Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 02:23 AM GMT

PDB ID	:	2GV9
Title	:	Crystal structure of the Herpes Simplex virus type 1 DNA polymerase
Authors	:	Liu, S.
Deposited on	:	2006-05-02
Resolution	:	2.68 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

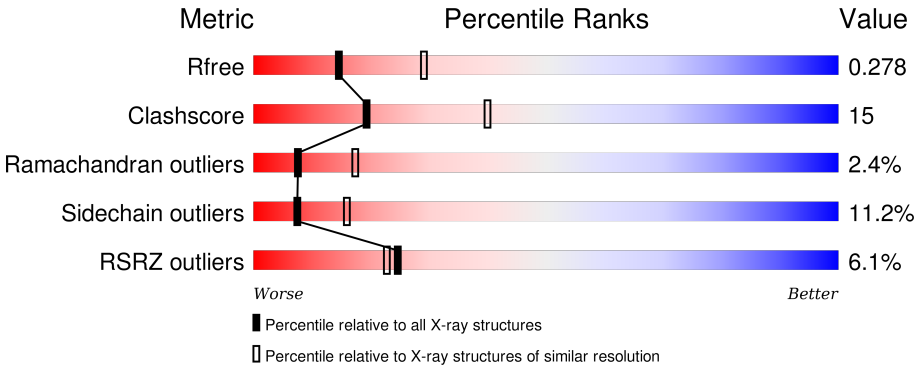
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.68 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}	91344	2780 (2.70-2.66)
Clashscore	102246	3138 (2.70-2.66)
Ramachandran outliers	100387	3089 (2.70-2.66)
Sidechain outliers	100360	3089 (2.70-2.66)
RSRZ outliers	91569	2789 (2.70-2.66)

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 <=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	1193	7%, 52%, 25%, 5%, 18%
1	B	1193	3%, 61%, 21%, 5%, 13%

2 Entry composition

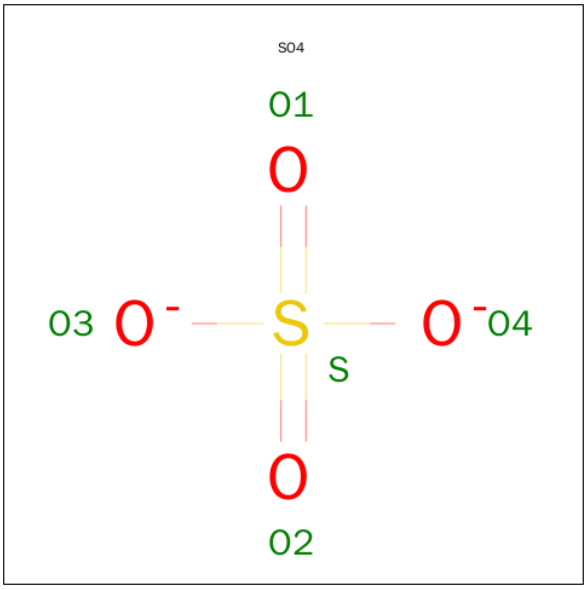
There are 5 unique types of molecules in this entry. The entry contains 16007 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	981	Total	C	N	O	S	0	0	0
			7725	4965	1329	1392	39			
1	B	1035	Total	C	N	O	S	0	0	0
			8180	5247	1422	1471	40			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

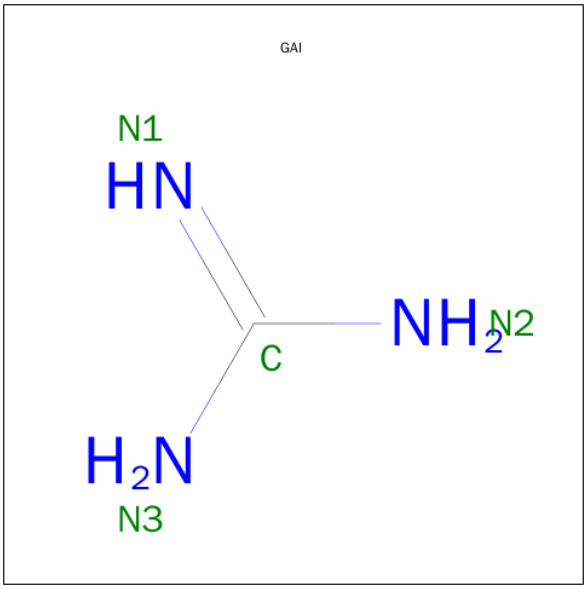


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	O	S		0	0
			5	4	1			
2	B	1	Total	O	S		0	0
			5	4	1			

- Molecule 3 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Hg 1 1	0	0

- Molecule 4 is GUANIDINE (three-letter code: GAI) (formula: CH_5N_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N 4 1 3	0	0

- Molecule 5 is water.

