Full wwPDB X-ray Structure Validation Report (i)

Aug 15, 2023 – 04:59 PM EDT

PDB ID	:	1SQL
Title	:	Crystal structure of 7,8-dihydroneopterin aldolase in complex with guanine
Authors	:	Bauer, S.; Schott, A.K.; Illarionova, V.; Bacher, A.; Huber, R.; Fischer, M.
Deposited on	:	2004-03-19
Resolution	:	2.20 Å(reported)

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

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

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

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

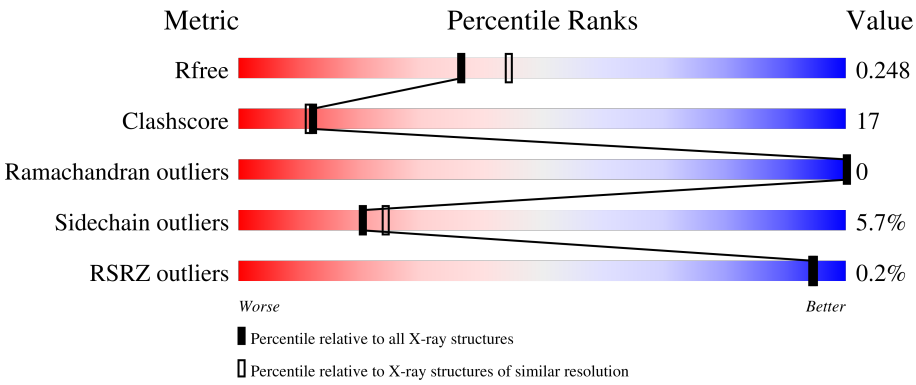
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	146	57% 25% 18%
1	B	146	60% 21% • 17%
1	C	146	60% 23% • 16%
1	D	146	54% 27% • 18%
1	E	146	56% 22% • 18%

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Mol	Chain	Length	Quality of chain
1	F	146	55% 26% • 17%
1	G	146	58% 22% • 17%
1	H	146	63% 20% • 16%
1	I	146	63% 19% • 17%
1	J	146	59% 23% • 16%
1	K	146	58% 21% • 18%
1	L	146	% 55% 26% • 16%
1	M	146	% 52% 30% • 16%
1	N	146	58% 22% • 17%
1	O	146	61% 19% • 18%
1	P	146	60% 19% • 16%

2 Entry composition (i)

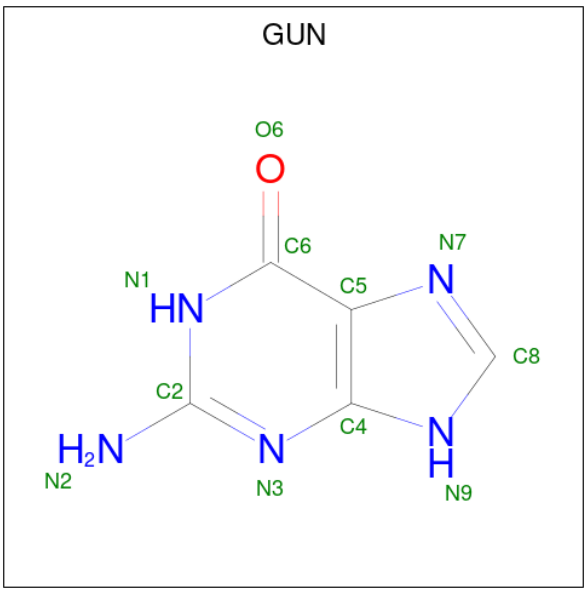
There are 3 unique types of molecules in this entry. The entry contains 16400 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 dihydroneopterin aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	120	947	611	158	177	1	5	0	0
1	B	121	955	615	160	179	1	0	0	0
1	C	122	962	619	161	181	1	7	0	0
1	D	120	947	611	158	177	1	0	0	0
1	E	120	947	611	158	177	1	0	0	0
1	F	121	955	615	160	179	1	0	0	0
1	G	121	955	615	160	179	1	6	0	0
1	H	122	962	619	161	181	1	0	0	0
1	I	121	955	615	160	179	1	6	0	0
1	J	123	968	622	162	183	1	0	0	0
1	K	120	947	611	158	177	1	0	0	0
1	L	122	962	619	161	181	1	0	0	0
1	M	123	968	622	162	183	1	7	0	0
1	N	121	955	615	160	179	1	0	0	0
1	O	120	947	611	158	177	1	0	0	0
1	P	122	963	621	161	180	1	0	0	0

- Molecule 2 is GUANINE (three-letter code: GUN) (formula: $C_5H_5N_5O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	11	5	5	1	0	0
2	B	1	11	5	5	1	0	0
2	B	1	11	5	5	1	0	0
2	D	1	11	5	5	1	0	0
2	F	1	11	5	5	1	0	0
2	G	1	11	5	5	1	0	0
2	G	1	11	5	5	1	0	0
2	H	1	11	5	5	1	0	0
2	I	1	11	5	5	1	0	0
2	J	1	11	5	5	1	0	0
2	J	1	11	5	5	1	0	0
2	L	1	11	5	5	1	0	0
2	M	1	11	5	5	1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	O	1	11	5	5	1	0	0
			Total	C	N	O		
2	P	1	11	5	5	1	0	0
			Total	C	N	O		
2	P	1	11	5	5	1	0	0

- Molecule 3 is water.

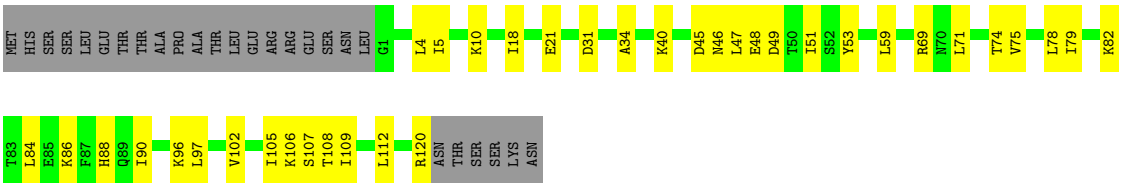
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	59	59	59	0	0
			Total	O		
3	B	67	67	67	0	0
			Total	O		
3	C	51	51	51	0	0
			Total	O		
3	D	50	50	50	0	0
			Total	O		
3	E	52	52	52	0	0
			Total	O		
3	F	52	52	52	0	0
			Total	O		
3	G	69	69	69	0	0
			Total	O		
3	H	67	67	67	0	0
			Total	O		
3	I	60	60	60	0	0
			Total	O		
3	J	70	70	70	0	0
			Total	O		
3	K	56	56	56	0	0
			Total	O		
3	L	54	54	54	0	0
			Total	O		
3	M	50	50	50	0	0
			Total	O		
3	N	53	53	53	0	0
			Total	O		
3	O	60	60	60	0	0
			Total	O		
3	P	59	59	59	0	0

3 Residue-property plots (i)

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

• Molecule 1: dihydroneopterin aldolase

Chain A: 57% 25% 18%

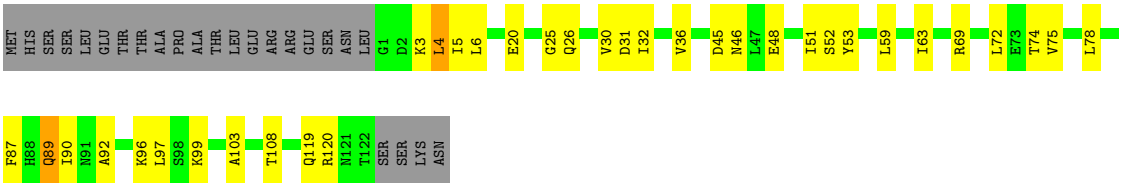


• Molecule 1: dihydroneopterin aldolase

Chain B: 60% 21% • 17%

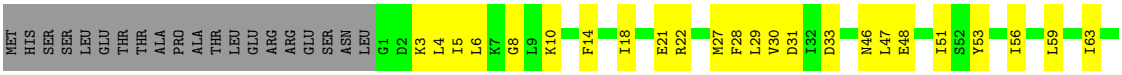
• Molecule 1: dihydroneopterin aldolase

Chain C: 60% 23% • 16%



• Molecule 1: dihydroneopterin aldolase

Chain D: 54% 27% • 18%



P68 R69 N70 L71 L72 E85 K86 F87 H88 Q89 R94 V95 K96 L97 S98 K99 V102 A103 L104 I105 D115 R120 ASN THR SER SER LYS ASN

• Molecule 1: dihydroneopterin aldolase

Chain E: 56% 22% • 18%

MET HIS SER SER LEU GLU THR THR ALA PRO ALA THR LEU GLU ARG ARG GLU SER ASN LEU G1 L4 I5 L6 K7 G8 L9 K10 R22 M27 V30 D31 W35 V36 L47 I51 S52 Y53 P68 R69 L72 A76 E77 L78 K82 F87 H88 Q89

I90 R94 V95 K96 L97 S98 K99 V102 I105 I109 D110 D115 I116 F117 R120 ASN THR SER SER LYS ASN

• Molecule 1: dihydroneopterin aldolase

Chain F: 55% 26% • 17%

MET HIS SER SER LEU GLU THR THR ALA PRO ALA THR LEU GLU ARG ARG GLU SER ASN LEU G1 L4 I5 L6 K7 K10 I18 A19 E20 E21 L24 L29 V30 D31 I32 D33 A34 W35 L38 L47 I51 S52 Y53 K61 E62 I63 V64 E65 R69

V75 L78 K82 F87 H88 Q89 I90 R94 V95 K96 L97 S98 K99 P100 A103 L104 I105 I109 Q119 R120 N121 THR SER SER LYS ASN

• Molecule 1: dihydroneopterin aldolase

Chain G: 58% 22% • 17%

MET HIS SER SER LEU GLU THR THR ALA PRO ALA THR LEU GLU ARG ARG GLU SER ASN LEU G1 D2 K3 L4 I5 L6 K7 G8 F14 R22 L29 V30 D31 V36 K39 L47 E48 I51 S52 Y53 V54 F57 S58 L59 A60 V64 P68 L72

