45		
8	I	33	Total	O	0	0
			33	33		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

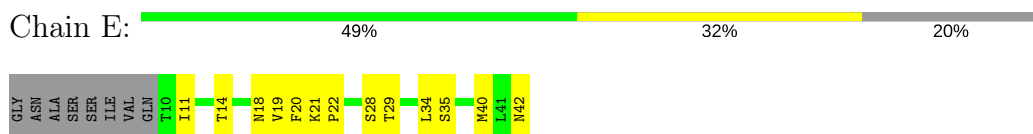
• Molecule 1: PROTEIN MU-1



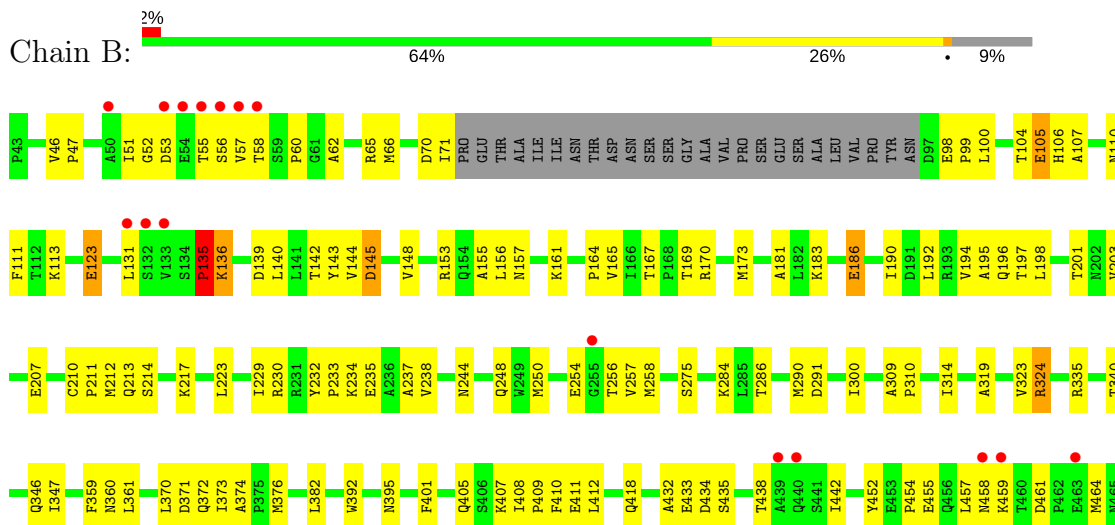
• Molecule 1: PROTEIN MU-1

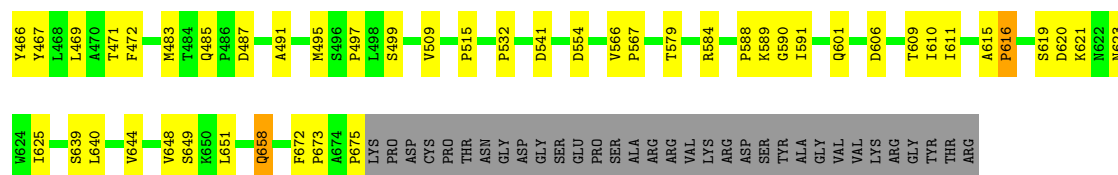


• Molecule 1: PROTEIN MU-1

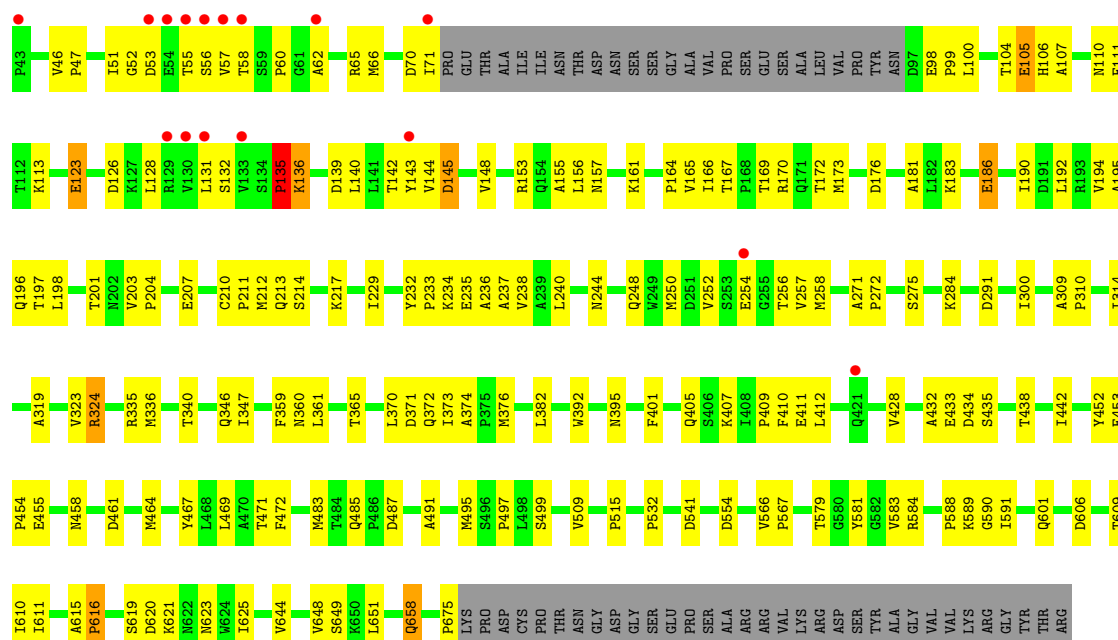


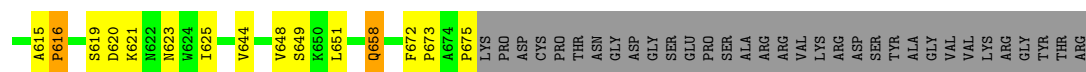
• Molecule 2: PROTEIN MU-1



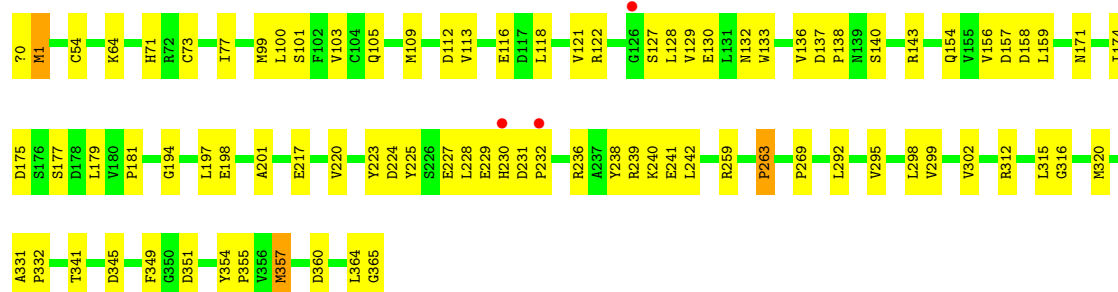
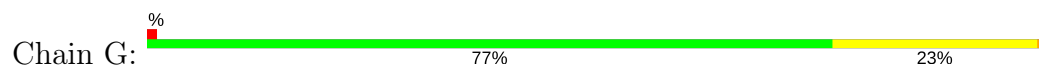


• Molecule 2: PROTEIN MU-1

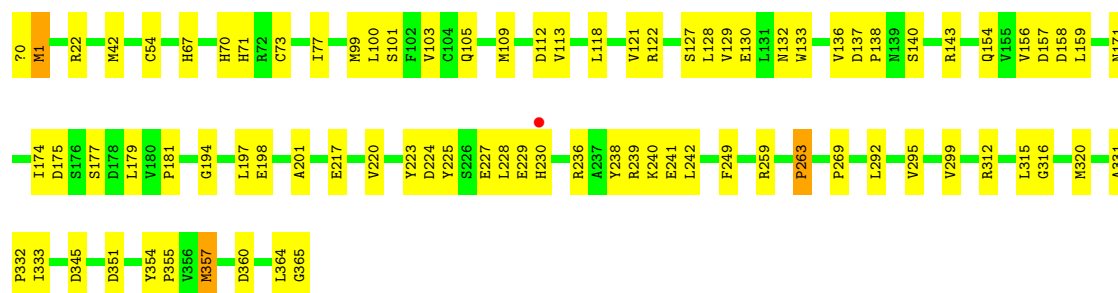




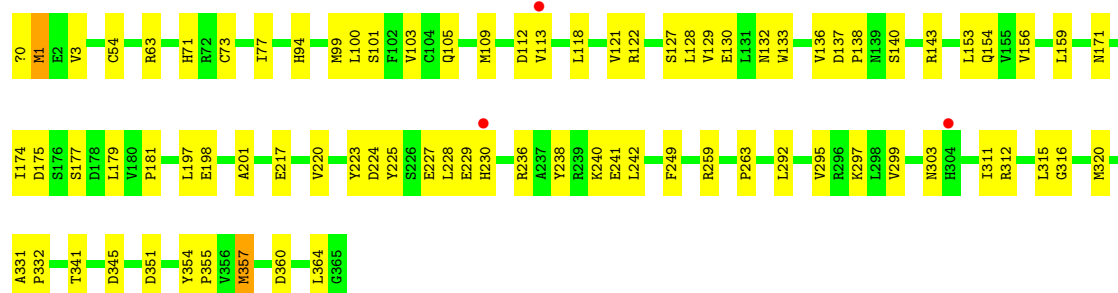
• Molecule 3: SIGMA 3 PROTEIN



• Molecule 3: SIGMA 3 PROTEIN



• Molecule 3: SIGMA 3 PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	180.29Å 184.94Å 284.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.80 34.70 – 2.81	Depositor EDS
% Data completeness (in resolution range)	93.6 (35.00-2.80) 93.7 (34.70-2.81)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.87 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.216 , 0.241 0.216 , 0.240	Depositor DCC
R_{free} test set	5422 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.838	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.006 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23657	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BOG, SO4, ACE, CL