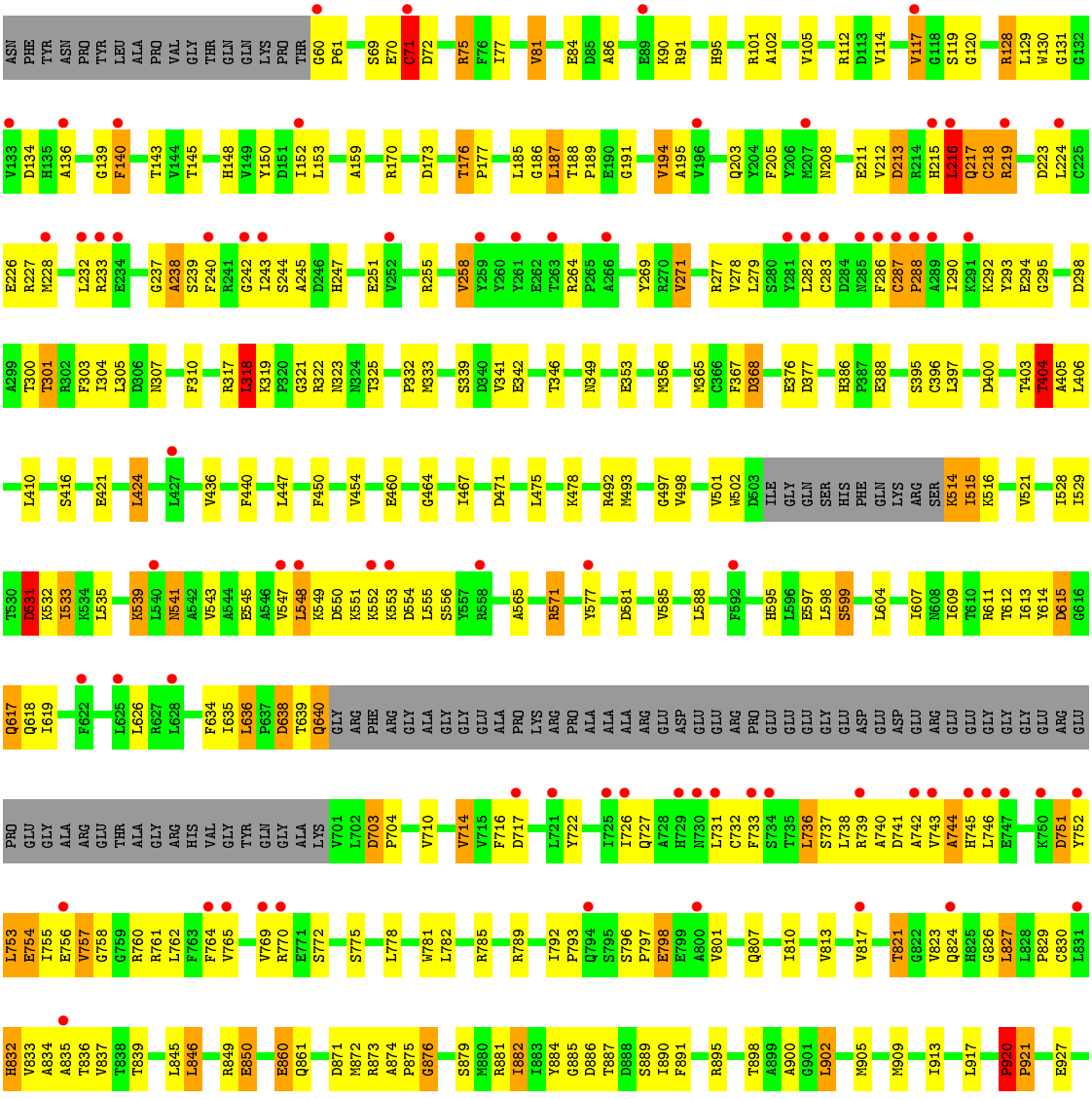
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	33	Total O 33 33	0	0
5	B	54	Total O 54 54	0	0

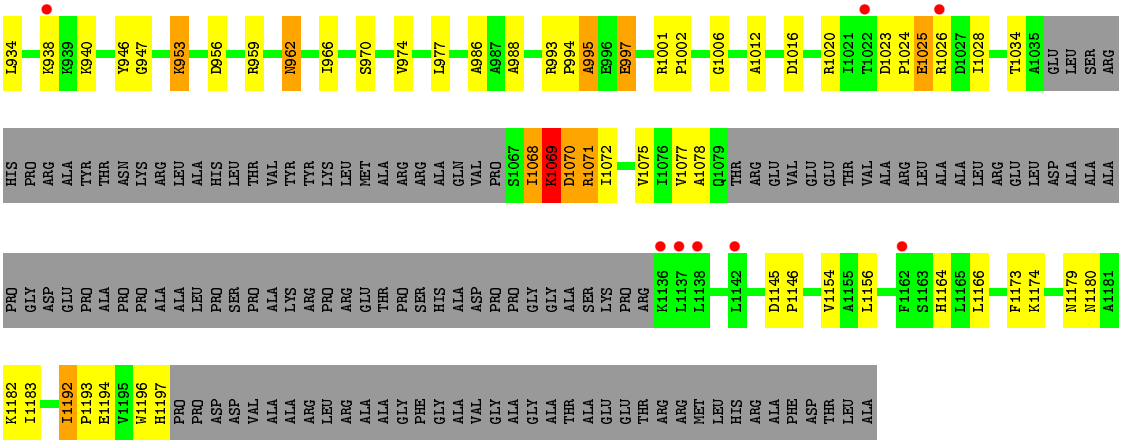
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: DNA polymerase

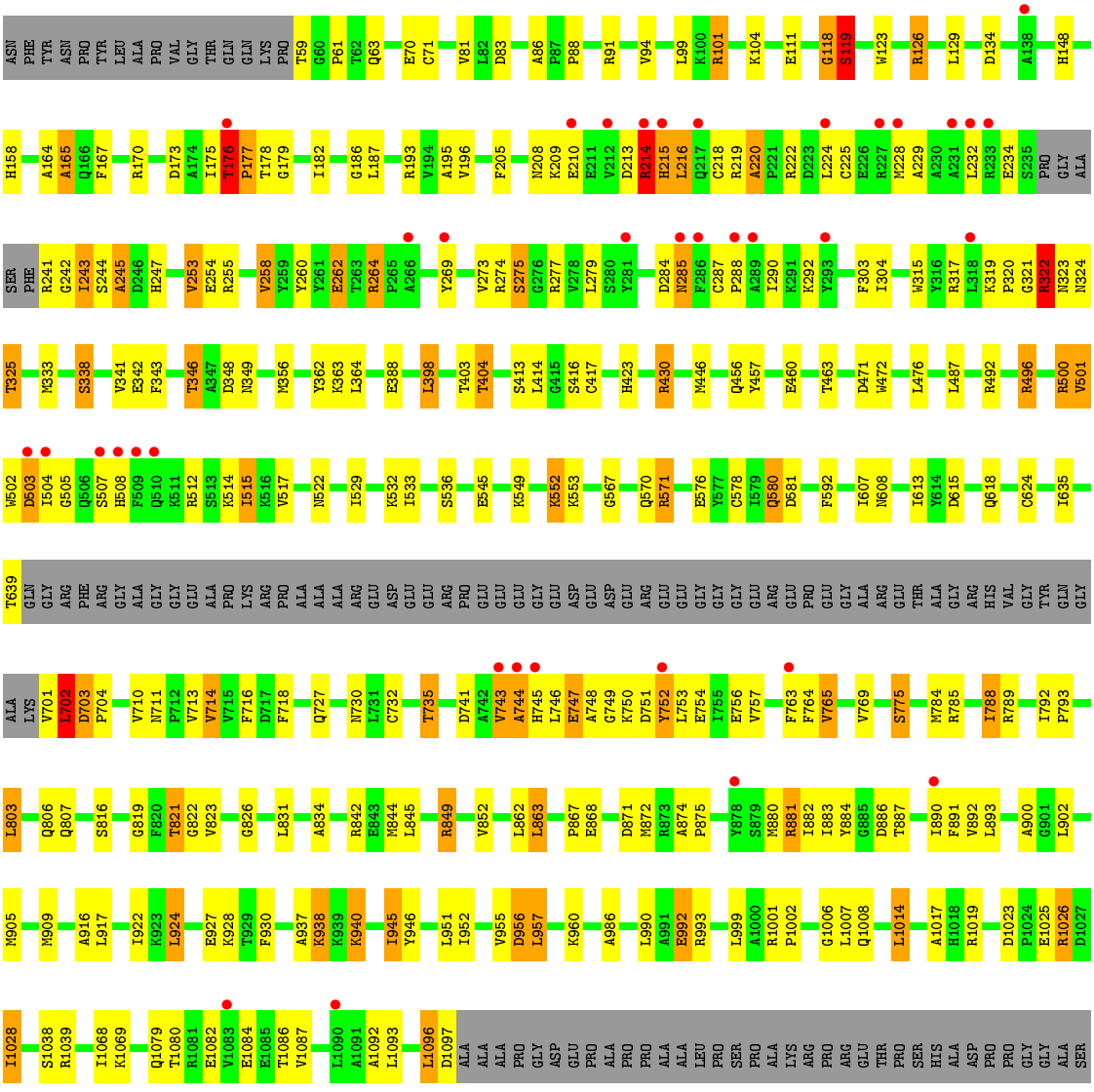
Chain A:

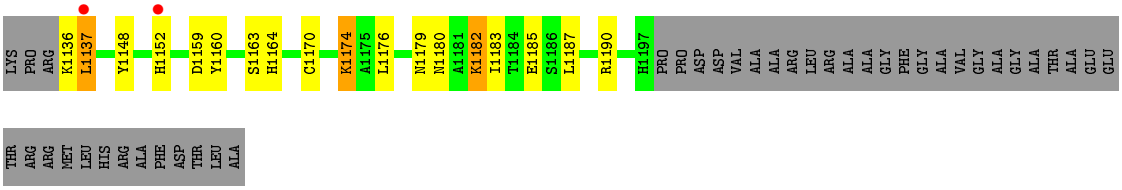




- Molecule 1: DNA polymerase

Chain B:




LYS PRO ARG K1136 L1137 Y1148 H1152 D1159 Y1160 S1163 H1164 C1170 K1174 A1175 L1176 N1179 N1180 A1181 K1182 I1183 T1184 E1185 S1186 L1187 R1190 H1197 PRO PRO ASP ASP VAL ALA ALA ARG LEU ARG ALA ALA GLY PHE GLY ALA VAL GLY ALA GLY ALA THR ALA GLU GLU
THR ARG ARG MET LEU HIS ARG ALA PHE ASP THR LEU ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	103.92Å 125.55Å 220.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.30 – 2.68 48.71 – 2.68	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.30-2.68) 98.9 (48.71-2.68)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.222 , 0.281 0.221 , 0.278	Depositor DCC
R_{free} test set	4067 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	67.5	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 63.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 81223 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16007	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: SO4, GAI, HG

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	0.81	4/7908 (0.1%)	0.89	16/10727 (0.1%)
1	B	0.90	8/8371 (0.1%)	0.91	13/11352 (0.1%)
All	All	0.86	12/16279 (0.1%)	0.90	29/22079 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	1
All	All	0	8

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	CYS	CB-SG	15.93	2.09	1.82
1	B	262	GLU	CD-OE2	8.40	1.34	1.25
1	A	850	GLU	CG-CD	6.78	1.62	1.51
1	B	1170	CYS	CB-SG	-6.35	1.71	1.82
1	B	578	CYS	CB-SG	-5.58	1.72	1.81
1	B	417	CYS	CB-SG	-5.38	1.73	1.81
1	B	624	CYS	CB-SG	-5.33	1.73	1.81
1	B	992	GLU	CG-CD	5.31	1.59	1.51
1	A	368	ASP	CB-CG	5.28	1.62	1.51
1	B	71	CYS	CB-SG	-5.18	1.73	1.81
1	B	262	GLU	CD-OE1	5.12	1.31	1.25
1	A	860	GLU	CG-CD	5.05	1.59	1.51

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	920	PRO	C-N-CD	-16.53	84.23	120.60
1	A	920	PRO	C-N-CA	9.82	163.25	122.00
1	A	75	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	B	126	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	A	187	LEU	CA-CB-CG	7.23	131.93	115.30
1	B	322	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	A	176	THR	C-N-CD	6.78	142.63	128.40
1	A	318	LEU	CA-CB-CG	6.72	130.77	115.30
1	B	176	THR	C-N-CD	6.62	142.30	128.40
1	A	75	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	B	496	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	A	921	PRO	CA-N-CD	-6.44	102.48	111.50
1	B	492	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	B	126	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	B	571	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	A	277	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	B	187	LEU	CA-CB-CG	5.99	129.07	115.30
1	A	1068	ILE	CB-CA-C	-5.78	100.03	111.60
1	A	571	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	B	118	GLY	N-CA-C	-5.62	99.05	113.10
1	A	571	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	B	218	CYS	N-CA-C	5.29	125.28	111.00
1	A	845	LEU	CA-CB-CG	5.27	127.43	115.30
1	B	258	VAL	CB-CA-C	-5.18	101.57	111.40
1	A	638	ASP	CB-CG-OD2	5.16	122.95	118.30
1	A	173	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	A	71	CYS	N-CA-CB	5.14	119.85	110.60
1	B	1190	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	B	388	GLU	CB-CA-C	-5.01	100.38	110.40

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1026	ARG	Peptide
1	A	216	LEU	Peptide
1	A	514	LYS	Peptide
1	A	703	ASP	Peptide
1	A	744	ALA	Peptide
1	A	920	PRO	Peptide
1	A	927	GLU	Peptide
1	B	214	ARG	Peptide

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	7725	0	7706	262	0
1	B	8180	0	8181	220	0
2	B	10	0	0	0	0
3	B	1	0	0	0	0
4	B	4	0	4	0	0
5	A	33	0	0	4	0
5	B	54	0	0	2	0
All	All	16007	0	15891	479	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 15.