L78 K82 F87 H88 Q89 I90 K96 L97 S98 K99 P100 A103 L104 I105 K106 R120 N121 THR SER SER LYS ASN

• Molecule 1: dihydroneopterin aldolase

Chain H: 63% 20% • 16%

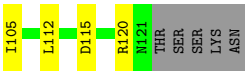
MET HIS SER SER LEU GLU THR THR ALA PRO ALA THR LEU GLU ARG ARG GLU SER ASN LEU G1 D2 K3 L4 I5 L9 R22 L29 V30 V36 I51 S52 Y53 S58 L59 E62 I63 S67 P68 R69 N70 L71 H88 Q89 I90 N91 A92 K96 L97

P100 A103 L104 I105 K106 I109 Q119 T122 SER SER LYS ASN

• Molecule 1: dihydroneopterin aldolase

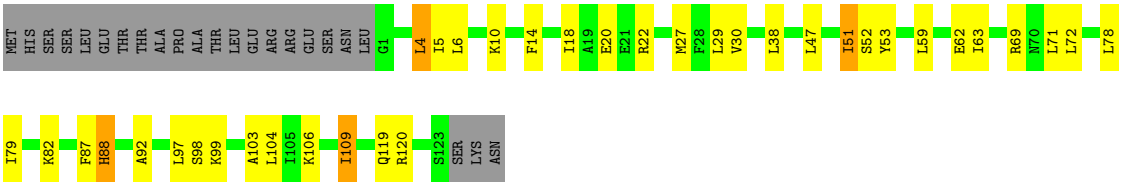
Chain I: 63% 19% • 17%

MET HIS SER SER LEU GLU THR THR ALA PRO ALA THR LEU GLU ARG ARG GLU SER ASN LEU G1 D2 K3 L4 I5 L6 K7 G8 L9 L24 L29 V30 D31 I51 S52 Y53 L59 L72 S81 K82 F87 H88 Q89 I90 K96 K99 P100 N101 V102 A103 L104



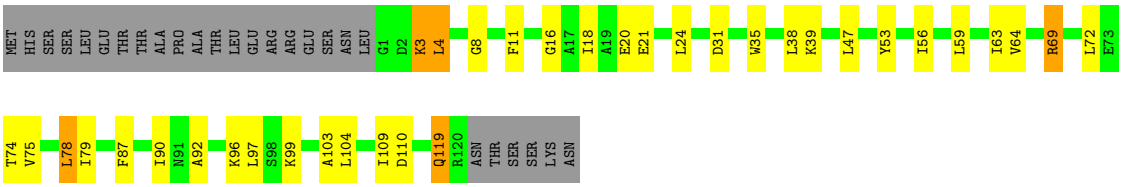
• Molecule 1: dihydroneopterin aldolase

Chain J:



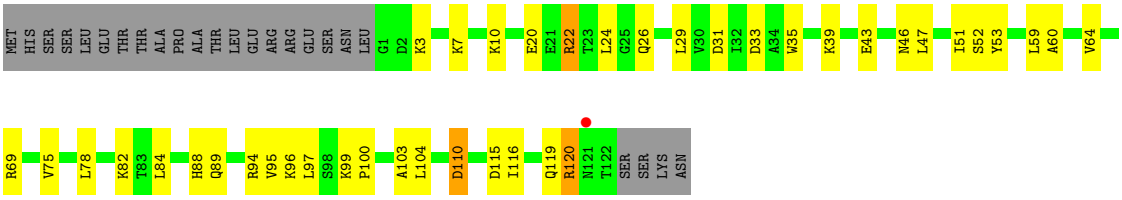
• Molecule 1: dihydroneopterin aldolase

Chain K:



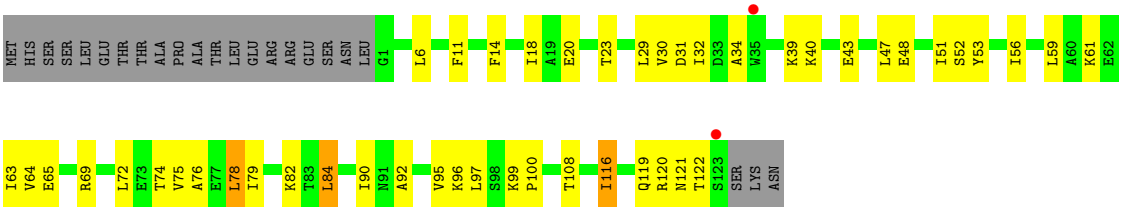
• Molecule 1: dihydroneopterin aldolase

Chain L:



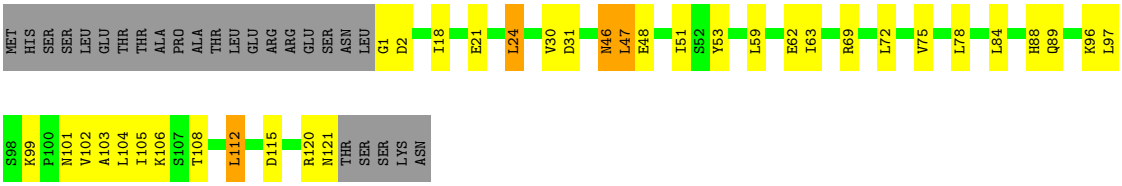
• Molecule 1: dihydroneopterin aldolase

Chain M:



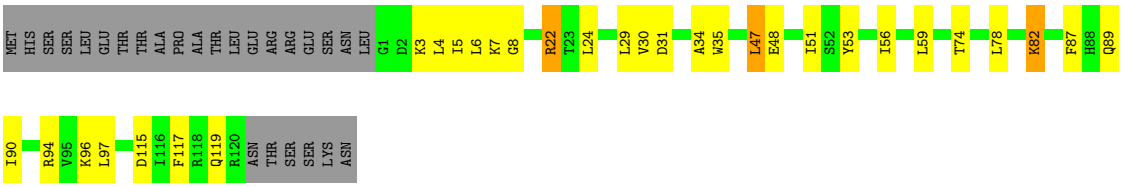
• Molecule 1: dihydroneopterin aldolase

Chain N:



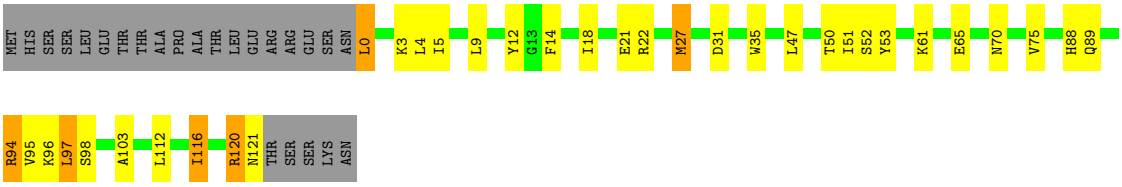
- Molecule 1: dihydroneopterin aldolase

Chain O:



- Molecule 1: dihydroneopterin aldolase

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	63.55Å 84.22Å 89.05Å 90.14° 89.99° 76.17°	Depositor
Resolution (Å)	20.00 – 2.20 15.94 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.20) 94.9 (15.94-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.90 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.204 , 0.260 0.185 , 0.248	Depositor DCC
R_{free} test set	3837 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å^2)	20.0	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 34.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.477 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16400	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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: GUN

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	0.40	0/961	0.68	0/1294
1	B	0.39	0/969	0.66	0/1305
1	C	0.37	0/976	0.64	0/1315
1	D	0.40	0/961	0.64	0/1294
1	E	0.40	0/961	0.67	0/1294
1	F	0.39	0/969	0.64	0/1305
1	G	0.40	0/969	0.65	0/1305
1	H	0.38	0/976	0.64	0/1315
1	I	0.38	0/969	0.65	0/1305
1	J	0.38	0/982	0.65	0/1323
1	K	0.39	0/961	0.66	0/1294
1	L	0.39	0/976	0.65	0/1315
1	M	0.37	0/982	0.66	0/1323
1	N	0.39	0/969	0.63	0/1305
1	O	0.38	0/961	0.68	0/1294
1	P	0.39	0/977	0.66	0/1316
All	All	0.39	0/15519	0.65	0/20902

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	947	0	983	30	0
1	B	955	0	989	43	0
1	C	962	0	996	37	0
1	D	947	0	983	40	0
1	E	947	0	983	48	0
1	F	955	0	989	38	0
1	G	955	0	989	33	0
1	H	962	0	996	21	0
1	I	955	0	989	32	0
1	J	968	0	1001	36	0
1	K	947	0	983	26	0
1	L	962	0	996	41	0
1	M	968	0	1001	43	0
1	N	955	0	989	31	0
1	O	947	0	983	31	0
1	P	963	0	1000	36	0
2	A	11	0	5	0	0
2	B	22	0	10	1	0
2	D	11	0	5	0	0
2	F	11	0	5	1	0
2	G	22	0	10	1	0
2	H	11	0	5	0	0
2	I	11	0	5	2	0
2	J	22	0	10	0	0
2	L	11	0	5	1	0
2	M	11	0	5	0	0
2	O	11	0	5	0	0
2	P	22	0	10	2	0
3	A	59	0	0	3	0
3	B	67	0	0	2	0
3	C	51	0	0	2	0
3	D	50	0	0	1	0
3	E	52	0	0	2	0
3	F	52	0	0	1	0
3	G	69	0	0	4	0
3	H	67	0	0	1	0
3	I	60	0	0	2	0
3	J	70	0	0	3	0
3	K	56	0	0	1	0
3	L	54	0	0	0	0
3	M	50	0	0	4	0
3	N	53	0	0	6	0
3	O	60	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	59	0	0	1	0
All	All	16400	0	15930	533	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 17.