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	0.42	0/233	0.63	0/317
1	C	0.40	0/233	0.63	0/317
1	E	0.39	0/233	0.63	0/317
2	B	0.44	0/4737	0.62	0/6466
2	D	0.44	0/4737	0.62	0/6466
2	F	0.44	0/4737	0.62	0/6466
3	G	0.44	0/2958	0.60	0/4007
3	H	0.43	0/2958	0.61	0/4007
3	I	0.42	0/2958	0.61	0/4007
All	All	0.44	0/23784	0.61	0/32370

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	230	0	227	16	0
1	C	230	0	227	14	0
1	E	230	0	227	15	0
2	B	4641	0	4673	158	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	4641	0	4673	160	0
2	F	4641	0	4673	165	0
3	G	2888	0	2814	59	0
3	H	2888	0	2814	60	0
3	I	2888	0	2814	59	0
4	B	20	0	28	2	0
4	D	20	0	28	1	0
4	F	20	0	28	1	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
6	B	5	0	0	0	0
6	D	5	0	0	0	0
6	F	5	0	0	0	0
6	G	10	0	0	0	0
6	H	10	0	0	0	0
6	I	10	0	0	0	0
7	A	1	0	0	0	0
8	A	5	0	0	2	0
8	B	42	0	0	0	0
8	C	2	0	0	0	0
8	D	46	0	0	0	0
8	E	1	0	0	0	0
8	F	56	0	0	3	0
8	G	41	0	0	0	0
8	H	45	0	0	1	0
8	I	33	0	0	2	0
All	All	23657	0	23226	633	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 14.