All (479) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:CYS:SG	1:A:71:CYS:CB	2.09	1.41
1:A:501:VAL:HG13	1:A:515:ILE:HG22	1.24	1.16
1:A:898:THR:HG22	1:A:900:ALA:H	1.04	1.09
1:B:501:VAL:HG13	1:B:502:TRP:O	1.51	1.08
1:B:702:LEU:O	1:B:702:LEU:HD23	1.54	1.05
1:A:283:CYS:SG	1:A:292:LYS:NZ	2.29	1.05
1:B:287:CYS:SG	1:B:290:ILE:HD13	1.98	1.03
1:A:882:ILE:HD13	1:A:882:ILE:C	1.83	0.99
1:B:346:THR:HG23	1:B:348:ASP:OD1	1.64	0.97
1:B:730:ASN:O	1:B:735:THR:HG21	1.64	0.95
1:A:905:MET:HG2	1:A:909:MET:CE	1.98	0.93
1:A:741:ASP:O	1:A:743:VAL:HG23	1.69	0.92
1:A:403:THR:O	1:A:404:THR:HB	1.69	0.90
1:A:105:VAL:HG22	1:A:114:VAL:HG22	1.54	0.89
1:A:898:THR:HG22	1:A:900:ALA:N	1.88	0.89
1:A:1034:THR:HG22	1:A:1070:ASP:C	1.95	0.87
1:A:714:VAL:HG22	1:A:902:LEU:HD13	1.57	0.87
1:A:194:VAL:HG13	1:A:341:VAL:HG23	1.57	0.86
1:A:529:ILE:HD11	1:A:588:LEU:HD13	1.58	0.85
1:A:403:THR:HG22	1:A:405:ALA:H	1.40	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:765:VAL:HG13	1:A:769:VAL:HB	1.58	0.85
1:B:403:THR:O	1:B:404:THR:HB	1.77	0.84
1:B:414:LEU:N	1:B:446:MET:HE3	1.94	0.83
1:B:430:ARG:HH11	1:B:430:ARG:HG2	1.46	0.81
1:A:529:ILE:HD13	1:A:543:VAL:HG11	1.63	0.80
1:A:872:MET:SD	1:A:905:MET:HE2	2.21	0.79
1:B:346:THR:CG2	1:B:348:ASP:OD1	2.30	0.79
1:B:264:ARG:HD2	1:B:264:ARG:H	1.47	0.79
1:B:872:MET:SD	1:B:905:MET:HE2	2.23	0.77
1:A:367:PHE:HA	1:A:395:SER:O	1.85	0.77
1:A:753:LEU:HD12	1:A:754:GLU:H	1.50	0.77
1:A:905:MET:HG2	1:A:909:MET:HE3	1.67	0.76
1:B:845:LEU:HD22	1:B:890:ILE:CD1	2.16	0.76
1:B:999:LEU:HD23	1:B:1187:LEU:HD21	1.66	0.76
1:A:882:ILE:O	1:A:882:ILE:HD13	1.85	0.75
1:A:1023:ASP:HB2	1:A:1025:GLU:HG2	1.69	0.75
1:A:541:ASN:HD22	1:A:541:ASN:H	1.34	0.74
1:A:293:TYR:HB3	1:A:635:ILE:CG2	2.17	0.74
1:A:170:ARG:HH22	1:A:349:ASN:HD21	1.35	0.74
1:B:472:TRP:HE1	1:B:522:ASN:HD21	1.36	0.73
1:A:947:GLY:HA2	1:B:868:GLU:HG3	1.70	0.73
1:B:99:LEU:HD21	1:B:101:ARG:NH1	2.04	0.73
1:B:413:SER:C	1:B:446:MET:CE	2.57	0.73
1:B:872:MET:SD	1:B:905:MET:CE	2.76	0.73
1:B:472:TRP:HE1	1:B:522:ASN:ND2	1.85	0.73
1:A:727:GLN:HE22	1:A:782:LEU:HD12	1.53	0.73
1:A:716:PHE:HB2	1:A:890:ILE:HG22	1.71	0.73
1:B:290:ILE:HD12	1:B:290:ILE:N	2.02	0.73
1:A:187:LEU:HA	1:A:194:VAL:HG23	1.71	0.73
1:B:845:LEU:HD22	1:B:890:ILE:HD12	1.71	0.73
1:A:1068:ILE:O	1:A:1072:ILE:HD13	1.89	0.72
1:A:714:VAL:HG22	1:A:902:LEU:CD1	2.19	0.72
1:B:225:CYS:HA	1:B:228:MET:HE2	1.71	0.72
1:A:293:TYR:HB3	1:A:635:ILE:HG22	1.71	0.72
1:A:1023:ASP:O	1:A:1025:GLU:N	2.23	0.72
1:A:501:VAL:HG13	1:A:515:ILE:CG2	2.13	0.71
1:A:821:THR:CG2	1:A:834:ALA:HB2	2.20	0.71
1:B:701:VAL:HG21	1:B:842:ARG:NH1	2.04	0.71
1:A:228:MET:CE	1:A:282:LEU:HD13	2.20	0.71
1:B:1084:GLU:O	1:B:1087:VAL:HG23	1.91	0.71
1:A:212:VAL:HG23	1:A:290:ILE:HG21	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:702:LEU:HD13	1:B:849:ARG:NH1	2.07	0.70
1:A:287:CYS:O	1:A:288:PRO:C	2.29	0.70
1:B:414:LEU:N	1:B:446:MET:CE	2.53	0.70
1:A:778:LEU:HD11	1:A:817:VAL:HG21	1.73	0.69
1:B:765:VAL:HG13	1:B:769:VAL:HB	1.74	0.69
1:A:962:ASN:ND2	5:A:1243:HOH:O	2.25	0.69
1:A:1069:LYS:O	1:A:1070:ASP:C	2.31	0.69
1:B:413:SER:C	1:B:446:MET:HE3	2.13	0.69
1:A:905:MET:HG2	1:A:909:MET:HE2	1.74	0.69
1:B:504:ILE:H	1:B:504:ILE:HD12	1.56	0.69
1:B:219:ARG:O	1:B:220:ALA:CB	2.40	0.69