All (533) 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:L:88:HIS:HA	1:L:120:ARG:NH1	1.80	0.95
1:J:88:HIS:H	1:J:88:HIS:CD2	1.64	0.95
1:L:88:HIS:HA	1:L:120:ARG:HH11	1.30	0.93
1:N:46:ASN:HB2	3:N:171:HOH:O	1.69	0.93
1:J:88:HIS:H	1:J:88:HIS:HD2	1.10	0.90
1:G:52:SER:OG	1:G:54:VAL:HG12	1.70	0.90
1:E:89:GLN:H	1:E:89:GLN:HE21	1.14	0.89
1:D:22:ARG:HE	1:D:68:PRO:HB2	1.36	0.88
1:E:95:VAL:HB	1:E:116:ILE:HD11	1.57	0.87
1:P:0:LEU:H3	1:P:35:TRP:HE1	1.19	0.86
1:L:95:VAL:HB	1:L:116:ILE:HD11	1.58	0.86
1:C:87:PHE:HB3	1:C:89:GLN:HE22	1.41	0.86
1:L:51:ILE:HD11	1:L:89:GLN:HB2	1.57	0.85
1:F:51:ILE:HD11	1:F:89:GLN:HB2	1.58	0.85
1:O:74:THR:O	1:O:78:LEU:HD13	1.77	0.84
1:C:72:LEU:HD21	1:C:99:LYS:HE3	1.61	0.83
1:F:94:ARG:HE	1:F:96:LYS:HE2	1.44	0.83
1:E:89:GLN:H	1:E:89:GLN:NE2	1.76	0.83
1:J:18:ILE:HG22	1:J:20:GLU:HG2	1.61	0.82
1:C:89:GLN:H	1:C:89:GLN:NE2	1.76	0.82
1:H:29:LEU:HD12	1:H:100:PRO:HG3	1.61	0.82
1:G:36:VAL:HG13	1:G:90:ILE:HA	1.62	0.82
1:D:89:GLN:H	1:D:89:GLN:HE21	1.27	0.81
1:C:120:ARG:HG2	1:C:120:ARG:HH21	1.46	0.81
1:J:88:HIS:CD2	1:J:88:HIS:N	2.45	0.80
1:D:89:GLN:H	1:D:89:GLN:NE2	1.80	0.79
1:L:3:LYS:HZ2	1:L:35:TRP:HE1	1.28	0.79
1:M:116:ILE:HD13	1:M:116:ILE:H	1.48	0.78
1:G:89:GLN:CD	1:G:89:GLN:H	1.83	0.78
1:P:0:LEU:N	1:P:35:TRP:HE1	1.82	0.77
1:C:92:ALA:HB2	1:C:119:GLN:HG3	1.64	0.76
1:E:94:ARG:HH21	1:E:94:ARG:HG3	1.49	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:22:ARG:HG2	1:O:22:ARG:HH21	1.50	0.75
1:N:46:ASN:ND2	1:N:48:GLU:H	1.85	0.74
1:M:95:VAL:HB	1:M:116:ILE:HD11	1.69	0.74
1:B:36:VAL:HG12	1:B:90:ILE:HA	1.69	0.74
1:B:94:ARG:CG	1:B:94:ARG:HH21	2.01	0.73
1:E:69:ARG:HH22	1:E:78:LEU:CD2	2.00	0.73
1:E:102:VAL:HB	1:E:105:ILE:HD12	1.69	0.73
1:F:69:ARG:NH2	1:F:78:LEU:HD11	2.03	0.73
1:A:74:THR:O	1:A:78:LEU:HD13	1.88	0.73
1:J:10:LYS:HE2	1:J:27:MET:HB3	1.69	0.73
1:D:46:ASN:ND2	1:D:48:GLU:HB2	2.03	0.73
1:H:51:ILE:HD11	1:H:89:GLN:HB2	1.71	0.73
1:A:102:VAL:HG12	1:A:105:ILE:HD13	1.71	0.73
1:A:5:ILE:HD11	1:D:115:ASP:HB3	1.70	0.72
1:P:94:ARG:HH21	1:P:94:ARG:HB2	1.55	0.72
1:D:48:GLU:HG3	3:D:1033:HOH:O	1.89	0.71
1:I:51:ILE:HD11	1:I:89:GLN:HB2	1.73	0.71
1:B:36:VAL:HG11	1:B:90:ILE:HD13	1.70	0.70
1:B:120:ARG:O	1:B:121:ASN:HB2	1.91	0.70
1:L:31:ASP:HB2	1:L:96:LYS:HB2	1.72	0.70
1:J:71:LEU:HD21	1:K:47:LEU:HD13	1.74	0.70
1:P:95:VAL:HB	1:P:116:ILE:HD11	1.74	0.70
1:J:51:ILE:HD12	1:J:52:SER:N	2.06	0.69
1:A:5:ILE:HD12	1:A:5:ILE:N	2.07	0.69
1:C:51:ILE:HD11	1:C:89:GLN:NE2	2.07	0.69
1:H:58:SER:O	1:H:62:GLU:HG3	1.93	0.69
1:E:72:LEU:HD22	1:E:97:LEU:CD1	2.22	0.69
1:E:110:ASP:HB2	1:F:7:LYS:O	1.93	0.69
1:F:69:ARG:HH22	1:F:78:LEU:HD11	1.56	0.69
1:M:120:ARG:HG2	1:M:120:ARG:HH21	1.58	0.69
1:K:87:PHE:HB2	1:K:90:ILE:HD12	1.74	0.68
1:H:9:LEU:HB2	1:H:30:VAL:HG13	1.75	0.68
1:E:89:GLN:HE21	1:E:89:GLN:N	1.91	0.68
1:I:29:LEU:HD13	1:I:100:PRO:HD3	1.75	0.68
1:B:16:GLY:O	1:B:22:ARG:HD3	1.94	0.67
1:M:63:ILE:HD12	1:M:79:ILE:HD13	1.76	0.67
1:P:4:LEU:C	1:P:5:ILE:HD12	2.15	0.67
1:F:10:LYS:HG2	1:F:29:LEU:HD23	1.76	0.67
1:P:120:ARG:HB2	1:P:120:ARG:NH2	2.10	0.67
1:M:34:ALA:HB1	1:M:90:ILE:HD12	1.78	0.66
1:F:94:ARG:HE	1:F:96:LYS:CE	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:90:ILE:N	1:I:90:ILE:HD12	2.11	0.66
1:I:120:ARG:HH21	1:I:120:ARG:HG3	1.61	0.66
1:P:14:PHE:O	1:P:22:ARG:HD3	1.96	0.66
1:G:29:LEU:HD13	1:G:100:PRO:HD3	1.76	0.66
1:E:94:ARG:HG3	1:E:94:ARG:NH2	2.09	0.65
1:M:120:ARG:HD2	1:M:122:THR:O	1.96	0.65
1:N:18:ILE:HB	1:N:21:GLU:HG3	1.78	0.65
1:J:78:LEU:HD22	1:J:82:LYS:HE3	1.77	0.65
1:C:108:THR:HB	3:C:139:HOH:O	1.96	0.65
1:A:46:ASN:OD1	1:A:48:GLU:HG2	1.97	0.65
1:M:31:ASP:HB2	1:M:96:LYS:HB2	1.76	0.65
1:E:72:LEU:HD22	1:E:97:LEU:HD11	1.78	0.65
1:E:95:VAL:HB	1:E:116:ILE:CD1	2.26	0.65
1:I:3:LYS:NZ	1:L:94:ARG:HH22	1.94	0.65
1:N:102:VAL:HG21	1:N:112:LEU:HD22	1.79	0.65
1:E:10:LYS:HB3	1:E:27:MET:CE	2.27	0.64
1:G:22:ARG:HG2	1:G:68:PRO:HB2	1.80	0.64
1:H:22:ARG:HD3	1:H:68:PRO:HB2	1.78	0.64
1:N:120:ARG:NH2	1:N:120:ARG:HB2	2.13	0.64
1:I:102:VAL:HG12	1:I:105:ILE:HD13	1.79	0.64
3:O:1025:HOH:O	1:P:61:LYS:HE3	1.97	0.64
1:B:51:ILE:HG13	1:B:90:ILE:HD11	1.80	0.64
1:P:120:ARG:HB2	1:P:120:ARG:HH21	1.63	0.64
1:G:78:LEU:O	1:G:82:LYS:HB2	1.97	0.64
1:J:88:HIS:HD2	1:J:88:HIS:N	1.90	0.63
1:J:18:ILE:CG2	1:J:20:GLU:HG2	2.28	0.63
1:L:22:ARG:HH21	1:L:22:ARG:HB3	1.62	0.63
1:O:4:LEU:C	1:O:5:ILE:HD12	2.19	0.63
1:E:22:ARG:HG2	1:E:68:PRO:HB2	1.79	0.63
1:G:39:LYS:HD2	3:G:1058:HOH:O	1.99	0.63
1:E:35:TRP:HZ3	1:E:94:ARG:HB2	1.62	0.63
1:E:47:LEU:HD13	1:H:71:LEU:HD21	1.81	0.63
1:E:95:VAL:O	1:E:116:ILE:HD13	1.99	0.62
1:G:3:LYS:HE2	1:G:5:ILE:HD11	1.81	0.62
1:F:31:ASP:HB2	1:F:96:LYS:HB2	1.81	0.62
1:E:69:ARG:HH22	1:E:78:LEU:HD22	1.63	0.62
1:G:36:VAL:CG1	1:G:90:ILE:HA	2.30	0.62
1:J:72:LEU:HD21	1:J:99:LYS:HE3	1.82	0.62
1:I:72:LEU:HD21	1:I:99:LYS:HE3	1.81	0.61
1:L:26:GLN:OE1	1:L:99:LYS:HE3	2.00	0.61
1:B:36:VAL:CG1	1:B:90:ILE:HA	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:120:ARG:HG2	1:L:120:ARG:HH21	1.65	0.61
1:O:78:LEU:O	1:O:82:LYS:HB2	2.00	0.61
1:O:22:ARG:HG2	1:O:22:ARG:NH2	2.16	0.61
1:F:10:LYS:HG2	1:F:29:LEU:CD2	2.31	0.61
1:N:102:VAL:HG12	1:N:105:ILE:HD13	1.83	0.61
1:A:5:ILE:HD11	1:D:115:ASP:CB	2.31	0.60
1:K:110:ASP:HB2	1:L:7:LYS:O	2.01	0.60
1:M:108:THR:HB	3:M:1043:HOH:O	2.02	0.60
1:B:120:ARG:HG3	1:B:120:ARG:HH11	1.66	0.60
1:K:69:ARG:HD2	1:K:74:THR:HG21	1.82	0.60
1:I:102:VAL:CG1	1:I:105:ILE:HD13	2.32	0.60
1:L:35:TRP:HZ3	1:L:94:ARG:HB2	1.66	0.60
1:B:51:ILE:HD11	1:B:89:GLN:HB2	1.84	0.60
1:D:89:GLN:HE21	1:D:89:GLN:N	1.98	0.59
1:P:31:ASP:HB2	1:P:96:LYS:HB2	1.84	0.59
1:N:1:GLY:HA2	3:N:173:HOH:O	2.03	0.59
1:H:59:LEU:O	1:H:63:ILE:HG12	2.03	0.59
1:N:120:ARG:HB2	1:N:120:ARG:CZ	2.31	0.59
1:P:116:ILE:HD13	1:P:116:ILE:H	1.67	0.59
1:G:72:LEU:HD21	1:G:99:LYS:HE3	1.83	0.59
1:I:90:ILE:N	1:I:90:ILE:CD1	2.65	0.59
1:J:51:ILE:HD13	1:J:87:PHE:CE1	2.38	0.59
1:J:104:LEU:O	1:J:106:LYS:HD2	2.02	0.58
1:A:109:ILE:HD12	1:A:112:LEU:HD13	1.86	0.58
1:B:94:ARG:NH1	3:B:1030:HOH:O	2.36	0.58
1:C:89:GLN:H	1:C:89:GLN:HE21	1.51	0.58
1:P:22:ARG:NH1	1:P:70:ASN:OD1	2.36	0.58
1:D:46:ASN:HD21	1:D:48:GLU:HB2	1.68	0.58
1:D:72:LEU:HD21	1:D:99:LYS:HE3	1.85	0.58
1:B:94:ARG:NH2	1:B:115:ASP:OD2	2.36	0.58
1:D:31:ASP:HB2	1:D:96:LYS:HB2	1.84	0.58
1:F:32:ILE:HD12	1:F:95:VAL:HG22	1.84	0.58
1:L:69:ARG:NH2	1:L:78:LEU:HD11	2.18	0.58
1:N:120:ARG:HG2	1:N:121:ASN:ND2	2.18	0.58
1:C:59:LEU:O	1:C:63:ILE:HG12	2.04	0.58
1:E:69:ARG:HH22	1:E:78:LEU:HD21	1.67	0.58
1:J:14:PHE:O	1:J:22:ARG:HD3	2.04	0.58
1:O:30:VAL:HG22	1:O:97:LEU:CD1	2.34	0.57
1:E:87:PHE:HB2	1:E:90:ILE:HG12	1.85	0.57
1:F:88:HIS:HA	1:F:120:ARG:NH1	2.17	0.57
1:C:69:ARG:HD2	1:C:74:THR:HG21	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ILE:H	1:A:18:ILE:HD12	1.67	0.57
1:J:30:VAL:HG22	1:J:97:LEU:HD13	1.86	0.57
1:H:51:ILE:HD13	1:H:90:ILE:HG13	1.87	0.57
1:F:10:LYS:HE2	1:F:29:LEU:HD21	1.86	0.57
1:K:56:ILE:HD13	1:K:87:PHE:CE2	2.39	0.57
1:P:5:ILE:HD12	1:P:5:ILE:N	2.19	0.57
1:L:78:LEU:O	1:L:82:LYS:HB2	2.04	0.57
1:E:116:ILE:HD13	1:E:116:ILE:H	1.69	0.57
1:B:59:LEU:C	1:B:59:LEU:HD23	2.25	0.57
1:C:87:PHE:HB3	1:C:89:GLN:NE2	2.16	0.57
1:J:92:ALA:HB2	1:J:119:GLN:HG2	1.87	0.57
1:O:5:ILE:HD12	1:O:5:ILE:N	2.19	0.57
1:F:63:ILE:HD11	1:F:82:LYS:HD2	1.86	0.56
1:G:89:GLN:HG2	3:G:1069:HOH:O	2.03	0.56
1:H:92:ALA:HB2	1:H:119:GLN:HG2	1.86	0.56
1:A:107:SER:HB2	3:A:1002:HOH:O	2.05	0.56
1:H:103:ALA:O	1:H:104:LEU:HB2	2.04	0.56
1:I:115:ASP:HB2	1:J:5:ILE:CD1	2.36	0.56
1:L:116:ILE:HD12	1:L:116:ILE:O	2.04	0.56
1:D:14:PHE:O	1:D:22:ARG:HD2	2.04	0.56
1:D:94:ARG:HE	1:D:96:LYS:CE	2.18	0.56
1:M:95:VAL:O	1:M:116:ILE:HD13	2.05	0.56
1:B:94:ARG:CZ	1:B:96:LYS:HZ3	2.19	0.56
1:P:121:ASN:HD22	1:P:121:ASN:N	2.02	0.56
1:I:3:LYS:HZ1	1:L:94:ARG:HH22	1.54	0.56
1:A:107:SER:O	1:A:108:THR:HB	2.06	0.56
1:F:4:LEU:HD11	1:F:38:LEU:HD21	1.87	0.56
1:L:95:VAL:HB	1:L:116:ILE:CD1	2.32	0.56
1:A:18:ILE:HD12	1:A:18:ILE:N	2.20	0.56
1:A:82:LYS:O	1:A:86:LYS:HG2	2.05	0.56
1:F:4:LEU:CD1	1:F:38:LEU:HD21	2.36	0.56
1:B:36:VAL:CG1	1:B:90:ILE:HD13	2.36	0.55
1:F:87:PHE:HB2	1:F:90:ILE:HD12	1.88	0.55
1:M:39:LYS:HE3	1:M:43:GLU:OE1	2.05	0.55