All (633) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:153:ARG:HH11	2:D:153:ARG:HB2	1.24	1.03
1:E:42:ASN:HB3	2:F:104:THR:HG21	1.42	1.00
1:C:42:ASN:HB3	2:D:104:THR:HG21	1.44	0.97
2:F:579:THR:HA	2:F:584:ARG:HH22	1.30	0.97
1:A:42:ASN:HB3	2:B:104:THR:HG21	1.46	0.96
3:G:171:ASN:HD22	3:G:259:ARG:HH11	1.02	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:153:ARG:HH11	2:F:153:ARG:HB2	1.30	0.96
2:B:153:ARG:HH11	2:B:153:ARG:HB2	1.28	0.95
3:G:171:ASN:HD22	3:G:259:ARG:NH1	1.65	0.93
2:D:471:THR:HG22	2:D:472:PHE:H	1.32	0.93
3:H:171:ASN:HD22	3:H:259:ARG:HH11	1.06	0.93
2:B:579:THR:HA	2:B:584:ARG:HH22	1.31	0.93
3:I:171:ASN:HD22	3:I:259:ARG:HH11	1.07	0.92
3:H:171:ASN:HD22	3:H:259:ARG:NH1	1.68	0.92
2:D:579:THR:HA	2:D:584:ARG:HH22	1.35	0.92
2:B:471:THR:HG22	2:B:472:PHE:H	1.31	0.90
3:I:171:ASN:HD22	3:I:259:ARG:NH1	1.69	0.90
2:B:435:SER:HB3	2:B:442:ILE:HB	1.54	0.89
2:B:644:VAL:HG22	2:D:186:GLU:HG2	1.52	0.89
3:G:171:ASN:ND2	3:G:259:ARG:HH11	1.70	0.89
2:B:186:GLU:HG2	2:F:644:VAL:HG22	1.54	0.88
2:F:471:THR:HG22	2:F:472:PHE:H	1.36	0.88
2:D:153:ARG:NH1	2:D:153:ARG:HB2	1.87	0.88
2:B:153:ARG:HB2	2:B:153:ARG:NH1	1.90	0.87
2:D:644:VAL:HG22	2:F:186:GLU:HG2	1.56	0.86
2:D:435:SER:HB3	2:D:442:ILE:HB	1.56	0.86
3:H:171:ASN:ND2	3:H:259:ARG:HH11	1.73	0.85
3:I:171:ASN:ND2	3:I:259:ARG:HH11	1.75	0.85
2:F:66:MET:HE1	2:F:144:VAL:HG11	1.59	0.85
2:F:435:SER:HB3	2:F:442:ILE:HB	1.59	0.84
2:D:66:MET:CE	2:D:144:VAL:HG11	2.09	0.83
2:B:66:MET:HE1	2:B:144:VAL:HG11	1.60	0.82
2:F:153:ARG:HB2	2:F:153:ARG:NH1	1.94	0.81
2:F:66:MET:CE	2:F:144:VAL:HG11	2.11	0.80
2:B:66:MET:CE	2:B:144:VAL:HG11	2.11	0.80
2:B:131:LEU:HD21	2:B:135:PRO:HD3	1.66	0.78
3:G:109:MET:HE1	3:G:129:VAL:HG13	1.65	0.77
2:D:382:LEU:HD23	2:D:491:ALA:HB2	1.67	0.76
2:F:372:GLN:O	2:F:509:VAL:HG23	1.86	0.75
2:D:471:THR:HG22	2:D:472:PHE:N	2.02	0.75
2:D:131:LEU:HD21	2:D:135:PRO:HD3	1.67	0.74
2:B:471:THR:HG22	2:B:472:PHE:N	2.02	0.73
2:B:579:THR:HA	2:B:584:ARG:NH2	2.04	0.73
2:D:372:GLN:O	2:D:509:VAL:HG23	1.88	0.73
2:F:131:LEU:HD21	2:F:135:PRO:HD3	1.67	0.73
3:I:109:MET:HE1	3:I:129:VAL:HG13	1.71	0.73
2:B:382:LEU:HD23	2:B:491:ALA:HB2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:579:THR:HA	2:F:584:ARG:NH2	2.02	0.72
2:D:66:MET:HE1	2:D:144:VAL:HG11	1.72	0.72
2:F:382:LEU:HD23	2:F:491:ALA:HB2	1.70	0.71
3:G:109:MET:CE	3:G:129:VAL:HG13	2.19	0.71
3:G:143:ARG:HG2	3:G:143:ARG:HH11	1.55	0.71
2:F:376:MET:HG2	2:F:495:MET:HE3	1.73	0.70
2:F:212:MET:O	2:F:212:MET:HE3	1.91	0.70
2:B:376:MET:HG2	2:B:495:MET:HE3	1.73	0.70
2:B:372:GLN:O	2:B:509:VAL:HG23	1.91	0.70
1:E:42:ASN:HB3	2:F:104:THR:CG2	2.21	0.70
3:H:109:MET:CE	3:H:129:VAL:HG13	2.21	0.70
3:H:143:ARG:HH11	3:H:143:ARG:HG2	1.57	0.70
2:D:376:MET:HG2	2:D:495:MET:HE3	1.73	0.69
2:D:579:THR:HA	2:D:584:ARG:NH2	2.07	0.69
3:I:109:MET:CE	3:I:129:VAL:HG13	2.23	0.69
2:D:46:VAL:HG11	2:D:65:ARG:NE	2.08	0.69
2:F:471:THR:HG22	2:F:472:PHE:N	2.06	0.68
2:B:566:VAL:HG11	2:D:194:VAL:HG13	1.75	0.67
3:G:118:LEU:O	3:G:122:ARG:HG2	1.94	0.67
2:D:212:MET:O	2:D:212:MET:HE3	1.95	0.67
1:E:18:ASN:HB3	2:F:212:MET:HG2	1.77	0.67
2:F:46:VAL:HG11	2:F:65:ARG:CD	2.25	0.67
1:E:42:ASN:CB	2:F:104:THR:HG21	2.23	0.67
2:F:70:ASP:C	2:F:71:ILE:HD12	2.14	0.67
3:I:143:ARG:HG2	3:I:143:ARG:HH11	1.60	0.67
2:B:46:VAL:HG11	2:B:65:ARG:CD	2.25	0.66
2:B:70:ASP:C	2:B:71:ILE:HD12	2.15	0.66
1:C:18:ASN:HB3	2:D:212:MET:HG2	1.76	0.66
1:A:18:ASN:HB3	2:B:212:MET:HG2	1.77	0.66
2:D:46:VAL:HG11	2:D:65:ARG:CD	2.25	0.66
2:D:70:ASP:C	2:D:71:ILE:HD12	2.16	0.66
1:C:42:ASN:HB3	2:D:104:THR:CG2	2.24	0.66
2:B:46:VAL:HG11	2:B:65:ARG:NE	2.11	0.66
2:F:46:VAL:HG11	2:F:65:ARG:NE	2.11	0.66
2:D:60:PRO:HG2	2:D:153:ARG:HH12	1.62	0.65
2:D:66:MET:HE2	2:D:71:ILE:HD11	1.79	0.65
2:D:213:GLN:O	2:D:217:LYS:HG2	1.97	0.65
2:F:395:ASN:HB2	2:F:432:ALA:HB3	1.78	0.65
2:B:212:MET:HE3	2:B:212:MET:O	1.96	0.64
2:F:213:GLN:O	2:F:217:LYS:HG2	1.97	0.64
2:B:371:ASP:O	2:B:372:GLN:HB2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:118:LEU:O	3:H:122:ARG:HG2	1.98	0.64
2:B:213:GLN:O	2:B:217:LYS:HG2	1.97	0.63
2:B:53:ASP:HB3	2:B:56:SER:OG	1.98	0.63
2:D:53:ASP:HB3	2:D:56:SER:OG	1.99	0.63
2:D:395:ASN:HB2	2:D:432:ALA:HB3	1.79	0.63
2:B:588:PRO:HD2	2:B:591:ILE:HD12	1.81	0.63
1:C:42:ASN:CB	2:D:104:THR:HG21	2.25	0.62
3:G:299:VAL:HG13	3:G:320:MET:HG2	1.80	0.62
2:F:409:PRO:HD2	2:F:412:LEU:HD12	1.81	0.62
3:H:22:ARG:NH1	8:H:704:HOH:O	2.32	0.62
2:D:60:PRO:HG2	2:D:153:ARG:NH1	2.13	0.62
2:D:371:ASP:O	2:D:372:GLN:HB2	2.00	0.62
3:H:109:MET:HE1	3:H:129:VAL:HG13	1.80	0.62
2:F:60:PRO:HG2	2:F:153:ARG:HH12	1.64	0.62
2:F:53:ASP:HB3	2:F:56:SER:OG	1.99	0.62
2:D:140:LEU:HD12	2:D:140:LEU:N	2.15	0.62
2:B:194:VAL:HG13	2:F:566:VAL:HG11	1.80	0.62
2:F:371:ASP:O	2:F:372:GLN:HB2	2.00	0.61
3:I:118:LEU:O	3:I:122:ARG:HG2	2.00	0.61
1:A:42:ASN:HB3	2:B:104:THR:CG2	2.25	0.61
2:D:471:THR:CG2	2:D:472:PHE:H	2.11	0.61
3:I:299:VAL:HG13	3:I:320:MET:HG2	1.82	0.61
2:D:405:GLN:HB3	2:D:464:MET:CE	2.30	0.61
2:B:60:PRO:HG2	2:B:153:ARG:HH12	1.65	0.61
2:D:140:LEU:HD12	2:D:140:LEU:H	1.66	0.61
3:I:113:VAL:HG11	3:I:128:LEU:HD11	1.82	0.61
2:B:284:LYS:HD3	2:F:291:ASP:OD1	2.01	0.60
2:F:405:GLN:HB3	2:F:464:MET:CE	2.31	0.60
2:F:405:GLN:HB3	2:F:464:MET:HE3	1.83	0.60
2:F:60:PRO:HG2	2:F:153:ARG:NH1	2.16	0.60
2:B:346:GLN:HG2	2:B:360:ASN:OD1	2.02	0.60
2:B:395:ASN:HB2	2:B:432:ALA:HB3	1.82	0.60
3:H:236:ARG:HE	3:H:240:LYS:HD2	1.67	0.60
3:G:236:ARG:HE	3:G:240:LYS:HD2	1.66	0.60
2:D:324:ARG:NH1	2:D:487:ASP:OD1	2.35	0.59
2:F:588:PRO:HD2	2:F:591:ILE:HD12	1.83	0.59
2:B:66:MET:CE	2:B:71:ILE:HD11	2.33	0.59
2:D:346:GLN:HG2	2:D:360:ASN:OD1	2.02	0.59
2:D:405:GLN:HB3	2:D:464:MET:HE3	1.85	0.59
2:F:66:MET:CE	2:F:71:ILE:HD11	2.33	0.59
2:D:258:MET:SD	2:F:99:PRO:HG3	2.41	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASN:HB2	8:A:603:HOH:O	2.01	0.59
2:B:60:PRO:HG2	2:B:153:ARG:NH1	2.16	0.59
3:G:132:ASN:HA	3:G:360:ASP:OD1	2.02	0.59
2:D:566:VAL:HG11	2:F:194:VAL:HG13	1.84	0.59
2:B:183:LYS:O	2:B:186:GLU:HB2	2.03	0.59
2:B:99:PRO:HG3	2:F:258:MET:SD	2.43	0.59
1:A:42:ASN:CB	2:B:104:THR:HG21	2.27	0.59
2:B:405:GLN:HB3	2:B:464:MET:CE	2.33	0.59
1:E:14:THR:O	1:E:14:THR:HG22	2.02	0.58
3:H:113:VAL:HG11	3:H:128:LEU:HD11	1.85	0.58
1:C:14:THR:HG22	1:C:14:THR:O	2.02	0.58
2:D:588:PRO:HD2	2:D:591:ILE:HD12	1.85	0.58
2:F:183:LYS:O	2:F:186:GLU:HB2	2.04	0.58
2:B:140:LEU:N	2:B:140:LEU:HD12	2.18	0.58
2:F:140:LEU:HD12	2:F:140:LEU:N	2.19	0.58
1:A:14:THR:O	1:A:14:THR:HG22	2.01	0.58
2:D:347:ILE:HD11	2:D:359:PHE:CE1	2.39	0.58
2:B:471:THR:CG2	2:B:472:PHE:H	2.11	0.57
2:F:335:ARG:HD2	2:F:411:GLU:OE2	2.04	0.57
2:B:235:GLU:N	2:B:235:GLU:OE1	2.37	0.57
2:F:46:VAL:HG11	2:F:65:ARG:HD2	1.87	0.57
2:B:46:VAL:HG11	2:B:65:ARG:HD2	1.86	0.57
2:D:66:MET:CE	2:D:71:ILE:HD11	2.35	0.57
2:B:153:ARG:HD3	2:F:132:SER:O	2.05	0.57
2:D:284:LYS:HE3	2:D:284:LYS:HA	1.86	0.57
2:F:235:GLU:N	2:F:235:GLU:OE1	2.38	0.57
2:F:347:ILE:HD11	2:F:359:PHE:CE1	2.40	0.57
3:I:132:ASN:HA	3:I:360:ASP:OD1	2.05	0.57
2:D:46:VAL:HG11	2:D:65:ARG:CZ	2.34	0.57
3:G:113:VAL:HG11	3:G:128:LEU:HD11	1.86	0.57