1:A:216:LEU:HA	1:A:217:GLN:HB2	1.74	0.69
1:B:743:VAL:HG23	1:B:744:ALA:H	1.58	0.69
1:B:743:VAL:O	1:B:745:HIS:N	2.27	0.68
1:A:400:ASP:HB3	1:A:403:THR:HB	1.74	0.68
1:A:995:ALA:HB1	1:A:1183:ILE:HD13	1.74	0.68
1:A:128:ARG:HD2	1:A:134:ASP:OD1	1.93	0.68
1:B:123:TRP:HE1	1:B:456:GLN:NE2	1.92	0.67
1:B:88:PRO:HA	1:B:91:ARG:HD2	1.77	0.67
1:A:286:PHE:O	1:A:288:PRO:HD2	1.94	0.67
1:A:821:THR:HG22	1:A:834:ALA:HB2	1.76	0.67
1:B:928:LYS:CD	1:B:945:ILE:HD11	2.25	0.67
1:A:298:ASP:OD1	1:A:301:THR:HG22	1.95	0.67
1:A:872:MET:CE	1:A:905:MET:HE2	2.25	0.66
1:A:765:VAL:CG1	1:A:769:VAL:HB	2.24	0.66
1:A:541:ASN:H	1:A:541:ASN:ND2	1.94	0.65
1:B:118:GLY:O	1:B:119:SER:O	2.14	0.65
1:A:757:VAL:HG21	1:A:762:LEU:HD12	1.78	0.65
1:B:788:ILE:CD1	1:B:803:LEU:O	2.45	0.65
1:A:835:ALA:O	1:A:839:THR:HG23	1.97	0.65
1:A:346:THR:H	1:A:349:ASN:HD22	1.45	0.65
1:B:753:LEU:HD13	1:B:763:PHE:HD2	1.60	0.64
1:A:195:ALA:HB3	1:A:342:GLU:HG2	1.80	0.64
1:B:164:ALA:C	1:B:165:ALA:O	2.31	0.64
1:B:1080:THR:HG22	1:B:1082:GLU:N	2.13	0.63
1:A:410:LEU:HD23	1:A:436:VAL:HB	1.80	0.63
1:B:788:ILE:CD1	1:B:807:GLN:HB3	2.28	0.63
1:A:317:ARG:HD3	5:A:1240:HOH:O	1.99	0.63
1:B:874:ALA:HB1	1:B:875:PRO:HD2	1.80	0.62
1:A:882:ILE:CD1	1:A:882:ILE:C	2.61	0.62
1:A:226:GLU:HG3	1:A:245:ALA:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ASP:OD1	1:A:219:ARG:HA	2.00	0.62
1:B:61:PRO:N	1:B:333:MET:HE3	2.14	0.62
1:A:203:GLN:NE2	1:A:279:LEU:HD22	2.13	0.62
1:A:913:ILE:CG2	1:A:917:LEU:HD12	2.29	0.62
1:B:148:HIS:HD2	1:B:362:TYR:OH	1.83	0.62
1:A:732:CYS:HB2	1:A:772:SER:OG	2.00	0.62
1:A:128:ARG:HD3	1:A:136:ALA:HB2	1.81	0.62
1:A:598:LEU:HD22	1:A:612:THR:HG22	1.81	0.62
1:B:322:ARG:HH11	1:B:323:ASN:HD21	1.46	0.61
1:A:1070:ASP:O	1:A:1072:ILE:N	2.34	0.61
1:B:748:ALA:HB3	1:B:752:TYR:HD1	1.64	0.61
1:B:363:LYS:HG3	1:B:457:TYR:OH	2.00	0.61
1:B:322:ARG:HB3	1:B:323:ASN:HD22	1.66	0.61
1:A:753:LEU:CD1	1:A:754:GLU:H	2.12	0.61
1:A:287:CYS:SG	1:A:292:LYS:HB2	2.41	0.60
1:B:928:LYS:HD2	1:B:945:ILE:HD11	1.83	0.60
1:A:757:VAL:HG21	1:A:836:THR:HG22	1.83	0.60
1:A:213:ASP:OD1	1:A:219:ARG:N	2.34	0.60
1:A:170:ARG:HH22	1:A:349:ASN:ND2	2.00	0.60
1:B:242:GLY:O	1:B:243:ILE:HB	2.02	0.60
1:A:1077:VAL:HG11	1:A:1154:VAL:HG11	1.82	0.60
1:B:244:SER:O	1:B:245:ALA:CB	2.50	0.60
1:A:710:VAL:HG13	1:A:988:ALA:HB2	1.84	0.59
1:B:364:LEU:HD11	1:B:463:THR:HG22	1.84	0.59
1:A:905:MET:CG	1:A:909:MET:HE3	2.32	0.59
1:A:757:VAL:CG2	1:A:836:THR:HG22	2.32	0.59
1:B:398:LEU:HG	1:B:457:TYR:CE2	2.37	0.59
1:A:159:ALA:HB2	1:A:176:THR:HA	1.84	0.59
1:A:1023:ASP:CB	1:A:1025:GLU:HG2	2.32	0.59
1:B:735:THR:HG22	1:B:764:PHE:HD2	1.68	0.59
1:A:117:VAL:CG1	1:A:130:TRP:CD1	2.86	0.58
1:A:761:ARG:O	1:A:762:LEU:HD23	2.03	0.58
1:B:727:GLN:HA	1:B:775:SER:OG	2.04	0.58
1:A:986:ALA:HB2	1:A:1006:GLY:HA3	1.84	0.58
1:B:244:SER:HA	1:B:247:HIS:ND1	2.18	0.58
1:A:208:ASN:HD22	1:A:211:GLU:H	1.52	0.58
1:B:158:HIS:ND1	1:B:178:THR:HG22	2.18	0.58
1:A:321:GLY:O	1:A:323:ASN:N	2.36	0.58
1:B:501:VAL:CG1	1:B:502:TRP:O	2.39	0.57
1:B:253:VAL:HG13	1:B:255:ARG:HG3	1.85	0.57
1:A:832:HIS:O	1:A:836:THR:HG23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:845:LEU:HD22	1:B:890:ILE:HD11	1.86	0.57
1:A:216:LEU:HA	1:A:217:GLN:CB	2.34	0.57
1:B:992:GLU:O	1:B:993:ARG:HG3	2.04	0.57
1:B:430:ARG:NH1	1:B:430:ARG:HG2	2.17	0.57