1:D:51:ILE:HD11	1:D:89:GLN:OE1	2.06	0.55
1:G:89:GLN:H	1:G:89:GLN:NE2	2.02	0.55
1:I:4:LEU:C	1:I:5:ILE:HD12	2.27	0.55
1:I:59:LEU:HD11	1:I:82:LYS:HG3	1.89	0.55
1:A:88:HIS:HA	1:A:120:ARG:NH2	2.22	0.55
1:B:94:ARG:HH22	1:B:96:LYS:CG	2.19	0.55
1:F:94:ARG:NE	1:F:96:LYS:HE2	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:81:SER:HB3	3:I:1059:HOH:O	2.06	0.55
1:B:51:ILE:HG13	1:B:90:ILE:CD1	2.36	0.55
1:B:94:ARG:HH22	1:B:96:LYS:HD3	1.71	0.55
1:C:103:ALA:HB1	1:F:24:LEU:HG	1.88	0.55
1:I:112:LEU:HD22	1:J:6:LEU:HG	1.89	0.55
1:K:16:GLY:HA2	3:K:132:HOH:O	2.06	0.55
1:A:109:ILE:CD1	1:A:112:LEU:HD13	2.37	0.55
1:P:0:LEU:O	1:P:0:LEU:HD23	2.07	0.55
1:E:72:LEU:HB3	1:E:97:LEU:HD12	1.88	0.54
1:D:4:LEU:C	1:D:5:ILE:HD12	2.28	0.54
1:B:94:ARG:CZ	3:B:1030:HOH:O	2.55	0.54
1:J:69:ARG:NH1	3:J:1040:HOH:O	2.40	0.54
1:J:59:LEU:O	1:J:62:GLU:HG2	2.08	0.54
1:E:94:ARG:NE	1:E:115:ASP:OD2	2.32	0.54
1:P:95:VAL:HB	1:P:116:ILE:CD1	2.38	0.54
1:F:10:LYS:HE3	3:F:1040:HOH:O	2.08	0.54
1:F:29:LEU:HD12	1:F:100:PRO:HG3	1.90	0.54
1:I:51:ILE:HG12	1:I:90:ILE:HD11	1.88	0.54
1:B:29:LEU:HD13	1:B:100:PRO:HD3	1.90	0.53
1:H:30:VAL:HA	1:H:96:LYS:O	2.08	0.53
1:E:69:ARG:NH2	1:E:78:LEU:HD22	2.23	0.53
1:E:72:LEU:HD21	1:E:99:LYS:HE3	1.90	0.53
1:K:103:ALA:O	1:K:104:LEU:HB2	2.07	0.53
1:B:94:ARG:CG	1:B:94:ARG:NH2	2.64	0.53
1:I:87:PHE:CB	1:I:90:ILE:HD13	2.38	0.53
1:A:102:VAL:HG21	1:A:112:LEU:HD22	1.91	0.53
1:C:120:ARG:HH21	1:C:120:ARG:CG	2.19	0.53
1:C:3:LYS:HE3	1:C:5:ILE:HD11	1.91	0.53
1:G:51:ILE:HD12	1:G:52:SER:N	2.24	0.53
1:M:108:THR:CB	3:M:1043:HOH:O	2.57	0.53
1:H:104:LEU:O	1:H:106:LYS:HD2	2.09	0.53
1:D:5:ILE:HD12	1:D:5:ILE:N	2.24	0.52
1:M:75:VAL:O	1:M:79:ILE:HG12	2.09	0.52
1:P:120:ARG:HA	3:P:1067:HOH:O	2.10	0.52
1:C:59:LEU:C	1:C:59:LEU:HD23	2.29	0.52
1:I:5:ILE:HD12	1:I:5:ILE:N	2.24	0.52
1:K:72:LEU:HD21	1:K:99:LYS:HE3	1.90	0.52
1:I:7:LYS:O	1:L:110:ASP:HB2	2.10	0.52
1:P:18:ILE:HD12	1:P:18:ILE:H	1.75	0.52
1:B:94:ARG:NH2	1:B:94:ARG:HG2	2.23	0.52
1:E:76:ALA:HB1	1:E:116:ILE:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:31:ASP:HB2	1:I:96:LYS:HB2	1.91	0.52
1:A:31:ASP:HB2	1:A:96:LYS:HB2	1.89	0.52
1:A:46:ASN:CG	1:A:48:GLU:HG2	2.30	0.52
1:K:75:VAL:HB	1:K:97:LEU:CD2	2.40	0.52
1:F:105:ILE:HD12	1:G:57:PHE:CE2	2.45	0.52
1:G:30:VAL:HG22	1:G:97:LEU:CD1	2.39	0.52
1:G:48:GLU:HA	3:G:1061:HOH:O	2.09	0.52
1:M:61:LYS:HE3	1:M:65:GLU:OE1	2.10	0.52
1:D:59:LEU:O	1:D:63:ILE:HG12	2.08	0.52
1:K:31:ASP:HB2	1:K:96:LYS:HB2	1.93	0.51
1:D:51:ILE:HD11	1:D:89:GLN:CD	2.31	0.51
1:L:29:LEU:HD13	1:L:100:PRO:CG	2.40	0.51
1:O:3:LYS:HG3	1:O:5:ILE:HD11	1.92	0.51
1:G:4:LEU:HD11	1:G:51:ILE:HG23	1.93	0.51
1:N:72:LEU:HD21	1:N:99:LYS:HE3	1.93	0.51
1:P:18:ILE:HD12	1:P:18:ILE:N	2.26	0.51
1:E:10:LYS:HB3	1:E:27:MET:HE3	1.90	0.51
1:N:103:ALA:O	1:N:104:LEU:HB2	2.11	0.51
1:I:120:ARG:HG3	1:I:120:ARG:NH2	2.25	0.51
1:K:24:LEU:HD11	1:N:103:ALA:HB1	1.93	0.51
1:B:94:ARG:HH22	1:B:96:LYS:CD	2.23	0.51
1:M:59:LEU:HD23	1:M:59:LEU:C	2.31	0.51
1:P:88:HIS:HA	1:P:120:ARG:NH1	2.25	0.51
1:A:84:LEU:O	1:A:120:ARG:NH2	2.45	0.50
1:I:87:PHE:HB2	1:I:90:ILE:HD13	1.93	0.50
1:B:94:ARG:HH21	1:B:94:ARG:HG3	1.75	0.50
1:E:120:ARG:HH21	1:E:120:ARG:HG3	1.76	0.50
1:E:35:TRP:CZ3	1:E:117:PHE:HE1	2.29	0.50
1:M:51:ILE:HG21	1:M:56:ILE:HD11	1.93	0.50
1:B:94:ARG:NH1	1:B:96:LYS:HZ2	2.09	0.50
1:L:59:LEU:C	1:L:59:LEU:HD23	2.32	0.50
1:M:40:LYS:HB3	3:M:1025:HOH:O	2.12	0.50
1:C:74:THR:O	1:C:78:LEU:HD23	2.12	0.50
1:D:18:ILE:HB	1:D:21:GLU:HG3	1.94	0.50
1:E:5:ILE:N	1:E:5:ILE:HD12	2.25	0.50
1:N:51:ILE:HD11	1:N:89:GLN:HG3	1.94	0.50
1:L:39:LYS:O	1:L:43:GLU:HG3	2.11	0.50
1:M:116:ILE:HD13	1:M:116:ILE:N	2.23	0.50
1:L:94:ARG:HG3	1:L:94:ARG:HH11	1.77	0.50
1:B:94:ARG:NH1	1:B:96:LYS:NZ	2.60	0.50
1:C:108:THR:CB	3:C:139:HOH:O	2.57	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:103:ALA:O	1:F:104:LEU:HB2	2.12	0.50
1:M:6:LEU:HG	1:P:112:LEU:HD22	1.94	0.50
1:K:92:ALA:HB2	1:K:119:GLN:HB3	1.95	0.49
1:C:4:LEU:HD22	1:C:36:VAL:HG11	1.94	0.49
1:O:117:PHE:CE2	1:O:119:GLN:HG3	2.48	0.49
1:E:78:LEU:O	1:E:82:LYS:HB2	2.13	0.49
1:J:29:LEU:HD22	3:J:1024:HOH:O	2.13	0.49
1:L:29:LEU:HD22	1:L:100:PRO:HG3	1.95	0.49
1:F:51:ILE:HD11	1:F:89:GLN:CB	2.37	0.49
1:L:29:LEU:HD13	1:L:100:PRO:HG2	1.94	0.49
1:N:46:ASN:OD1	1:N:48:GLU:HB2	2.13	0.49
1:O:35:TRP:CZ3	1:O:94:ARG:HB2	2.48	0.49
1:P:52:SER:HA	2:P:1016:GUN:N3	2.27	0.49
1:A:10:LYS:HE3	3:A:1030:HOH:O	2.13	0.49
1:A:105:ILE:N	1:A:105:ILE:HD12	2.27	0.49
1:G:60:ALA:O	1:G:64:VAL:HG23	2.12	0.49
1:C:31:ASP:HB2	1:C:96:LYS:HB2	1.94	0.49
1:E:76:ALA:HB1	1:E:116:ILE:CD1	2.43	0.49
1:P:51:ILE:HD11	1:P:89:GLN:HB2	1.94	0.49
1:D:33:ASP:HB2	1:D:94:ARG:HB3	1.95	0.49
1:F:18:ILE:HG22	1:F:20:GLU:HG2	1.94	0.49
1:N:31:ASP:HB2	1:N:96:LYS:HB2	1.94	0.49
1:O:6:LEU:HD12	1:O:6:LEU:N	2.28	0.49
1:O:47:LEU:O	1:O:47:LEU:HD22	2.13	0.49
1:C:89:GLN:NE2	1:C:89:GLN:N	2.56	0.48
1:D:46:ASN:CG	1:D:48:GLU:HB2	2.33	0.48
1:H:3:LYS:HG3	1:H:5:ILE:HD11	1.95	0.48
1:C:4:LEU:HD22	1:C:36:VAL:CG1	2.44	0.48
1:E:4:LEU:C	1:E:5:ILE:HD12	2.33	0.48
1:O:51:ILE:HD11	1:O:89:GLN:HB2	1.95	0.48
1:I:51:ILE:HD12	1:I:51:ILE:N	2.27	0.48
1:P:121:ASN:N	1:P:121:ASN:ND2	2.60	0.48
1:O:31:ASP:HB2	1:O:96:LYS:HB2	1.96	0.48
1:J:20:GLU:HB2	1:O:24:LEU:HG	1.96	0.48
1:O:29:LEU:HD21	3:O:1066:HOH:O	2.13	0.48
1:A:51:ILE:N	1:A:51:ILE:HD12	2.29	0.48
1:H:36:VAL:HG23	3:H:1063:HOH:O	2.13	0.48
1:B:110:ASP:O	1:B:111:TYR:HB3	2.14	0.48
1:D:22:ARG:HG3	1:D:22:ARG:HH21	1.79	0.48
1:J:88:HIS:HA	1:J:120:ARG:NH1	2.29	0.48
1:O:34:ALA:HB1	1:O:90:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ILE:O	1:B:22:ARG:HG2	2.14	0.47
1:B:120:ARG:HG3	1:B:120:ARG:NH1	2.28	0.47
1:E:9:LEU:HB2	1:E:30:VAL:HB	1.96	0.47
1:H:51:ILE:HD13	1:H:90:ILE:CG1	2.43	0.47
1:J:51:ILE:HD13	1:J:87:PHE:CD1	2.49	0.47
1:M:120:ARG:HG2	1:M:120:ARG:NH2	2.27	0.47
1:N:101:ASN:HA	3:N:144:HOH:O	2.14	0.47
1:G:30:VAL:HG22	1:G:97:LEU:HD13	1.95	0.47
1:I:115:ASP:HB2	1:J:5:ILE:HD12	1.95	0.47
1:L:22:ARG:HH21	1:L:22:ARG:CB	2.26	0.47
1:J:103:ALA:O	1:J:104:LEU:HB2	2.13	0.47
1:D:3:LYS:HG3	1:D:5:ILE:HD11	1.95	0.47
1:K:69:ARG:HH21	1:K:69:ARG:CG	2.27	0.47
1:L:120:ARG:HG2	1:L:120:ARG:NH2	2.28	0.47
1:C:46:ASN:HD21	1:C:48:GLU:HB2	1.80	0.47
1:D:6:LEU:HD21	1:D:56:ILE:HB	1.95	0.47
1:D:102:VAL:HB	1:D:105:ILE:HD12	1.95	0.47
1:E:6:LEU:HD12	1:E:6:LEU:N	2.30	0.47
1:I:103:ALA:O	1:I:104:LEU:HB2	2.15	0.47
1:L:3:LYS:NZ	1:L:35:TRP:HE1	2.06	0.47
1:N:30:VAL:HG22	1:N:97:LEU:CD1	2.44	0.47
1:G:1:GLY:HA3	3:G:1074:HOH:O	2.15	0.47
1:P:27:MET:HA	1:P:27:MET:CE	2.44	0.47
1:B:94:ARG:NH2	1:B:96:LYS:HZ3	2.13	0.47
1:C:89:GLN:HE21	1:C:89:GLN:N	2.12	0.47
1:G:59:LEU:C	1:G:59:LEU:HD23	2.35	0.47
1:K:47:LEU:HD22	1:K:47:LEU:N	2.30	0.47
1:N:46:ASN:HD22	1:N:47:LEU:N	2.13	0.47
1:N:59:LEU:O	1:N:63:ILE:HG12	2.15	0.47
1:F:32:ILE:CD1	1:F:95:VAL:HG22	2.45	0.46
1:A:45:ASP:OD2	1:D:70:ASN:HB2	2.15	0.46
1:P:120:ARG:C	1:P:121:ASN:HD22	2.18	0.46
1:B:94:ARG:CZ	1:B:96:LYS:NZ	2.78	0.46
1:C:20:GLU:HB2	1:F:24:LEU:HD13	1.97	0.46
1:D:22:ARG:HG3	1:D:22:ARG:NH2	2.30	0.46
1:B:70:ASN:HB2	1:B:71:LEU:HD22	1.98	0.46
1:G:36:VAL:HG12	1:G:89:GLN:O	2.15	0.46
1:L:69:ARG:HH22	1:L:78:LEU:HD11	1.80	0.46
1:F:6:LEU:N	1:F:6:LEU:HD12	2.31	0.46
1:C:75:VAL:HB	1:C:97:LEU:CD2	2.46	0.46
1:D:22:ARG:NE	1:D:68:PRO:HB2	2.17	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4:LEU:CD2	1:J:51:ILE:HG23	2.46	0.46
1:J:63:ILE:HD13	1:J:79:ILE:HA	1.98	0.46
1:N:115:ASP:HB3	1:O:5:ILE:HD11	1.98	0.46
1:P:3:LYS:HG3	1:P:5:ILE:HD11	1.97	0.45
1:D:8:GLY:HA2	1:D:29:LEU:HD11	1.98	0.45
1:M:48:GLU:HG3	3:M:1029:HOH:O	2.16	0.45
1:M:69:ARG:HG2	1:M:74:THR:CG2	2.47	0.45
1:I:52:SER:HA	2:I:1009:GUN:N3	2.31	0.45
1:P:61:LYS:HE2	1:P:65:GLU:OE2	2.17	0.45
1:B:102:VAL:HG12	1:B:105:ILE:HD13	1.98	0.45
1:F:51:ILE:N	1:F:51:ILE:HD12	2.32	0.45
1:I:9:LEU:HB2	1:I:30:VAL:HB	1.99	0.45
1:A:75:VAL:O	1:A:79:ILE:HG13	2.17	0.45
1:L:20:GLU:HG2	1:M:23:THR:OG1	2.17	0.45
1:E:69:ARG:HH21	1:E:69:ARG:HG3	1.81	0.45
1:L:33:ASP:HB2	1:L:94:ARG:HB3	1.98	0.45
1:O:30:VAL:HG22	1:O:97:LEU:HD13	1.99	0.45
1:E:35:TRP:CH2	3:E:164:HOH:O	2.56	0.45
1:G:47:LEU:HD13	1:G:47:LEU:O	2.17	0.45
1:J:104:LEU:O	1:J:106:LYS:CD	2.65	0.45