2:D:409:PRO:HD2	2:D:412:LEU:HD12	1.86	0.56
2:F:346:GLN:HG2	2:F:360:ASN:OD1	2.05	0.56
3:H:223:TYR:OH	3:H:351:ASP:HB3	2.05	0.56
3:H:132:ASN:HA	3:H:360:ASP:OD1	2.04	0.56
2:F:237:ALA:HA	4:F:709:BOG:H8'1	1.88	0.56
3:G:223:TYR:OH	3:G:351:ASP:HB3	2.05	0.56
2:D:183:LYS:O	2:D:186:GLU:HB2	2.05	0.56
2:F:347:ILE:HD11	2:F:359:PHE:CZ	2.39	0.56
2:F:324:ARG:NH1	2:F:487:ASP:OD1	2.37	0.56
2:D:347:ILE:HD11	2:D:359:PHE:CZ	2.40	0.56
2:B:347:ILE:HD11	2:B:359:PHE:CE1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:335:ARG:HD2	2:B:411:GLU:OE2	2.05	0.56
2:B:409:PRO:HD2	2:B:412:LEU:HD12	1.86	0.56
2:B:140:LEU:H	2:B:140:LEU:HD12	1.70	0.56
2:B:284:LYS:HE3	2:B:284:LYS:HA	1.87	0.56
2:B:347:ILE:HD11	2:B:359:PHE:CZ	2.40	0.56
2:F:100:LEU:HD23	2:F:167:THR:HG22	1.88	0.56
2:B:407:LYS:HE2	2:B:461:ASP:OD1	2.06	0.55
2:F:471:THR:CG2	2:F:472:PHE:H	2.15	0.55
2:D:100:LEU:HD13	2:D:165:VAL:HG11	1.88	0.55
2:D:340:THR:HG22	2:D:340:THR:O	2.06	0.55
2:B:66:MET:HE2	2:B:71:ILE:HD11	1.89	0.55
2:D:309:ALA:HB3	2:D:310:PRO:HD3	1.89	0.55
2:D:235:GLU:N	2:D:235:GLU:OE1	2.39	0.55
2:D:46:VAL:HG11	2:D:65:ARG:HD2	1.87	0.55
1:E:11:ILE:O	2:F:234:LYS:HE3	2.06	0.55
3:H:299:VAL:HG13	3:H:320:MET:HG2	1.89	0.55
2:B:309:ALA:HB3	2:B:310:PRO:HD3	1.88	0.55
2:B:499:SER:HA	2:D:601:GLN:HB3	1.87	0.55
2:D:335:ARG:HD2	2:D:411:GLU:OE2	2.07	0.55
2:D:66:MET:HE3	2:D:144:VAL:HG11	1.86	0.55
2:F:66:MET:HE2	2:F:71:ILE:HD11	1.88	0.55
3:I:223:TYR:OH	3:I:351:ASP:HB3	2.06	0.55
2:D:140:LEU:HB3	2:D:170:ARG:HD3	1.89	0.55
3:I:236:ARG:HE	3:I:240:LYS:HD2	1.70	0.55
2:B:340:THR:O	2:B:340:THR:HG22	2.05	0.55
2:F:309:ALA:HB3	2:F:310:PRO:HD3	1.89	0.55
2:B:324:ARG:NH1	2:B:487:ASP:OD1	2.40	0.54
2:D:145:ASP:OD2	2:D:161:LYS:HG2	2.07	0.54
3:H:241:GLU:O	3:H:242:LEU:HD23	2.06	0.54
2:F:140:LEU:HD12	2:F:140:LEU:H	1.70	0.54
2:B:123:GLU:HG3	2:B:238:VAL:HG11	1.89	0.54
3:H:101:SER:O	3:H:105:GLN:HG3	2.07	0.54
2:B:433:GLU:HG2	2:B:434:ASP:H	1.72	0.54
3:I:241:GLU:O	3:I:242:LEU:HD23	2.08	0.54
2:D:237:ALA:HA	4:D:709:BOG:H8'1	1.89	0.54
2:D:291:ASP:OD1	2:F:284:LYS:HD3	2.08	0.54
3:H:174:ILE:HD13	3:H:181:PRO:HG3	1.90	0.54
1:C:11:ILE:O	2:D:234:LYS:HE3	2.08	0.54
2:F:340:THR:O	2:F:340:THR:HG22	2.07	0.53
2:F:46:VAL:HG11	2:F:65:ARG:CZ	2.38	0.53
3:H:137:ASP:N	3:H:138:PRO:HD3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:113:LYS:HE2	1:E:40:MET:O	2.08	0.53
2:F:148:VAL:O	2:F:155:ALA:HA	2.09	0.53
2:B:275:SER:HA	2:B:651:LEU:CD1	2.39	0.53
2:D:407:LYS:HE2	2:D:461:ASP:OD1	2.07	0.53
2:F:123:GLU:HG3	2:F:238:VAL:HG11	1.90	0.53
2:F:284:LYS:HE3	2:F:284:LYS:HA	1.89	0.53
2:F:275:SER:HA	2:F:651:LEU:CD1	2.39	0.53
3:G:174:ILE:HD13	3:G:181:PRO:HG3	1.89	0.53
1:A:11:ILE:O	2:B:234:LYS:HE3	2.08	0.53
2:B:46:VAL:HG11	2:B:65:ARG:CZ	2.38	0.53
2:D:433:GLU:HG2	2:D:434:ASP:H	1.74	0.53
2:B:136:LYS:O	2:B:139:ASP:HB2	2.08	0.53
2:B:237:ALA:HA	4:B:709:BOG:H8'1	1.89	0.53
2:F:248:GLN:HE21	2:F:257:VAL:HG12	1.74	0.53
2:B:291:ASP:OD1	2:D:284:LYS:HD3	2.08	0.52
2:B:411:GLU:H	2:B:411:GLU:CD	2.12	0.52
2:F:213:GLN:OE1	2:F:675:PRO:HD2	2.09	0.52
3:I:177:SER:HB2	3:I:179:LEU:HG	1.91	0.52
2:D:123:GLU:HG3	2:D:238:VAL:HG11	1.91	0.52
2:D:452:TYR:CE2	2:D:454:PRO:HG3	2.44	0.52
2:F:452:TYR:CE2	2:F:454:PRO:HG3	2.43	0.52
2:F:407:LYS:HE2	2:F:461:ASP:OD1	2.10	0.52
3:G:177:SER:HB2	3:G:179:LEU:HG	1.90	0.52
3:I:198:GLU:HG3	3:I:355:PRO:HB2	1.91	0.52
3:I:101:SER:O	3:I:105:GLN:HG3	2.10	0.52
2:B:248:GLN:HE21	2:B:257:VAL:HG12	1.75	0.52
2:F:411:GLU:CD	2:F:411:GLU:H	2.13	0.52
2:D:248:GLN:HE21	2:D:257:VAL:HG12	1.75	0.52
2:F:100:LEU:HD13	2:F:165:VAL:HG11	1.92	0.52
2:F:192:LEU:O	2:F:196:GLN:HG3	2.10	0.52
2:F:376:MET:CG	2:F:495:MET:HE3	2.40	0.52
2:B:192:LEU:O	2:B:196:GLN:HG3	2.09	0.52
2:B:145:ASP:OD2	2:B:161:LYS:HG2	2.10	0.52
2:D:232:TYR:N	2:D:233:PRO:HD3	2.25	0.52
2:B:340:THR:HG21	3:G:341:THR:HB	1.92	0.52
2:F:131:LEU:HD13	2:F:181:ALA:HB2	1.92	0.52
2:F:373:ILE:O	2:F:374:ALA:HB3	2.10	0.52
3:I:3:VAL:HA	8:I:711:HOH:O	2.10	0.52
2:B:376:MET:CG	2:B:495:MET:HE3	2.39	0.51
2:F:433:GLU:HG2	2:F:434:ASP:H	1.74	0.51
2:B:100:LEU:HD23	2:B:167:THR:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:100:LEU:HD23	2:D:167:THR:HG22	1.91	0.51
3:I:174:ILE:HD13	3:I:181:PRO:HG3	1.91	0.51
3:I:137:ASP:OD2	3:I:140:SER:HB3	2.10	0.51
2:D:411:GLU:CD	2:D:411:GLU:H	2.14	0.51
3:H:177:SER:HB2	3:H:179:LEU:HG	1.92	0.51
2:D:275:SER:HA	2:D:651:LEU:CD1	2.40	0.51
3:G:241:GLU:O	3:G:242:LEU:HD23	2.11	0.51
2:B:373:ILE:O	2:B:374:ALA:HB3	2.10	0.51
2:D:428:VAL:HG11	8:F:713:HOH:O	2.11	0.51
2:F:140:LEU:HB3	2:F:170:ARG:HD3	1.93	0.51
3:G:143:ARG:CG	3:G:143:ARG:HH11	2.23	0.51
2:B:410:PHE:HB2	2:B:467:TYR:CE1	2.45	0.51
1:A:40:MET:O	2:F:113:LYS:HE2	2.11	0.51
2:B:100:LEU:HD13	2:B:165:VAL:HG11	1.92	0.51
2:F:145:ASP:OD2	2:F:161:LYS:HG2	2.12	0.51
3:G:101:SER:O	3:G:105:GLN:HG3	2.10	0.51
2:F:352:ASN:HB3	3:G:64:LYS:HA	1.92	0.51
2:B:213:GLN:OE1	2:B:675:PRO:HD2	2.11	0.50
2:D:136:LYS:O	2:D:139:ASP:HB2	2.11	0.50
2:B:131:LEU:HD13	2:B:181:ALA:HB2	1.93	0.50
2:B:405:GLN:HB3	2:B:464:MET:HE1	1.93	0.50
3:H:198:GLU:HG3	3:H:355:PRO:HB2	1.93	0.50
2:D:58:THR:O	2:D:156:LEU:HD21	2.11	0.50
3:G:137:ASP:N	3:G:138:PRO:HD3	2.25	0.50
3:H:229:GLU:HG2	3:H:230:HIS:N	2.26	0.50
2:D:131:LEU:HD13	2:D:181:ALA:HB2	1.93	0.50
2:B:232:TYR:N	2:B:233:PRO:HD3	2.27	0.50
2:B:452:TYR:CE2	2:B:454:PRO:HG3	2.46	0.50
1:C:34:LEU:HB3	2:D:110:ASN:HD22	1.76	0.50
2:B:148:VAL:O	2:B:155:ALA:HA	2.10	0.50
2:D:148:VAL:O	2:D:155:ALA:HA	2.11	0.50
2:D:192:LEU:O	2:D:196:GLN:HG3	2.12	0.50
3:G:198:GLU:HG3	3:G:355:PRO:HB2	1.93	0.50
3:I:137:ASP:N	3:I:138:PRO:HD3	2.26	0.49
2:D:373:ILE:O	2:D:374:ALA:HB3	2.11	0.49
2:D:132:SER:O	2:F:153:ARG:HD3	2.12	0.49
2:F:71:ILE:HD12	2:F:71:ILE:N	2.28	0.49
3:H:99:MET:O	3:H:103:VAL:HG23	2.12	0.49
2:B:250:MET:CB	2:B:257:VAL:HG22	2.42	0.49
2:D:131:LEU:O	2:D:131:LEU:HD23	2.13	0.49
2:B:601:GLN:HB3	2:F:499:SER:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:610:ILE:HG13	2:F:611:ILE:HG23	1.94	0.49
3:G:136:VAL:O	3:G:143:ARG:HD3	2.13	0.49
3:H:137:ASP:OD2	3:H:140:SER:HB3	2.13	0.49
1:A:34:LEU:HB3	2:B:110:ASN:HD22	1.77	0.49
2:B:433:GLU:CG	2:B:434:ASP:H	2.25	0.49
1:E:34:LEU:HB3	2:F:110:ASN:HD22	1.77	0.49
2:B:123:GLU:HG3	2:B:238:VAL:CG1	2.43	0.49
2:B:567:PRO:HG3	2:D:197:THR:HB	1.94	0.49
2:F:232:TYR:N	2:F:233:PRO:HD3	2.26	0.49
2:F:51:ILE:HG22	2:F:62:ALA:O	2.12	0.49
2:F:136:LYS:O	2:F:139:ASP:HB2	2.11	0.49
2:F:143:TYR:N	8:F:736:HOH:O	2.37	0.49
2:F:250:MET:CB	2:F:257:VAL:HG22	2.42	0.49
3:H:122:ARG:CD	3:H:177:SER:HB3	2.43	0.49
2:B:113:LYS:HE2	1:C:40:MET:O	2.12	0.48
2:D:250:MET:CB	2:D:257:VAL:HG22	2.43	0.48
2:F:410:PHE:HB2	2:F:467:TYR:CE1	2.48	0.48
2:F:314:ILE:HD11	2:F:541:ASP:HB2	1.95	0.48
3:I:122:ARG:CD	3:I:177:SER:HB3	2.43	0.48
2:D:589:LYS:HG3	2:D:590:GLY:N	2.29	0.48
2:B:198:LEU:CD1	2:F:566:VAL:HB	2.44	0.48
2:D:100:LEU:HB3	2:D:165:VAL:CG1	2.44	0.48
2:B:644:VAL:HG22	2:D:186:GLU:CG	2.35	0.48
3:H:143:ARG:CG	3:H:143:ARG:HH11	2.24	0.48
2:B:314:ILE:HD11	2:B:541:ASP:HB2	1.96	0.48
2:D:410:PHE:HB2	2:D:467:TYR:CE1	2.47	0.48
2:D:376:MET:CG	2:D:495:MET:HE3	2.42	0.48