1:A:727:GLN:HE22	1:A:782:LEU:CD1	2.18	0.56
1:B:1023:ASP:O	1:B:1026:ARG:HG3	2.03	0.56
1:B:788:ILE:HD11	1:B:807:GLN:HB3	1.86	0.56
1:B:1080:THR:HG22	1:B:1082:GLU:H	1.70	0.56
1:B:413:SER:CA	1:B:446:MET:CE	2.83	0.56
1:B:225:CYS:HA	1:B:228:MET:CE	2.35	0.56
1:A:213:ASP:OD1	1:A:219:ARG:CA	2.53	0.56
1:A:117:VAL:HG12	1:A:130:TRP:CD1	2.40	0.56
1:A:1075:VAL:CG1	1:A:1156:LEU:CD2	2.84	0.56
1:B:702:LEU:O	1:B:702:LEU:CD2	2.42	0.56
1:B:702:LEU:HD13	1:B:849:ARG:HH12	1.70	0.56
1:A:539:LYS:O	1:A:543:VAL:HG23	2.05	0.56
1:A:1192:ILE:CD1	1:A:1196:TRP:HB2	2.35	0.56
1:B:219:ARG:O	1:B:220:ALA:HB3	2.06	0.56
1:B:515:ILE:CG2	1:B:515:ILE:O	2.53	0.56
1:B:701:VAL:HG21	1:B:842:ARG:HH11	1.69	0.55
1:B:930:PHE:CE2	1:B:945:ILE:HD13	2.41	0.55
1:A:467:ILE:HA	1:A:471:ASP:HB2	1.88	0.55
1:A:514:LYS:N	1:A:614:TYR:CD2	2.75	0.55
1:B:552:LYS:HD2	1:B:553:LYS:O	2.06	0.55
1:A:785:ARG:O	1:A:789:ARG:HG3	2.07	0.55
1:A:129:LEU:HD21	1:A:332:PRO:O	2.06	0.55
1:A:703:ASP:HB2	1:A:704:PRO:CD	2.37	0.55
1:B:413:SER:N	1:B:446:MET:HE2	2.21	0.55
1:A:1034:THR:HG22	1:A:1070:ASP:O	2.06	0.55
1:B:515:ILE:HG22	1:B:515:ILE:O	2.07	0.55
1:A:533:ILE:HD13	1:A:547:VAL:HG22	1.88	0.55
1:B:788:ILE:HD11	1:B:803:LEU:O	2.06	0.55
1:B:1092:ALA:O	1:B:1096:LEU:HD12	2.07	0.55
1:A:258:VAL:HA	1:A:634:PHE:CD2	2.42	0.55
1:A:424:LEU:HD13	5:A:1257:HOH:O	2.07	0.55
1:B:1080:THR:HG23	1:B:1082:GLU:OE1	2.07	0.54
1:A:223:ASP:O	1:A:227:ARG:HG3	2.06	0.54
1:A:152:ILE:HG21	1:A:300:THR:HG23	1.89	0.54
1:B:322:ARG:HB3	1:B:323:ASN:ND2	2.21	0.54
1:B:321:GLY:HA3	1:B:325:THR:HG22	1.88	0.54
1:A:703:ASP:HB2	1:A:704:PRO:HD3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:SER:HB3	1:A:895:ARG:HB2	1.88	0.54
1:B:905:MET:HG2	1:B:909:MET:CE	2.38	0.54
1:A:732:CYS:SG	1:A:733:PHE:N	2.81	0.54
1:A:397:LEU:HD13	1:A:406:LEU:HD21	1.90	0.54
1:A:1012:ALA:O	1:A:1016:ASP:HB2	2.08	0.53
1:A:611:ARG:HG2	1:A:615:ASP:OD2	2.08	0.53
1:A:722:TYR:O	1:A:726:ILE:HG13	2.09	0.53
1:A:798:GLU:O	1:A:801:VAL:HG22	2.08	0.53
1:A:194:VAL:HG13	1:A:341:VAL:CG2	2.36	0.53
1:B:883:ILE:HD12	1:B:883:ILE:O	2.07	0.53
1:A:1028:ILE:H	1:A:1028:ILE:HD12	1.73	0.53
1:A:237:GLY:O	1:A:238:ALA:HB3	2.07	0.53
1:B:714:VAL:HG13	1:B:902:LEU:HG	1.90	0.53
1:B:863:LEU:HD22	1:B:863:LEU:O	2.08	0.53
1:B:952:ILE:HD12	1:B:957:LEU:HD22	1.89	0.53
1:A:874:ALA:HB1	1:A:875:PRO:HD2	1.90	0.53
1:B:264:ARG:HD2	1:B:264:ARG:N	2.21	0.53
1:B:748:ALA:HB3	1:B:752:TYR:CD1	2.43	0.53
1:B:1097:ASP:O	5:B:1275:HOH:O	2.18	0.53
1:A:148:HIS:O	1:A:186:GLY:HA3	2.09	0.53
1:B:63:GLN:HB3	1:B:496:ARG:NH2	2.24	0.53
1:B:884:TYR:HB3	1:B:891:PHE:HB2	1.90	0.53
1:A:1075:VAL:HG11	1:A:1156:LEU:CD2	2.39	0.52
1:A:294:GLU:OE2	1:A:636:LEU:HD22	2.09	0.52
1:A:618:GLN:OE1	1:A:827:LEU:HD12	2.10	0.52
1:B:423:HIS:ND1	1:B:576:GLU:HG3	2.24	0.52
1:A:365:MET:CE	1:A:396:CYS:SG	2.97	0.52
1:B:403:THR:O	1:B:404:THR:CB	2.51	0.52
1:A:994:PRO:HD2	1:A:997:GLU:HG3	1.91	0.52
1:A:464:GLY:HA2	1:A:585:VAL:HG11	1.91	0.52
1:A:514:LYS:O	1:A:515:ILE:HG22	2.09	0.52
1:B:1080:THR:CG2	1:B:1082:GLU:HB2	2.39	0.52
1:B:874:ALA:HB1	1:B:875:PRO:CD	2.39	0.52
1:A:176:THR:O	1:A:177:PRO:C	2.37	0.52
1:A:731:LEU:HD22	1:A:764:PHE:CD2	2.45	0.52
1:A:618:GLN:HE22	1:A:826:GLY:HA3	1.75	0.52
1:B:487:LEU:HD12	1:B:500:ARG:HD2	1.91	0.52
1:B:545:GLU:O	1:B:549:LYS:HA	2.10	0.52