1:K:69:ARG:HD2	1:K:74:THR:CG2	2.45	0.45
1:L:94:ARG:HG3	1:L:94:ARG:NH1	2.31	0.45
1:M:52:SER:HA	2:P:1013:GUN:N3	2.32	0.45
1:O:29:LEU:HD22	3:O:1041:HOH:O	2.15	0.45
1:G:3:LYS:CE	1:G:5:ILE:HD11	2.47	0.45
1:N:62:GLU:HG2	3:N:157:HOH:O	2.17	0.45
1:F:35:TRP:CZ3	1:F:94:ARG:HB2	2.52	0.45
1:O:7:LYS:HD3	1:O:8:GLY:N	2.31	0.45
1:O:89:GLN:HB2	3:O:1039:HOH:O	2.17	0.45
1:M:72:LEU:HD11	1:M:99:LYS:HG3	1.98	0.44
1:G:7:LYS:HG3	1:G:8:GLY:N	2.30	0.44
1:K:69:ARG:HH21	1:K:69:ARG:HG3	1.81	0.44
1:M:59:LEU:HD23	1:M:59:LEU:O	2.18	0.44
1:N:75:VAL:HA	1:N:78:LEU:HD12	2.00	0.44
1:C:25:GLY:O	1:C:26:GLN:HB3	2.16	0.44
1:D:30:VAL:HG22	1:D:97:LEU:CD1	2.48	0.44
1:F:75:VAL:HB	1:F:97:LEU:CD1	2.48	0.44
1:M:6:LEU:HB2	1:M:32:ILE:HB	1.99	0.44
1:D:103:ALA:O	1:D:104:LEU:HB2	2.17	0.44
1:F:119:GLN:HE21	1:F:119:GLN:HB3	1.68	0.44
1:N:88:HIS:HA	1:N:120:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:29:LEU:HD23	1:O:30:VAL:N	2.32	0.44
1:E:31:ASP:HB2	1:E:96:LYS:HB2	1.99	0.44
1:E:36:VAL:HG11	1:E:51:ILE:HD11	2.00	0.44
1:G:14:PHE:O	1:G:22:ARG:HG3	2.17	0.44
1:H:29:LEU:CD1	1:H:100:PRO:HG3	2.41	0.44
1:I:51:ILE:HD11	1:I:89:GLN:CB	2.45	0.44
1:A:74:THR:O	1:A:78:LEU:CD1	2.62	0.44
1:F:31:ASP:O	1:F:32:ILE:HD13	2.18	0.44
1:M:11:PHE:HB2	1:M:64:VAL:HG11	2.00	0.44
1:M:76:ALA:HB1	1:M:116:ILE:CD1	2.47	0.44
1:N:108:THR:HA	3:N:160:HOH:O	2.16	0.44
1:O:35:TRP:HZ3	1:O:94:ARG:HB2	1.82	0.44
1:A:34:ALA:HB1	1:A:90:ILE:HD12	1.99	0.44
1:C:51:ILE:CD1	1:C:90:ILE:HG13	2.48	0.43
1:D:6:LEU:N	1:D:6:LEU:HD12	2.32	0.43
1:D:10:LYS:HE3	1:D:27:MET:HG3	2.00	0.43
1:D:51:ILE:HD12	1:D:87:PHE:CD1	2.53	0.43
1:F:61:LYS:O	1:F:65:GLU:HG3	2.17	0.43
1:L:60:ALA:O	1:L:64:VAL:HG23	2.18	0.43
1:M:29:LEU:CD1	1:M:100:PRO:HG3	2.48	0.43
1:N:102:VAL:CG1	1:N:105:ILE:HD13	2.47	0.43
1:B:88:HIS:HA	1:B:120:ARG:NH2	2.33	0.43
1:D:28:PHE:HE2	1:D:99:LYS:HE2	1.82	0.43
1:E:78:LEU:HD12	1:E:78:LEU:HA	1.91	0.43
1:F:47:LEU:HD13	1:F:47:LEU:O	2.17	0.43
1:O:115:ASP:HB3	1:P:5:ILE:HD11	1.99	0.43
1:A:96:LYS:NZ	3:A:1039:HOH:O	2.49	0.43
2:I:1009:GUN:H8	3:I:1049:HOH:O	2.18	0.43
1:L:94:ARG:NH2	1:L:115:ASP:OD1	2.51	0.43
1:L:94:ARG:HE	1:L:96:LYS:NZ	2.16	0.43
1:P:18:ILE:O	1:P:21:GLU:HB2	2.18	0.43
1:E:69:ARG:NH2	1:E:78:LEU:CD2	2.76	0.43
1:A:40:LYS:HD2	1:A:49:ASP:CG	2.39	0.43
1:K:20:GLU:HB3	1:N:24:LEU:HD22	2.00	0.43
1:M:116:ILE:HG22	1:N:2:ASP:HB3	2.01	0.43
1:N:106:LYS:HB3	1:N:106:LYS:HE2	1.85	0.43
1:B:71:LEU:HD23	1:C:45:ASP:HA	1.99	0.43
1:F:32:ILE:HD11	1:F:95:VAL:HG13	2.00	0.43
1:L:24:LEU:HD21	1:M:18:ILE:HG21	2.00	0.43
1:A:18:ILE:HD13	1:A:21:GLU:OE2	2.19	0.43
1:I:115:ASP:HB2	1:J:5:ILE:HD11	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:30:VAL:HG22	1:M:97:LEU:CD1	2.49	0.43
1:K:18:ILE:HB	1:K:21:GLU:HG3	2.01	0.43
1:C:120:ARG:HG2	1:C:120:ARG:NH2	2.22	0.43
1:G:22:ARG:CG	1:G:68:PRO:HB2	2.47	0.43
1:E:7:LYS:HD2	1:E:31:ASP:OD1	2.19	0.42
1:E:47:LEU:CD1	1:H:71:LEU:HD21	2.47	0.42
1:F:52:SER:HA	2:F:1006:GUN:N3	2.35	0.42
1:M:30:VAL:HG22	1:M:97:LEU:HD13	2.00	0.42
1:L:103:ALA:O	1:L:104:LEU:HB2	2.19	0.42
1:B:35:TRP:CZ3	1:B:94:ARG:HB2	2.53	0.42
1:B:112:LEU:HD22	1:C:6:LEU:HG	2.00	0.42
1:J:51:ILE:HD12	1:J:51:ILE:C	2.39	0.42
1:B:33:ASP:HB2	1:B:94:ARG:HB3	2.02	0.42
1:C:6:LEU:HB2	1:C:32:ILE:HB	2.00	0.42
1:N:18:ILE:HB	1:N:21:GLU:CG	2.48	0.42
1:P:50:THR:OG1	1:P:51:ILE:N	2.53	0.42
1:G:104:LEU:N	1:G:104:LEU:HD22	2.35	0.42
1:P:47:LEU:HD13	1:P:47:LEU:O	2.19	0.42
1:C:30:VAL:HG22	1:C:97:LEU:HD13	2.02	0.42
1:G:103:ALA:O	1:G:104:LEU:HB2	2.20	0.42
1:M:61:LYS:O	1:M:65:GLU:HG3	2.20	0.42
1:A:4:LEU:C	1:A:5:ILE:HD12	2.39	0.42
1:I:24:LEU:HD11	1:P:103:ALA:HB1	2.00	0.42
1:J:20:GLU:CB	1:O:24:LEU:HG	2.50	0.42
1:K:3:LYS:HE3	1:K:35:TRP:CZ2	2.55	0.42
1:K:59:LEU:O	1:K:63:ILE:HG12	2.20	0.42
1:M:78:LEU:O	1:M:82:LYS:HB2	2.20	0.42
1:M:84:LEU:HD12	1:M:84:LEU:HA	1.83	0.42
1:P:27:MET:HA	1:P:27:MET:HE3	2.01	0.42
1:E:120:ARG:HG3	1:E:120:ARG:NH2	2.34	0.42
1:K:4:LEU:HD13	1:K:38:LEU:HD21	2.01	0.42
1:M:14:PHE:CD1	1:M:14:PHE:N	2.87	0.42
1:D:28:PHE:CE2	1:D:99:LYS:HE2	2.55	0.42
2:G:1008:GUN:N3	1:H:52:SER:HA	2.35	0.42
1:L:116:ILE:HD12	1:L:116:ILE:C	2.41	0.42
1:N:101:ASN:ND2	3:N:136:HOH:O	2.45	0.42
1:O:22:ARG:NH2	1:O:22:ARG:CG	2.83	0.42
1:F:21:GLU:OE2	1:F:99:LYS:NZ	2.53	0.41
1:L:52:SER:HA	2:L:1012:GUN:N3	2.35	0.41
1:M:63:ILE:CD1	1:M:79:ILE:HD13	2.47	0.41
1:B:50:THR:OG1	1:B:51:ILE:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:LEU:HD11	1:D:99:LYS:HG3	2.01	0.41
1:H:92:ALA:CB	1:H:119:GLN:HG2	2.49	0.41
1:J:4:LEU:HD13	1:J:38:LEU:HD21	2.02	0.41
1:M:92:ALA:HB2	1:M:119:GLN:HB3	2.02	0.41
1:C:120:ARG:CG	1:C:120:ARG:NH2	2.80	0.41
1:E:97:LEU:C	1:E:97:LEU:HD13	2.41	0.41
1:G:120:ARG:HH21	1:G:120:ARG:HG3	1.85	0.41
1:L:84:LEU:HD22	1:L:120:ARG:NH2	2.35	0.41
1:B:6:LEU:HD12	1:B:6:LEU:N	2.35	0.41
1:D:59:LEU:HD11	1:D:86:LYS:HD3	2.02	0.41
1:G:89:GLN:CD	1:G:89:GLN:N	2.61	0.41
1:H:3:LYS:HG3	1:H:5:ILE:CD1	2.51	0.41
1:I:104:LEU:N	1:I:104:LEU:HD22	2.35	0.41
1:K:78:LEU:HD12	1:K:78:LEU:HA	1.91	0.41
1:E:8:GLY:O	1:H:109:ILE:HA	2.21	0.41
1:K:75:VAL:O	1:K:79:ILE:HG13	2.21	0.41
1:L:75:VAL:HB	1:L:97:LEU:CD2	2.50	0.41
1:B:71:LEU:HD22	1:B:71:LEU:N	2.36	0.41
1:B:75:VAL:HB	1:B:97:LEU:CD1	2.51	0.41
1:C:89:GLN:H	1:C:89:GLN:CD	2.24	0.41
1:E:69:ARG:HD3	1:E:69:ARG:HA	1.90	0.41
1:J:109:ILE:HA	1:K:8:GLY:O	2.21	0.41
1:M:32:ILE:CD1	1:M:95:VAL:HG22	2.50	0.41
1:O:4:LEU:HD23	1:O:4:LEU:HA	1.88	0.41
1:B:35:TRP:HZ3	1:B:94:ARG:HB2	1.84	0.41
2:B:1003:GUN:N3	1:C:52:SER:HA	2.35	0.41
1:C:87:PHE:CB	1:C:89:GLN:HE22	2.23	0.41
1:M:121:ASN:HD22	1:M:121:ASN:HA	1.63	0.41
1:N:120:ARG:NH2	1:N:120:ARG:CB	2.83	0.41
1:B:3:LYS:HG3	1:B:5:ILE:HD11	2.03	0.41
1:E:5:ILE:HG23	3:E:137:HOH:O	2.20	0.41
1:G:51:ILE:HD13	1:G:87:PHE:CD1	2.56	0.41
1:K:11:PHE:HB2	1:K:64:VAL:HG11	2.02	0.41
1:P:12:TYR:CD2	1:P:27:MET:HE3	2.56	0.41
1:L:10:LYS:HG2	1:L:29:LEU:HD12	2.03	0.41
1:O:56:ILE:HD13	1:O:87:PHE:CE2	2.55	0.41
1:D:94:ARG:HE	1:D:96:LYS:HE2	1.85	0.40
1:F:33:ASP:HB2	1:F:94:ARG:HB3	2.04	0.40
1:G:31:ASP:HB2	1:G:96:LYS:HB2	2.01	0.40
1:P:75:VAL:HB	1:P:97:LEU:CD1	2.51	0.40
1:C:46:ASN:ND2	1:C:48:GLU:HB2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:VAL:HG22	1:D:97:LEU:HD12	2.03	0.40
1:I:87:PHE:HB3	1:I:90:ILE:HD13	2.04	0.40
1:J:29:LEU:C	1:J:29:LEU:HD23	2.41	0.40
1:J:20:GLU:HB2	1:O:24:LEU:CG	2.52	0.40
3:J:1026:HOH:O	1:K:39:LYS:HD2	2.21	0.40
1:M:32:ILE:HD11	1:M:79:ILE:HG21	2.03	0.40
1:A:84:LEU:O	1:A:120:ARG:CZ	2.70	0.40
1:M:20:GLU:OE2	1:M:20:GLU:N	2.53	0.40
1:O:30:VAL:HG22	1:O:97:LEU:HD12	2.03	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	118/146 (81%)	115 (98%)	3 (2%)	0	100	100
1	B	119/146 (82%)	116 (98%)	3 (2%)	0	100	100
1	C	120/146 (82%)	116 (97%)	4 (3%)	0	100	100
1	D	118/146 (81%)	113 (96%)	5 (4%)	0	100	100
1	E	118/146 (81%)	116 (98%)	2 (2%)	0	100	100
1	F	119/146 (82%)	114 (96%)	5 (4%)	0	100	100
1	G	119/146 (82%)	115 (97%)	4 (3%)	0	100	100
1	H	120/146 (82%)	117 (98%)	3 (2%)	0	100	100
1	I	119/146 (82%)	118 (99%)	1 (1%)	0	100	100
1	J	121/146 (83%)	119 (98%)	2 (2%)	0	100	100
1	K	118/146 (81%)	114 (97%)	4 (3%)	0	100	100
1	L	120/146 (82%)	116 (97%)	4 (3%)	0	100	100
1	M	121/146 (83%)	115 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	119/146 (82%)	114 (96%)	5 (4%)	0	100	100
1	O	118/146 (81%)	117 (99%)	1 (1%)	0	100	100
1	P	120/146 (82%)	116 (97%)	4 (3%)	0	100	100
All	All	1907/2336 (82%)	1851 (97%)	56 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	103/127 (81%)	96 (93%)	7 (7%)	16	17
1	B	104/127 (82%)	99 (95%)	5 (5%)	25	32
1	C	105/127 (83%)	102 (97%)	3 (3%)	42	54
1	D	103/127 (81%)	98 (95%)	5 (5%)	25	31
1	E	103/127 (81%)	95 (92%)	8 (8%)	12	13
1	F	104/127 (82%)	99 (95%)	5 (5%)	25	32
1	G	104/127 (82%)	98 (94%)	6 (6%)	20	23
1	H	105/127 (83%)	99 (94%)	6 (6%)	20	24
1	I	104/127 (82%)	102 (98%)	2 (2%)	57	71
1	J	106/127 (84%)	99 (93%)	7 (7%)	16	19
1	K	103/127 (81%)	96 (93%)	7 (7%)	16	17
1	L	105/127 (83%)	98 (93%)	7 (7%)	16	18
1	M	106/127 (84%)	101 (95%)	5 (5%)	26	33
1	N	104/127 (82%)	97 (93%)	7 (7%)	16	18
1	O	103/127 (81%)	97 (94%)	6 (6%)	20	23
1	P	105/127 (83%)	96 (91%)	9 (9%)	10	10
All	All	1667/2032 (82%)	1572 (94%)	95 (6%)	20	24