2:F:566:VAL:CG2	2:F:567:PRO:HD3	2.43	0.48
3:I:113:VAL:CG1	3:I:128:LEU:HD11	2.43	0.48
2:B:157:ASN:O	2:F:136:LYS:NZ	2.38	0.48
2:B:405:GLN:HB3	2:B:464:MET:HE3	1.94	0.48
2:D:250:MET:HA	2:D:257:VAL:HG22	1.96	0.48
2:D:300:ILE:O	2:D:515:PRO:HG2	2.13	0.48
3:G:354:TYR:CD1	3:G:354:TYR:N	2.81	0.48
2:D:433:GLU:CG	2:D:434:ASP:H	2.27	0.48
2:D:453:GLU:OE1	3:I:63:ARG:NH2	2.42	0.48
3:I:354:TYR:N	3:I:354:TYR:CD1	2.82	0.48
2:F:123:GLU:HG3	2:F:238:VAL:CG1	2.43	0.47
2:F:648:VAL:CG2	2:F:649:SER:N	2.77	0.47
2:B:589:LYS:HG3	2:B:590:GLY:N	2.28	0.47
3:G:71:HIS:NE2	3:G:73:CYS:HB2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:MET:HB2	2:B:257:VAL:HG22	1.96	0.47
2:B:371:ASP:O	2:B:372:GLN:CB	2.62	0.47
3:H:121:VAL:HG21	3:H:128:LEU:HD13	1.95	0.47
3:I:143:ARG:CG	3:I:143:ARG:HH11	2.26	0.47
2:B:258:MET:SD	2:D:99:PRO:HG3	2.55	0.47
2:F:250:MET:HB2	2:F:257:VAL:HG22	1.96	0.47
2:F:589:LYS:HG3	2:F:590:GLY:N	2.29	0.47
3:G:99:MET:O	3:G:103:VAL:HG23	2.14	0.47
2:B:71:ILE:HD12	2:B:71:ILE:N	2.29	0.47
3:G:154:GLN:O	3:G:156:VAL:HG23	2.14	0.47
3:G:239:ARG:HD2	3:G:365:GLY:OXT	2.15	0.47
2:B:143:TYR:CE2	2:B:164:PRO:HG3	2.50	0.47
2:B:566:VAL:CG2	2:B:567:PRO:HD3	2.45	0.47
3:I:136:VAL:O	3:I:143:ARG:HD3	2.14	0.47
2:F:300:ILE:O	2:F:515:PRO:HG2	2.14	0.47
2:B:105:GLU:HG2	2:B:106:HIS:N	2.30	0.47
2:B:58:THR:O	2:B:156:LEU:HD21	2.14	0.47
2:D:65:ARG:HB3	2:D:65:ARG:HH11	1.79	0.47
3:H:0:ACE:O	3:H:1:MET:CB	2.63	0.47
3:H:225:TYR:O	3:H:228:LEU:HB3	2.15	0.47
2:D:213:GLN:OE1	2:D:675:PRO:HD2	2.15	0.47
2:B:324:ARG:NH2	2:B:485:GLN:OE1	2.48	0.47
2:F:275:SER:C	2:F:651:LEU:HD11	2.35	0.47
2:D:123:GLU:HG3	2:D:238:VAL:CG1	2.45	0.47
2:F:620:ASP:HB3	2:F:623:ASN:ND2	2.31	0.47
8:A:604:HOH:O	2:B:213:GLN:HG2	2.14	0.46
2:D:190:ILE:O	2:D:194:VAL:HG23	2.15	0.46
2:F:58:THR:O	2:F:156:LEU:HD21	2.15	0.46
3:I:99:MET:O	3:I:103:VAL:HG23	2.15	0.46
2:D:621:LYS:O	2:D:625:ILE:HG13	2.16	0.46
3:H:292:LEU:O	3:H:295:VAL:HG22	2.15	0.46
3:I:292:LEU:O	3:I:295:VAL:HG22	2.15	0.46
2:B:610:ILE:HG13	2:B:611:ILE:HG23	1.98	0.46
2:F:105:GLU:HG2	2:F:106:HIS:N	2.31	0.46
3:G:312:ARG:HD2	3:G:316:GLY:O	2.16	0.46
3:H:136:VAL:O	3:H:143:ARG:HD3	2.15	0.46
3:H:312:ARG:HD2	3:H:316:GLY:O	2.15	0.46
2:D:319:ALA:HB3	2:D:532:PRO:HG3	1.98	0.46
3:H:0:ACE:O	3:H:1:MET:HB3	2.15	0.46
2:F:324:ARG:HD3	8:F:759:HOH:O	2.16	0.46
2:F:606:ASP:O	2:F:609:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:225:TYR:O	3:G:228:LEU:HB3	2.15	0.46
2:D:143:TYR:CE2	2:D:164:PRO:HG3	2.50	0.46
2:F:433:GLU:CG	2:F:434:ASP:H	2.29	0.46
3:G:54:CYS:HA	3:G:77:ILE:HG12	1.98	0.46
2:B:71:ILE:HG21	2:B:142:THR:HG21	1.98	0.46
2:B:190:ILE:O	2:B:194:VAL:HG23	2.16	0.46
2:F:340:THR:HG21	3:I:341:THR:HB	1.96	0.46
3:G:229:GLU:HG2	3:G:230:HIS:N	2.30	0.46
3:H:239:ARG:HD2	3:H:365:GLY:OXT	2.16	0.46
2:B:66:MET:HE3	2:B:71:ILE:HD11	1.98	0.46
3:G:1:MET:HG2	3:G:1:MET:O	2.16	0.46
3:I:229:GLU:HG2	3:I:230:HIS:N	2.31	0.46
2:B:275:SER:C	2:B:651:LEU:HD11	2.37	0.46
2:D:566:VAL:CG2	2:D:567:PRO:HD3	2.45	0.46
3:G:231:ASP:HA	3:G:232:PRO:HD3	1.75	0.46
2:D:314:ILE:HD11	2:D:541:ASP:HB2	1.97	0.45
2:F:143:TYR:CE2	2:F:164:PRO:HG3	2.50	0.45
3:H:113:VAL:CG1	3:H:128:LEU:HD11	2.45	0.45
2:B:250:MET:HA	2:B:257:VAL:HG22	1.97	0.45
2:D:98:GLU:OE2	2:D:169:THR:HB	2.17	0.45
2:B:319:ALA:HB3	2:B:532:PRO:HG3	1.99	0.45
2:F:65:ARG:HB3	2:F:65:ARG:HH11	1.82	0.45
2:D:648:VAL:CG2	2:D:649:SER:N	2.80	0.45
2:F:71:ILE:HG21	2:F:142:THR:HG21	1.97	0.45
2:F:370:LEU:O	2:F:373:ILE:HG12	2.16	0.45
3:I:225:TYR:O	3:I:228:LEU:HB3	2.16	0.45
2:D:105:GLU:HG2	2:D:106:HIS:N	2.31	0.45
2:D:203:VAL:CG2	2:D:658:GLN:HA	2.46	0.45
3:G:133:TRP:HB2	3:G:220:VAL:HB	1.99	0.45
3:G:137:ASP:OD2	3:G:140:SER:HB3	2.16	0.45
2:B:140:LEU:HB3	2:B:170:ARG:HD3	1.97	0.45
2:D:405:GLN:HB3	2:D:464:MET:HE1	1.99	0.45
2:F:131:LEU:HD23	2:F:131:LEU:O	2.16	0.45
2:F:250:MET:HA	2:F:257:VAL:HG22	1.99	0.45
3:I:133:TRP:HB2	3:I:220:VAL:HB	1.98	0.45
2:B:100:LEU:HB3	2:B:165:VAL:CG1	2.46	0.45
2:B:606:ASP:O	2:B:609:THR:HG23	2.17	0.45
2:D:51:ILE:HG22	2:D:62:ALA:O	2.17	0.45
1:E:21:LYS:HD3	2:F:207:GLU:OE1	2.17	0.45
2:F:190:ILE:O	2:F:194:VAL:HG23	2.17	0.45
2:F:324:ARG:NH2	2:F:485:GLN:OE1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:250:MET:HB2	2:D:257:VAL:HG22	1.98	0.45
2:D:610:ILE:HG13	2:D:611:ILE:HG23	1.98	0.45
3:G:292:LEU:O	3:G:295:VAL:HG22	2.17	0.45
2:B:201:THR:CG2	2:B:244:ASN:ND2	2.80	0.45
2:B:223:LEU:O	2:F:589:LYS:HE3	2.17	0.45
3:G:113:VAL:CG1	3:G:128:LEU:HD11	2.47	0.45
3:I:312:ARG:HD2	3:I:316:GLY:O	2.16	0.45
2:B:51:ILE:HG22	2:B:62:ALA:O	2.17	0.45
3:G:121:VAL:HG21	3:G:128:LEU:HD13	1.98	0.45
3:G:238:TYR:CE1	3:G:242:LEU:HD12	2.52	0.45
3:I:297:LYS:HB2	8:I:716:HOH:O	2.17	0.45
2:F:442:ILE:O	2:F:442:ILE:HG23	2.17	0.44
3:I:71:HIS:NE2	3:I:73:CYS:HB2	2.31	0.44
2:D:371:ASP:O	2:D:372:GLN:CB	2.64	0.44
2:D:71:ILE:N	2:D:71:ILE:HD12	2.31	0.44
2:F:98:GLU:OE2	2:F:169:THR:HB	2.17	0.44
3:G:122:ARG:CD	3:G:177:SER:HB3	2.47	0.44
3:G:242:LEU:O	3:G:349:PHE:HB2	2.18	0.44
1:A:18:ASN:CB	2:B:212:MET:HG2	2.45	0.44
2:B:211:PRO:O	2:B:214:SER:N	2.50	0.44
2:B:620:ASP:HB3	2:B:623:ASN:ND2	2.33	0.44
2:D:606:ASP:O	2:D:609:THR:HG23	2.18	0.44
3:G:315:LEU:N	3:G:315:LEU:HD22	2.32	0.44
2:B:621:LYS:O	2:B:625:ILE:HG13	2.17	0.44
2:D:201:THR:CG2	2:D:244:ASN:ND2	2.80	0.44
3:H:224:ASP:HB2	3:H:357:MET:CG	2.47	0.44
3:H:54:CYS:HA	3:H:77:ILE:HG12	1.99	0.44
3:I:154:GLN:O	3:I:156:VAL:HG23	2.17	0.44
2:B:370:LEU:O	2:B:373:ILE:HG12	2.18	0.44
2:B:47:PRO:HB2	2:B:66:MET:HB3	1.99	0.44
2:D:324:ARG:NH2	2:D:485:GLN:OE1	2.51	0.44
1:E:19:VAL:HB	2:F:248:GLN:HB2	1.99	0.44
3:I:54:CYS:HA	3:I:77:ILE:HG12	1.99	0.44
2:D:195:ALA:HB2	2:D:229:ILE:CD1	2.48	0.44
2:D:499:SER:HA	2:F:601:GLN:HB3	1.99	0.44
3:I:109:MET:HE1	3:I:130:GLU:N	2.33	0.44
2:F:100:LEU:HB3	2:F:165:VAL:CG1	2.48	0.44
2:D:136:LYS:NZ	2:F:157:ASN:O	2.46	0.44
2:D:336:MET:CE	3:H:333:ILE:HD13	2.48	0.44
3:H:354:TYR:N	3:H:354:TYR:CD1	2.85	0.44
2:D:620:ASP:HB3	2:D:623:ASN:ND2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:47:PRO:HB2	2:F:66:MET:HB3	1.99	0.43
2:F:66:MET:HE3	2:F:71:ILE:HD11	1.99	0.43
3:G:354:TYR:HB3	3:G:355:PRO:HD2	1.99	0.43
3:H:133:TRP:HB2	3:H:220:VAL:HB	1.99	0.43
2:B:107:ALA:O	2:B:111:PHE:HD1	2.02	0.43
1:C:10:THR:O	2:D:252:VAL:HG23	2.18	0.43
3:H:71:HIS:NE2	3:H:73:CYS:HB2	2.32	0.43
2:D:566:VAL:N	2:D:567:PRO:CD	2.82	0.43
1:E:18:ASN:CB	2:F:212:MET:HG2	2.46	0.43
2:F:648:VAL:HG23	2:F:649:SER:N	2.33	0.43
3:H:109:MET:HE1	3:H:130:GLU:N	2.33	0.43
3:H:249:PHE:CD2	3:H:259:ARG:HG2	2.53	0.43
2:B:136:LYS:NZ	2:D:157:ASN:O	2.44	0.43
2:B:392:TRP:CE3	2:B:483:MET:HB2	2.54	0.43
2:B:203:VAL:CG2	2:B:658:GLN:HA	2.48	0.43
2:D:172:THR:HG22	2:D:176:ASP:OD2	2.18	0.43
2:D:370:LEU:O	2:D:373:ILE:HG12	2.18	0.43
3:H:354:TYR:HB3	3:H:355:PRO:HD2	2.00	0.43
2:B:198:LEU:HD12	2:F:566:VAL:HB	2.01	0.43
2:B:452:TYR:HE1	2:B:457:LEU:HD12	1.84	0.43
2:B:65:ARG:HB3	2:B:65:ARG:HH11	1.83	0.43
2:F:203:VAL:CG2	2:F:658:GLN:HA	2.49	0.43
1:A:19:VAL:HB	2:B:248:GLN:HB2	2.00	0.43
2:B:300:ILE:O	2:B:515:PRO:HG2	2.18	0.43
2:D:107:ALA:O	2:D:111:PHE:HD1	2.00	0.43
1:C:18:ASN:CB	2:D:212:MET:HG2	2.44	0.43