1:A:61:PRO:N	1:A:333:MET:HE3	2.25	0.52
1:A:212:VAL:CG2	1:A:290:ILE:HG21	2.39	0.51
1:A:913:ILE:HG23	1:A:917:LEU:HD12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1028:ILE:N	1:A:1028:ILE:HD12	2.26	0.51
1:B:254:GLU:O	1:B:255:ARG:HG2	2.11	0.51
1:B:765:VAL:CG1	1:B:769:VAL:HB	2.40	0.51
1:B:325:THR:HG23	1:B:349:ASN:HD21	1.75	0.51
1:B:315:TRP:CG	1:B:356:MET:HG2	2.45	0.51
1:B:165:ALA:HB1	1:B:167:PHE:CE2	2.45	0.51
1:A:203:GLN:NE2	1:A:279:LEU:CD2	2.74	0.51
1:B:148:HIS:O	1:B:186:GLY:HA3	2.10	0.51
1:B:273:VAL:HG12	1:B:275:SER:H	1.76	0.51
1:A:872:MET:CE	1:A:905:MET:CE	2.89	0.50
1:A:1068:ILE:HA	5:A:1256:HOH:O	2.11	0.50
1:B:61:PRO:CD	1:B:333:MET:HE3	2.41	0.50
1:A:205:PHE:CE2	1:A:271:VAL:HG22	2.46	0.50
1:B:930:PHE:CE2	1:B:945:ILE:CD1	2.95	0.50
1:B:552:LYS:NZ	1:B:581:ASP:OD1	2.42	0.50
1:B:999:LEU:HD23	1:B:1187:LEU:CD2	2.39	0.50
1:A:293:TYR:HB3	1:A:635:ILE:HG21	1.92	0.50
1:A:1069:LYS:O	1:A:1071:ARG:N	2.44	0.50
1:B:788:ILE:HD12	1:B:803:LEU:O	2.12	0.50
1:B:1174:LYS:NZ	1:B:1179:ASN:O	2.44	0.50
1:A:353:GLU:HG3	1:A:356:MET:HB3	1.92	0.50
1:B:990:LEU:HD12	1:B:1176:LEU:HD22	1.93	0.50
1:B:940:LYS:HB3	1:B:955:VAL:HG23	1.94	0.50
1:A:293:TYR:CB	1:A:635:ILE:HG21	2.41	0.49
1:A:305:LEU:HD12	1:A:626:LEU:HD23	1.94	0.49
1:A:188:THR:HB	1:A:189:PRO:HD2	1.93	0.49
1:B:1148:TYR:CE1	1:B:1152:HIS:CE1	3.00	0.49
1:B:1159:ASP:O	1:B:1163:SER:HB2	2.12	0.49
1:B:819:GLY:O	1:B:823:VAL:HG23	2.13	0.49
1:A:846:LEU:O	1:A:850:GLU:HG3	2.12	0.49
1:B:743:VAL:O	1:B:744:ALA:C	2.51	0.49
1:A:208:ASN:ND2	1:A:211:GLU:H	2.09	0.49
1:A:105:VAL:HG13	1:A:440:PHE:CZ	2.47	0.49
1:B:1182:LYS:O	1:B:1183:ILE:C	2.51	0.49
1:A:884:TYR:HB3	1:A:891:PHE:HB2	1.94	0.49
1:B:290:ILE:CD1	1:B:290:ILE:N	2.74	0.49
1:B:784:MET:O	1:B:788:ILE:HG23	2.12	0.49
1:A:874:ALA:HB1	1:A:875:PRO:CD	2.43	0.49
1:B:214:ARG:O	1:B:216:LEU:N	2.46	0.49
1:B:404:THR:CG2	1:B:404:THR:O	2.61	0.49
1:A:61:PRO:N	1:A:333:MET:CE	2.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:832:HIS:N	1:A:832:HIS:ND1	2.60	0.48
1:B:1174:LYS:HB2	1:B:1174:LYS:HZ2	1.78	0.48
1:A:1192:ILE:HD12	1:A:1193:PRO:O	2.13	0.48
1:A:727:GLN:NE2	1:A:782:LEU:HD12	2.26	0.48
1:A:736:LEU:HB2	1:A:764:PHE:CE2	2.48	0.48
1:B:323:ASN:N	1:B:323:ASN:HD22	2.11	0.48
1:B:205:PHE:HD2	1:B:279:LEU:HD11	1.77	0.48
1:B:821:THR:HG22	1:B:834:ALA:HB2	1.95	0.48
1:B:905:MET:HG2	1:B:909:MET:HE3	1.96	0.48
1:A:450:PHE:O	1:A:454:VAL:HG23	2.13	0.48
1:A:604:LEU:HD23	1:A:813:VAL:HG21	1.95	0.48
1:A:521:VAL:HG11	1:A:609:ILE:HD13	1.95	0.48
1:B:718:PHE:HE1	1:B:845:LEU:HD23	1.79	0.48
1:A:1075:VAL:CG1	1:A:1156:LEU:HD23	2.43	0.48
1:A:736:LEU:HG	1:A:737:SER:N	2.28	0.48
1:B:173:ASP:O	1:B:176:THR:OG1	2.32	0.48
1:B:129:LEU:HD23	1:B:134:ASP:HA	1.94	0.48
1:B:404:THR:O	1:B:404:THR:HG23	2.14	0.47
1:A:303:PHE:O	1:A:307:ASN:ND2	2.41	0.47
1:B:1026:ARG:NH1	1:B:1028:ILE:HD12	2.29	0.47
1:A:744:ALA:HB3	1:A:746:LEU:HG	1.96	0.47
1:B:244:SER:O	1:B:245:ALA:HB3	2.14	0.47
1:A:233:ARG:NH1	1:A:243:ILE:HD11	2.29	0.47
1:B:83:ASP:HB2	1:B:86:ALA:HB2	1.96	0.47
1:B:63:GLN:HB3	1:B:496:ARG:HH21	1.79	0.47
1:B:229:ALA:HB1	1:B:244:SER:HB2	1.96	0.47
1:B:325:THR:CG2	1:B:349:ASN:HD21	2.27	0.47
1:B:703:ASP:CB	1:B:704:PRO:CD	2.93	0.47
1:B:1001:ARG:HD3	1:B:1002:PRO:HD2	1.97	0.47
1:B:416:SER:O	1:B:571:ARG:HD2	2.14	0.47