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	A	53	TYR
1	A	59	LEU
1	A	69	ARG
1	A	71	LEU
1	A	97	LEU
1	A	106	LYS
1	B	30	VAL
1	B	53	TYR
1	B	94	ARG
1	B	97	LEU
1	B	121	ASN
1	C	4	LEU
1	C	53	TYR
1	C	89	GLN
1	D	47	LEU
1	D	53	TYR
1	D	85	GLU
1	D	88	HIS
1	D	89	GLN
1	E	35	TRP
1	E	51	ILE
1	E	53	TYR
1	E	89	GLN
1	E	94	ARG
1	E	109	ILE
1	E	110	ASP
1	E	116	ILE
1	F	4	LEU
1	F	53	TYR
1	F	97	LEU
1	F	109	ILE
1	F	119	GLN
1	G	7	LYS
1	G	36	VAL
1	G	51	ILE
1	G	78	LEU
1	G	89	GLN
1	G	106	LYS
1	H	53	TYR
1	H	67	SER
1	H	69	ARG

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Mol	Chain	Res	Type
1	H	88	HIS
1	H	97	LEU
1	H	109	ILE
1	I	53	TYR
1	I	90	ILE
1	J	4	LEU
1	J	47	LEU
1	J	51	ILE
1	J	53	TYR
1	J	88	HIS
1	J	98	SER
1	J	109	ILE
1	K	3	LYS
1	K	4	LEU
1	K	53	TYR
1	K	69	ARG
1	K	78	LEU
1	K	109	ILE
1	K	119	GLN
1	L	22	ARG
1	L	46	ASN
1	L	47	LEU
1	L	53	TYR
1	L	110	ASP
1	L	119	GLN
1	L	120	ARG
1	M	47	LEU
1	M	53	TYR
1	M	78	LEU
1	M	84	LEU
1	M	116	ILE
1	N	24	LEU
1	N	46	ASN
1	N	47	LEU
1	N	53	TYR
1	N	69	ARG
1	N	84	LEU
1	N	112	LEU
1	O	22	ARG
1	O	47	LEU
1	O	48	GLU
1	O	53	TYR