2:D:275:SER:C	2:D:651:LEU:HD11	2.39	0.43
2:F:361:LEU:HD21	2:F:469:LEU:HD22	2.00	0.43
2:F:566:VAL:HG23	2:F:567:PRO:HD3	1.99	0.43
3:H:42:MET:HB2	3:H:42:MET:HE3	1.89	0.43
3:I:113:VAL:HG21	3:I:128:LEU:HG	2.00	0.43
1:A:28:SER:O	1:A:29:THR:HG23	2.19	0.43
2:B:131:LEU:O	2:B:131:LEU:HD23	2.17	0.43
2:B:98:GLU:OE2	2:B:169:THR:HB	2.18	0.43
3:I:315:LEU:N	3:I:315:LEU:HD22	2.34	0.43
3:I:227:GLU:HG3	3:I:354:TYR:CD2	2.53	0.43
2:B:615:ALA:O	2:B:619:SER:HB2	2.19	0.43
2:D:153:ARG:HH11	2:D:153:ARG:CB	2.12	0.43
2:D:361:LEU:HD21	2:D:469:LEU:HD22	1.99	0.43
2:F:361:LEU:HD22	2:F:365:THR:HG21	2.00	0.43
3:H:197:LEU:HD13	3:H:201:ALA:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:133:TRP:HA	3:I:136:VAL:HG23	1.99	0.43
3:I:354:TYR:HB3	3:I:355:PRO:HD2	2.01	0.43
2:F:392:TRP:CE3	2:F:483:MET:HB2	2.54	0.43
3:G:100:LEU:HD22	3:G:159:LEU:HD12	2.00	0.43
3:H:238:TYR:CE1	3:H:242:LEU:HD12	2.53	0.43
3:I:0:ACE:O	3:I:1:MET:CB	2.67	0.43
2:B:361:LEU:HD21	2:B:469:LEU:HD22	2.01	0.42
2:D:271:ALA:HA	2:D:272:PRO:HD3	1.86	0.42
2:D:566:VAL:HB	2:F:198:LEU:CD1	2.49	0.42
3:G:224:ASP:HB2	3:G:357:MET:CG	2.49	0.42
3:G:295:VAL:O	3:G:299:VAL:HG23	2.19	0.42
3:H:100:LEU:HD22	3:H:159:LEU:HD12	2.00	0.42
3:H:295:VAL:O	3:H:299:VAL:HG23	2.19	0.42
3:G:197:LEU:HD13	3:G:201:ALA:O	2.19	0.42
2:B:408:ILE:HD12	2:B:418:GLN:HB3	2.00	0.42
2:B:566:VAL:N	2:B:567:PRO:CD	2.82	0.42
2:D:71:ILE:HG21	2:D:142:THR:HG21	2.01	0.42
1:E:22:PRO:HD2	2:F:208:VAL:HG23	2.02	0.42
2:F:371:ASP:O	2:F:372:GLN:CB	2.64	0.42
2:F:459:LYS:HA	2:F:466:TYR:OH	2.19	0.42
2:F:55:THR:C	2:F:57:VAL:H	2.22	0.42
3:G:113:VAL:HG21	3:G:128:LEU:HG	2.02	0.42
3:H:1:MET:O	3:H:1:MET:HG2	2.19	0.42
2:B:254:GLU:C	2:B:256:THR:N	2.73	0.42
2:D:615:ALA:O	2:D:619:SER:HB2	2.19	0.42
3:G:227:GLU:HG3	3:G:354:TYR:CD2	2.54	0.42
3:G:227:GLU:HG3	3:G:354:TYR:HD2	1.85	0.42
3:H:113:VAL:HG21	3:H:128:LEU:HG	2.01	0.42
3:H:331:ALA:HB3	3:H:332:PRO:HD3	2.01	0.42
3:I:121:VAL:HG21	3:I:128:LEU:HD13	2.01	0.42
3:I:227:GLU:HG3	3:I:354:TYR:HD2	1.85	0.42
2:D:47:PRO:HB2	2:D:66:MET:HB3	2.00	0.42
1:E:28:SER:O	1:E:29:THR:HG23	2.18	0.42
2:F:253:SER:HB3	2:F:254:GLU:OE2	2.19	0.42
2:F:205:ILE:O	2:F:658:GLN:HG3	2.19	0.42
2:F:46:VAL:HA	2:F:47:PRO:HD3	1.90	0.42
2:F:566:VAL:N	2:F:567:PRO:CD	2.83	0.42
2:F:621:LYS:O	2:F:625:ILE:HG13	2.19	0.42
3:I:238:TYR:CE1	3:I:242:LEU:HD12	2.53	0.42
2:B:46:VAL:HG13	2:B:47:PRO:HD2	2.01	0.42
3:H:315:LEU:N	3:H:315:LEU:HD22	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:648:VAL:HG23	2:D:649:SER:N	2.35	0.42
3:G:263:PRO:HG3	3:G:269:PRO:HG3	2.02	0.42
2:B:201:THR:CG2	2:B:201:THR:O	2.68	0.42
2:B:46:VAL:HG13	2:B:47:PRO:CD	2.50	0.42
2:F:497:PRO:HG3	2:F:532:PRO:HB2	2.01	0.42
2:F:672:PHE:N	2:F:673:PRO:HD3	2.34	0.42
1:C:19:VAL:HB	2:D:248:GLN:HB2	2.02	0.42
2:F:201:THR:CG2	2:F:244:ASN:ND2	2.83	0.42
2:D:581:TYR:O	3:H:70:HIS:HA	2.19	0.42
2:B:611:ILE:C	2:B:611:ILE:HD12	2.40	0.41
2:F:615:ALA:O	2:F:619:SER:HB2	2.20	0.41
3:I:224:ASP:HB2	3:I:357:MET:CG	2.50	0.41
1:A:20:PHE:HB3	2:B:210:CYS:O	2.19	0.41
2:B:195:ALA:HB2	2:B:229:ILE:CD1	2.49	0.41
2:D:126:ASP:C	2:D:128:LEU:H	2.24	0.41
2:B:197:THR:HB	2:F:567:PRO:HG3	2.02	0.41
1:C:21:LYS:HD3	2:D:207:GLU:OE1	2.20	0.41
2:F:143:TYR:CD1	2:F:143:TYR:N	2.88	0.41
2:F:271:ALA:HA	2:F:272:PRO:HD3	1.85	0.41
3:G:331:ALA:HB3	3:G:332:PRO:HD3	2.02	0.41
1:A:21:LYS:HD3	2:B:207:GLU:OE1	2.20	0.41
2:B:153:ARG:HH11	2:B:153:ARG:CB	2.15	0.41
2:B:55:THR:C	2:B:57:VAL:H	2.23	0.41
2:D:211:PRO:O	2:D:214:SER:N	2.53	0.41
2:F:284:LYS:O	2:F:288:GLN:HG3	2.21	0.41
3:H:157:ASP:O	3:H:158:ASP:HB2	2.21	0.41
3:I:1:MET:HG2	3:I:1:MET:O	2.20	0.41
1:A:35:SER:O	2:B:106:HIS:HE1	2.02	0.41
2:D:126:ASP:C	2:D:128:LEU:N	2.74	0.41
1:C:20:PHE:HB3	2:D:210:CYS:O	2.21	0.41
2:F:405:GLN:HB3	2:F:464:MET:HE1	2.02	0.41
3:I:100:LEU:HD22	3:I:159:LEU:HD12	2.01	0.41
2:F:620:ASP:OD2	3:I:1:MET:HA	2.21	0.41
3:I:197:LEU:HD13	3:I:201:ALA:O	2.19	0.41
2:D:203:VAL:HA	2:D:204:PRO:HD3	1.88	0.41
2:D:254:GLU:C	2:D:256:THR:N	2.74	0.41
2:D:566:VAL:HG23	2:D:567:PRO:HD3	2.02	0.41
2:F:165:VAL:HG12	2:F:166:ILE:N	2.36	0.41
2:F:587:ASN:HA	2:F:588:PRO:HD3	1.89	0.41
3:G:109:MET:HE1	3:G:130:GLU:N	2.35	0.41
3:G:116:GLU:H	3:G:116:GLU:CD	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:154:GLN:O	3:H:156:VAL:HG23	2.20	0.41
3:H:263:PRO:HG3	3:H:269:PRO:HG3	2.02	0.41
3:I:0:ACE:O	3:I:1:MET:HB3	2.20	0.41
3:I:249:PHE:CD2	3:I:259:ARG:HG2	2.56	0.41
2:B:230:ARG:HG2	2:B:230:ARG:HH11	1.86	0.41
2:F:123:GLU:HG3	2:F:238:VAL:HB	2.03	0.41
2:F:254:GLU:C	2:F:256:THR:N	2.74	0.41
2:B:672:PHE:N	2:B:673:PRO:HD3	2.35	0.41
2:D:46:VAL:HG13	2:D:47:PRO:HD2	2.02	0.41
2:D:611:ILE:C	2:D:611:ILE:HD12	2.42	0.41
3:G:0:ACE:O	3:G:1:MET:CB	2.69	0.41
3:H:227:GLU:HG3	3:H:354:TYR:CD2	2.56	0.41
2:B:131:LEU:HD21	2:B:135:PRO:CD	2.44	0.41
2:D:497:PRO:HG3	2:D:532:PRO:HB2	2.03	0.41
2:F:452:TYR:HE1	2:F:457:LEU:HD12	1.86	0.41
2:B:497:PRO:HG3	2:B:532:PRO:HB2	2.03	0.41
1:C:35:SER:H	2:D:110:ASN:ND2	2.18	0.41
2:D:361:LEU:HD22	2:D:365:THR:HG21	2.03	0.41
1:E:20:PHE:HB3	2:F:210:CYS:O	2.21	0.41
2:F:195:ALA:HB2	2:F:229:ILE:CD1	2.51	0.41
3:H:227:GLU:HG3	3:H:354:TYR:HD2	1.86	0.41
1:A:13:VAL:HG11	4:B:709:BOG:H5'1	2.03	0.40
2:B:143:TYR:CD1	2:B:143:TYR:N	2.89	0.40
2:B:639:SER:O	2:B:640:LEU:C	2.59	0.40
2:B:648:VAL:CG2	2:B:649:SER:N	2.83	0.40
2:D:198:LEU:HD12	2:D:198:LEU:HA	1.88	0.40
2:D:55:THR:C	2:D:57:VAL:H	2.24	0.40
2:F:46:VAL:HG13	2:F:47:PRO:HD2	2.04	0.40
3:G:298:LEU:O	3:G:302:VAL:HG23	2.21	0.40
3:G:127:SER:HA	3:G:364:LEU:HB3	2.02	0.40
3:I:303:ASN:HD22	3:I:311:ILE:HD13	1.87	0.40
2:F:107:ALA:O	2:F:111:PHE:HD1	2.03	0.40
3:H:109:MET:HE2	3:H:129:VAL:HG13	2.02	0.40
2:D:583:VAL:HG21	3:H:67:HIS:HB3	2.03	0.40
2:B:286:THR:O	2:B:290:MET:HG3	2.22	0.40
1:E:35:SER:O	2:F:106:HIS:HE1	2.04	0.40
2:F:368:VAL:HB	2:F:468:LEU:HB3	2.02	0.40
3:I:303:ASN:HD22	3:I:303:ASN:HA	1.69	0.40
3:I:331:ALA:HB3	3:I:332:PRO:HD3	2.03	0.40
2:B:566:VAL:HG23	2:B:567:PRO:HD3	2.03	0.40
2:D:165:VAL:HG12	2:D:166:ILE:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:114:ALA:O	2:F:117:ALA:HB3	2.21	0.40
3:H:127:SER:HA	3:H:364:LEU:HB3	2.03	0.40
3:I:127:SER:HA	3:I:364:LEU:HB3	2.03	0.40
3:I:94:HIS:CE1	3:I:153:LEU:HD23	2.56	0.40
2:B:459:LYS:HA	2:B:466:TYR:OH	2.21	0.40
2:D:236:ALA:O	2:D:240:LEU:HG	2.22	0.40
2:D:254:GLU:O	2:D:256:THR:N	2.55	0.40
2:D:392:TRP:CE3	2:D:483:MET:HB2	2.57	0.40
2:D:46:VAL:HG13	2:D:47:PRO:CD	2.52	0.40
2:F:211:PRO:O	2:F:214:SER:N	2.53	0.40
3:G:143:ARG:CG	3:G:143:ARG:NH1	2.81	0.40
3:G:157:ASP:O	3:G:158:ASP:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	31/41 (76%)	28 (90%)	3 (10%)	0	100	100
1	C	31/41 (76%)	28 (90%)	3 (10%)	0	100	100
1	E	31/41 (76%)	27 (87%)	4 (13%)	0	100	100
2	B	604/666 (91%)	560 (93%)	38 (6%)	6 (1%)	18	50
2	D	604/666 (91%)	561 (93%)	37 (6%)	6 (1%)	18	50
2	F	604/666 (91%)	561 (93%)	36 (6%)	7 (1%)	15	44
3	G	364/366 (100%)	336 (92%)	25 (7%)	3 (1%)	22	55
3	H	364/366 (100%)	336 (92%)	25 (7%)	3 (1%)	22	55
3	I	364/366 (100%)	336 (92%)	26 (7%)	2 (0%)	32	67
All	All	2997/3219 (93%)	2773 (92%)	197 (7%)	27 (1%)	20	52

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	616	PRO
2	D	616	PRO
2	F	616	PRO
3	G	1	MET
3	H	1	MET
3	I	1	MET
2	B	135	PRO
2	D	135	PRO
2	D	136	LYS
2	F	135	PRO
2	B	136	LYS
2	D	52	GLY
2	F	52	GLY
2	F	136	LYS
2	B	52	GLY
2	D	186	GLU
2	D	323	VAL
2	B	186	GLU
2	B	323	VAL
2	F	186	GLU
2	F	352	ASN
2	F	323	VAL
3	G	263	PRO
3	H	263	PRO
3	I	263	PRO
3	G	194	GLY
3	H	194	GLY

5.3.2 Protein sidechains ⓘ

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	28/34 (82%)	28 (100%)	0	100	100
1	C	28/34 (82%)	28 (100%)	0	100	100
1	E	28/34 (82%)	28 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	513/561 (91%)	500 (98%)	13 (2%)	53	84
2	D	513/561 (91%)	500 (98%)	13 (2%)	53	84
2	F	513/561 (91%)	500 (98%)	13 (2%)	53	84
3	G	317/317 (100%)	312 (98%)	5 (2%)	68	91
3	H	317/317 (100%)	312 (98%)	5 (2%)	68	91
3	I	317/317 (100%)	312 (98%)	5 (2%)	68	91
All	All	2574/2736 (94%)	2520 (98%)	54 (2%)	59	88