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Mol	Chain	Res	Type
1	O	59	LEU
1	O	82	LYS
1	P	0	LEU
1	P	9	LEU
1	P	27	MET
1	P	53	TYR
1	P	94	ARG
1	P	97	LEU
1	P	98	SER
1	P	116	ILE
1	P	120	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	26	GLN
1	C	89	GLN
1	C	121	ASN
1	D	70	ASN
1	D	89	GLN
1	E	46	ASN
1	E	89	GLN
1	F	119	GLN
1	G	91	ASN
1	G	101	ASN
1	H	121	ASN
1	I	119	GLN
1	I	121	ASN
1	J	88	HIS
1	J	91	ASN
1	J	101	ASN
1	J	121	ASN
1	K	119	GLN
1	L	46	ASN
1	L	88	HIS
1	L	89	GLN
1	M	121	ASN
1	N	46	ASN
1	N	121	ASN
1	O	91	ASN
1	P	119	GLN
1	P	121	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

16 ligands 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	$\#\|Z\| > 2$
2	GUN	B	1003	-	7,12,12	0.96	0	8,17,17	2.26	2 (25%)
2	GUN	A	1001	-	7,12,12	0.87	0	8,17,17	2.31	2 (25%)
2	GUN	J	1011	-	7,12,12	0.96	0	8,17,17	2.27	2 (25%)
2	GUN	P	1013	-	7,12,12	0.92	0	8,17,17	2.20	2 (25%)
2	GUN	G	1007	-	7,12,12	0.86	0	8,17,17	2.29	2 (25%)
2	GUN	O	1015	-	7,12,12	0.95	0	8,17,17	2.33	2 (25%)
2	GUN	B	1002	-	7,12,12	1.04	0	8,17,17	2.15	2 (25%)
2	GUN	D	1004	-	7,12,12	0.88	0	8,17,17	2.23	2 (25%)
2	GUN	L	1012	-	7,12,12	0.98	0	8,17,17	2.33	2 (25%)
2	GUN	I	1009	-	7,12,12	0.90	0	8,17,17	2.22	2 (25%)
2	GUN	M	1014	-	7,12,12	0.97	0	8,17,17	2.17	2 (25%)
2	GUN	J	1010	-	7,12,12	0.90	0	8,17,17	2.23	2 (25%)
2	GUN	H	1005	-	7,12,12	0.96	0	8,17,17	2.31	2 (25%)
2	GUN	G	1008	-	7,12,12	0.95	0	8,17,17	2.32	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GUN	P	1016	-	7,12,12	1.00	0	8,17,17	2.23	2 (25%)
2	GUN	F	1006	-	7,12,12	1.00	0	8,17,17	2.25	2 (25%)

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
2	GUN	B	1003	-	-	-	0/2/2/2
2	GUN	A	1001	-	-	-	0/2/2/2
2	GUN	J	1011	-	-	-	0/2/2/2
2	GUN	P	1013	-	-	-	0/2/2/2
2	GUN	G	1007	-	-	-	0/2/2/2
2	GUN	O	1015	-	-	-	0/2/2/2
2	GUN	B	1002	-	-	-	0/2/2/2
2	GUN	D	1004	-	-	-	0/2/2/2
2	GUN	L	1012	-	-	-	0/2/2/2
2	GUN	I	1009	-	-	-	0/2/2/2
2	GUN	M	1014	-	-	-	0/2/2/2
2	GUN	J	1010	-	-	-	0/2/2/2
2	GUN	H	1005	-	-	-	0/2/2/2
2	GUN	G	1008	-	-	-	0/2/2/2
2	GUN	P	1016	-	-	-	0/2/2/2
2	GUN	F	1006	-	-	-	0/2/2/2

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	GUN	C8-N7-C5	4.77	112.08	102.99
2	G	1008	GUN	C8-N7-C5	4.64	111.83	102.99
2	L	1012	GUN	C8-N7-C5	4.64	111.83	102.99
2	J	1010	GUN	C8-N7-C5	4.64	111.82	102.99
2	P	1016	GUN	C8-N7-C5	4.63	111.81	102.99
2	O	1015	GUN	C8-N7-C5	4.63	111.81	102.99
2	H	1005	GUN	C8-N7-C5	4.62	111.80	102.99
2	J	1011	GUN	C8-N7-C5	4.60	111.75	102.99
2	D	1004	GUN	C8-N7-C5	4.60	111.75	102.99
2	P	1013	GUN	C8-N7-C5	4.59	111.73	102.99
2	M	1014	GUN	C8-N7-C5	4.58	111.71	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1006	GUN	C8-N7-C5	4.52	111.60	102.99
2	B	1003	GUN	C8-N7-C5	4.51	111.58	102.99
2	I	1009	GUN	C8-N7-C5	4.48	111.52	102.99
2	G	1007	GUN	C8-N7-C5	4.44	111.45	102.99
2	B	1002	GUN	C8-N7-C5	4.41	111.40	102.99
2	L	1012	GUN	N2-C2-N1	2.94	122.98	116.71
2	B	1003	GUN	N2-C2-N1	2.93	122.95	116.71
2	O	1015	GUN	N2-C2-N1	2.89	122.86	116.71
2	G	1007	GUN	N2-C2-N1	2.86	122.81	116.71
2	H	1005	GUN	N2-C2-N1	2.81	122.70	116.71
2	F	1006	GUN	N2-C2-N1	2.80	122.68	116.71
2	I	1009	GUN	N2-C2-N1	2.80	122.68	116.71
2	J	1011	GUN	N2-C2-N1	2.80	122.67	116.71
2	P	1016	GUN	N2-C2-N1	2.77	122.61	116.71
2	A	1001	GUN	N2-C2-N1	2.75	122.57	116.71
2	B	1002	GUN	N2-C2-N1	2.69	122.43	116.71
2	G	1008	GUN	N2-C2-N1	2.63	122.32	116.71
2	P	1013	GUN	N2-C2-N1	2.63	122.31	116.71
2	J	1010	GUN	N2-C2-N1	2.60	122.25	116.71
2	D	1004	GUN	N2-C2-N1	2.60	122.24	116.71
2	M	1014	GUN	N2-C2-N1	2.46	121.94	116.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1003	GUN	1	0
2	P	1013	GUN	1	0
2	L	1012	GUN	1	0
2	I	1009	GUN	2	0
2	G	1008	GUN	1	0
2	P	1016	GUN	1	0
2	F	1006	GUN	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	120/146 (82%)	-0.62	0	100	100	11, 19, 33, 40	1 (0%)
1	B	121/146 (82%)	-0.61	0	100	100	12, 20, 33, 55	0
1	C	122/146 (83%)	-0.45	0	100	100	13, 23, 37, 59	1 (0%)
1	D	120/146 (82%)	-0.49	0	100	100	12, 21, 37, 49	0
1	E	120/146 (82%)	-0.53	0	100	100	12, 20, 32, 42	0
1	F	121/146 (82%)	-0.57	0	100	100	9, 20, 35, 46	0
1	G	121/146 (82%)	-0.63	0	100	100	11, 19, 32, 57	1 (0%)
1	H	122/146 (83%)	-0.61	0	100	100	10, 19, 34, 40	0
1	I	121/146 (82%)	-0.62	0	100	100	11, 19, 30, 52	1 (0%)
1	J	123/146 (84%)	-0.60	0	100	100	12, 19, 35, 46	0
1	K	120/146 (82%)	-0.54	0	100	100	13, 21, 31, 45	0
1	L	122/146 (83%)	-0.49	1 (0%)	86	85	10, 21, 36, 66	0
1	M	123/146 (84%)	-0.40	2 (1%)	72	70	15, 23, 40, 68	1 (0%)
1	N	121/146 (82%)	-0.48	0	100	100	13, 21, 37, 60	0
1	O	120/146 (82%)	-0.64	0	100	100	11, 20, 33, 43	0
1	P	122/146 (83%)	-0.56	0	100	100	12, 20, 33, 56	0
All	All	1939/2336 (83%)	-0.55	3 (0%)	95	94	9, 20, 36, 68	5 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	121	ASN	2.7
1	M	35	TRP	2.2
1	M	123	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GUN	I	1009	11/11	0.94	0.10	16,20,22,26	0
2	GUN	P	1013	11/11	0.94	0.11	18,23,26,28	0
2	GUN	A	1001	11/11	0.95	0.10	18,21,25,25	0
2	GUN	J	1011	11/11	0.95	0.12	24,27,32,34	0
2	GUN	B	1003	11/11	0.95	0.10	16,23,26,28	0
2	GUN	H	1005	11/11	0.96	0.09	21,23,25,25	0
2	GUN	B	1002	11/11	0.96	0.10	16,17,23,26	0
2	GUN	D	1004	11/11	0.96	0.09	16,20,26,27	0
2	GUN	M	1014	11/11	0.96	0.10	13,19,26,27	0
2	GUN	O	1015	11/11	0.96	0.09	13,16,18,21	0
2	GUN	F	1006	11/11	0.96	0.10	12,16,18,22	0
2	GUN	L	1012	11/11	0.97	0.09	15,18,22,23	0
2	GUN	G	1008	11/11	0.97	0.10	8,10,13,14	0
2	GUN	P	1016	11/11	0.97	0.09	15,17,22,24	0
2	GUN	G	1007	11/11	0.98	0.09	10,14,17,20	0
2	GUN	J	1010	11/11	0.98	0.06	5,14,19,20	0

6.5 Other polymers (i)

There are no such residues in this entry.