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	105	GLU
2	B	123	GLU
2	B	135	PRO
2	B	145	ASP
2	B	173	MET
2	B	324	ARG
2	B	401	PHE
2	B	438	THR
2	B	455	GLU
2	B	458	ASN
2	B	554	ASP
2	B	616	PRO
2	B	658	GLN
2	D	105	GLU
2	D	123	GLU
2	D	135	PRO
2	D	145	ASP
2	D	173	MET
2	D	324	ARG
2	D	401	PHE
2	D	438	THR
2	D	455	GLU
2	D	458	ASN
2	D	554	ASP
2	D	616	PRO
2	D	658	GLN
2	F	105	GLU
2	F	123	GLU
2	F	135	PRO

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Mol	Chain	Res	Type
2	F	145	ASP
2	F	173	MET
2	F	324	ARG
2	F	401	PHE
2	F	438	THR
2	F	455	GLU
2	F	458	ASN
2	F	554	ASP
2	F	616	PRO
2	F	658	GLN
3	G	112	ASP
3	G	175	ASP
3	G	217	GLU
3	G	345	ASP
3	G	357	MET
3	H	112	ASP
3	H	175	ASP
3	H	217	GLU
3	H	345	ASP
3	H	357	MET
3	I	112	ASP
3	I	175	ASP
3	I	217	GLU
3	I	345	ASP
3	I	357	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	106	HIS
2	B	110	ASN
2	B	248	GLN
2	B	356	ASN
2	D	106	HIS
2	D	110	ASN
2	D	248	GLN
2	D	356	ASN
2	F	106	HIS
2	F	110	ASN
2	F	248	GLN
2	F	356	ASN
3	G	7	ASN

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Mol	Chain	Res	Type
3	G	70	HIS
3	G	111	ASN
3	G	132	ASN
3	G	171	ASN
3	G	303	ASN
3	G	329	GLN
3	H	7	ASN
3	H	70	HIS
3	H	111	ASN
3	H	132	ASN
3	H	171	ASN
3	H	303	ASN
3	I	7	ASN
3	I	111	ASN
3	I	132	ASN
3	I	171	ASN
3	I	303	ASN
3	I	329	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](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	BOG	B	709	-	20,20,20	1.42	3 (15%)	25,25,25	0.70	0
6	SO4	B	710	-	4,4,4	0.49	0	6,6,6	0.17	0
4	BOG	D	709	-	20,20,20	1.41	4 (20%)	25,25,25	0.68	0
6	SO4	D	710	-	4,4,4	0.52	0	6,6,6	0.07	0
4	BOG	F	709	-	20,20,20	1.49	5 (25%)	25,25,25	0.69	0
6	SO4	F	710	-	4,4,4	0.51	0	6,6,6	0.16	0
6	SO4	G	504	-	4,4,4	0.64	0	6,6,6	0.17	0
6	SO4	G	507	-	4,4,4	0.65	0	6,6,6	0.08	0
6	SO4	H	505	-	4,4,4	0.74	0	6,6,6	0.13	0
6	SO4	H	508	-	4,4,4	0.67	0	6,6,6	0.17	0
6	SO4	I	506	-	4,4,4	0.73	0	6,6,6	0.12	0
6	SO4	I	509	-	4,4,4	0.65	0	6,6,6	0.14	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
4	BOG	B	709	-	-	0/11/31/31	0/1/1/1
6	SO4	B	710	-	-	0/0/0/0	0/0/0/0
4	BOG	D	709	-	-	0/11/31/31	0/1/1/1
6	SO4	D	710	-	-	0/0/0/0	0/0/0/0
4	BOG	F	709	-	-	0/11/31/31	0/1/1/1
6	SO4	F	710	-	-	0/0/0/0	0/0/0/0
6	SO4	G	504	-	-	0/0/0/0	0/0/0/0
6	SO4	G	507	-	-	0/0/0/0	0/0/0/0
6	SO4	H	505	-	-	0/0/0/0	0/0/0/0
6	SO4	H	508	-	-	0/0/0/0	0/0/0/0
6	SO4	I	506	-	-	0/0/0/0	0/0/0/0
6	SO4	I	509	-	-	0/0/0/0	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	709	BOG	C4-C3	2.04	1.57	1.52
4	F	709	BOG	C1-C2	2.14	1.58	1.52
4	F	709	BOG	C4-C3	2.21	1.58	1.52
4	B	709	BOG	C4-C5	2.53	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	709	BOG	C4-C5	2.58	1.58	1.53
4	F	709	BOG	O1-C1	2.59	1.44	1.40
4	D	709	BOG	O1-C1	2.60	1.44	1.40
4	F	709	BOG	C4-C5	2.89	1.59	1.53
4	B	709	BOG	O1-C1	2.91	1.45	1.40
4	B	709	BOG	O5-C1	3.28	1.50	1.41
4	D	709	BOG	O5-C1	3.48	1.50	1.41
4	F	709	BOG	O5-C1	3.49	1.50	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	709	BOG	2	0
4	D	709	BOG	1	0
4	F	709	BOG	1	0

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	33/41 (80%)	0.10	1 (3%) 51 39	51, 59, 71, 73	0
1	C	33/41 (80%)	0.03	0 100 100	52, 58, 70, 72	0
1	E	33/41 (80%)	0.01	0 100 100	53, 60, 71, 73	0
2	B	608/666 (91%)	-0.21	16 (2%) 56 45	32, 50, 87, 126	0
2	D	608/666 (91%)	-0.19	16 (2%) 56 45	32, 50, 87, 125	0
2	F	608/666 (91%)	-0.21	21 (3%) 44 33	33, 50, 87, 125	0
3	G	365/366 (99%)	-0.27	3 (0%) 86 81	34, 52, 84, 115	0
3	H	365/366 (99%)	-0.24	1 (0%) 93 92	34, 52, 84, 114	0
3	I	365/366 (99%)	-0.27	3 (0%) 86 81	36, 53, 84, 115	0
All	All	3018/3219 (93%)	-0.22	61 (2%) 65 56	32, 51, 86, 126	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	56	SER	5.8
2	D	57	VAL	5.8
2	D	55	THR	5.6
2	F	55	THR	5.1
2	D	62	ALA	4.7
2	B	55	THR	4.6
2	D	58	THR	4.4
2	F	56	SER	4.2
2	F	458	ASN	3.9
2	D	54	GLU	3.7
2	F	57	VAL	3.7
2	F	133	VAL	3.7
2	F	129	ARG	3.6
3	G	230	HIS	3.5
3	H	230	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	53	ASP	3.4
2	B	439	ALA	3.2
2	D	129	ARG	3.1
2	F	53	ASP	3.1
2	D	131	LEU	3.1
2	B	56	SER	3.1
2	D	71	ILE	3.0
2	F	252	VAL	3.0
3	I	230	HIS	3.0
2	F	58	THR	2.9
2	F	253	SER	2.9
2	D	133	VAL	2.9
2	B	459	LYS	2.9
3	I	113	VAL	2.8
2	D	143	TYR	2.8
2	B	131	LEU	2.7
2	B	54	GLU	2.7
2	F	54	GLU	2.6
3	I	304	HIS	2.6
2	B	50	ALA	2.6
2	B	58	THR	2.5
2	F	132	SER	2.5
2	B	133	VAL	2.5
2	F	459	LYS	2.5
2	B	440	GLN	2.4
2	F	51	ILE	2.4
2	B	132	SER	2.3
2	D	130	VAL	2.3
2	B	53	ASP	2.2
2	D	254	GLU	2.2
2	D	421	GLN	2.2
2	B	458	ASN	2.1
2	F	256	THR	2.1
2	F	69	LYS	2.1
2	F	579	THR	2.1
2	B	57	VAL	2.1
1	A	28	SER	2.1
2	B	255	GLY	2.1
2	D	43	PRO	2.1
3	G	232	PRO	2.0
2	F	456	GLN	2.0
2	F	59	SER	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	463	GLU	2.0
3	G	126	GLY	2.0
2	F	71	ILE	2.0
2	F	460	THR	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
7	CL	A	601	1/1	0.93	0.35	10.62	76,76,76,76	0
4	BOG	B	709	20/20	0.77	0.39	4.80	70,91,94,94	0
4	BOG	F	709	20/20	0.76	0.34	4.79	70,91,94,95	0
4	BOG	D	709	20/20	0.85	0.37	4.12	68,89,92,93	0
5	ZN	H	703	1/1	0.99	0.07	-1.43	45,45,45,45	0
6	SO4	F	710	5/5	0.97	0.09	-1.93	70,71,71,72	0
5	ZN	I	701	1/1	0.99	0.07	-2.23	52,52,52,52	0
6	SO4	B	710	5/5	0.96	0.10	-2.39	69,69,70,71	0
6	SO4	D	710	5/5	0.98	0.10	-2.75	69,69,70,70	0
5	ZN	G	702	1/1	1.00	0.05	-2.92	39,39,39,39	0
6	SO4	I	506	5/5	0.86	0.33	-	114,114,114,114	0
6	SO4	I	509	5/5	0.95	0.18	-	101,101,102,102	0
6	SO4	H	508	5/5	0.92	0.20	-	100,101,101,102	0
6	SO4	G	504	5/5	0.87	0.24	-	112,112,112,112	0
6	SO4	G	507	5/5	0.87	0.20	-	100,101,101,101	0
6	SO4	H	505	5/5	0.92	0.24	-	114,114,114,115	0

6.5 Other polymers [i](#)

There are no such residues in this entry.