1:A:886:ASP:OD1	1:A:887:THR:N	2.48	0.47
1:A:305:LEU:CD1	1:A:626:LEU:HD23	2.45	0.47
1:B:264:ARG:H	1:B:264:ARG:CD	2.24	0.47
1:A:1025:GLU:HA	1:A:1025:GLU:OE2	2.14	0.47
1:A:940:LYS:HA	1:A:953:LYS:O	2.15	0.47
1:B:213:ASP:OD1	1:B:269:TYR:OH	2.33	0.47
1:B:852:VAL:HG13	1:B:880:MET:CE	2.45	0.47
1:A:872:MET:HE1	1:A:902:LEU:HA	1.97	0.46
1:A:1192:ILE:HD13	1:A:1196:TRP:HB2	1.96	0.46
1:B:284:ASP:C	1:B:285:ASN:OD1	2.53	0.46
1:A:244:SER:HB3	1:A:247:HIS:NE2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:LEU:HD13	1:A:577:TYR:CD1	2.50	0.46
1:B:785:ARG:O	1:B:789:ARG:HG3	2.15	0.46
1:A:607:ILE:HD13	1:A:619:ILE:HG23	1.97	0.46
1:B:502:TRP:CE2	1:B:512:ARG:HG3	2.51	0.46
1:B:852:VAL:HG13	1:B:880:MET:HE1	1.97	0.46
1:B:747:GLU:HG3	1:B:752:TYR:CD2	2.50	0.46
1:A:716:PHE:O	1:A:889:SER:HA	2.16	0.46
1:A:997:GLU:O	1:A:1001:ARG:HG2	2.16	0.46
1:B:315:TRP:CD2	1:B:356:MET:HG2	2.51	0.46
1:A:1194:GLU:HA	1:A:1197:HIS:CD2	2.50	0.46
1:A:239:SER:O	1:A:242:GLY:N	2.47	0.46
1:A:365:MET:HE1	1:A:396:CYS:SG	2.55	0.46
1:A:72:ASP:O	1:A:101:ARG:N	2.49	0.46
1:A:548:LEU:HD21	1:A:588:LEU:HD23	1.97	0.46
1:B:126:ARG:HH22	1:B:460:GLU:CD	2.19	0.46
1:A:823:VAL:O	1:A:829:PRO:HB3	2.16	0.46
1:B:618:GLN:HE22	1:B:826:GLY:HA3	1.80	0.46
1:B:732:CYS:HB3	1:B:735:THR:HB	1.97	0.46
1:B:413:SER:CA	1:B:446:MET:HE1	2.45	0.46
1:B:1079:GLN:NE2	1:B:1137:LEU:HB2	2.31	0.46
1:B:615:ASP:OD2	1:B:615:ASP:N	2.49	0.46
1:A:994:PRO:O	1:A:995:ALA:C	2.55	0.45
1:A:595:HIS:O	1:A:599:SER:OG	2.31	0.45
1:A:1180:ASN:ND2	1:A:1183:ILE:CD1	2.79	0.45
1:A:153:LEU:HD11	1:A:185:LEU:HD11	1.97	0.45
1:B:175:ILE:HG22	1:B:179:GLY:HA3	1.98	0.45
1:A:86:ALA:HB1	1:A:91:ARG:HD2	1.98	0.45
1:A:872:MET:HE1	1:A:905:MET:HE2	1.97	0.45
1:B:195:ALA:HB3	1:B:342:GLU:HG2	1.98	0.45
1:A:1145:ASP:OD2	1:A:1146:PRO:HD2	2.16	0.45
1:B:253:VAL:CG1	1:B:255:ARG:HG3	2.45	0.45
1:A:533:ILE:HD11	1:A:535:LEU:HD11	1.98	0.45
1:A:279:LEU:HD21	1:A:295:GLY:O	2.16	0.45
1:A:555:LEU:HD13	1:A:577:TYR:HD1	1.82	0.45
1:B:713:VAL:HG22	1:B:893:LEU:HA	1.98	0.45
1:B:881:ARG:HH11	1:B:881:ARG:CG	2.30	0.45
1:A:885:GLY:HA2	1:A:890:ILE:HD12	1.99	0.45
1:A:232:LEU:HD11	1:A:278:VAL:HG13	1.98	0.45
1:B:765:VAL:HG21	1:B:769:VAL:HG11	1.99	0.45
1:A:757:VAL:HG12	1:A:758:GLY:N	2.32	0.45
1:A:117:VAL:HG11	1:A:130:TRP:CG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:SER:HB3	1:A:247:HIS:CD2	2.52	0.44
1:A:493:MET:CE	1:A:497:GLY:HA2	2.46	0.44
1:A:239:SER:O	1:A:240:PHE:C	2.56	0.44
1:A:541:ASN:N	1:A:541:ASN:ND2	2.64	0.44
1:B:99:LEU:CD2	1:B:101:ARG:NH1	2.79	0.44
1:A:397:LEU:HB3	1:A:406:LEU:HD11	1.98	0.44
1:B:567:GLY:HA2	1:B:571:ARG:NH2	2.31	0.44
1:A:77:ILE:HA	1:A:95:HIS:O	2.18	0.44
1:B:822:GLY:HA2	1:B:831:LEU:HD23	1.99	0.44
1:A:139:GLY:O	1:A:140:PHE:C	2.56	0.44
1:A:1072:ILE:HG22	1:A:1072:ILE:O	2.18	0.44
1:B:177:PRO:HD3	1:B:274:ARG:NH2	2.33	0.44
1:B:209:LYS:O	1:B:213:ASP:HB2	2.17	0.44
1:A:977:LEU:HD22	1:A:1173:PHE:CE2	2.52	0.44
1:B:999:LEU:CD2	1:B:1187:LEU:HD21	2.43	0.44
1:A:219:ARG:HA	1:A:269:TYR:OH	2.18	0.44
1:B:821:THR:CG2	1:B:834:ALA:HB2	2.48	0.44
1:A:187:LEU:HD13	1:A:191:GLY:HA2	1.99	0.44
1:A:228:MET:CE	1:A:282:LEU:CD1	2.93	0.44
1:A:467:ILE:HG22	1:A:471:ASP:CB	2.48	0.44
1:A:532:LYS:NZ	1:A:597:GLU:OE1	2.46	0.44
1:A:318:LEU:HA	1:A:349:ASN:O	2.18	0.44
1:B:515:ILE:HD13	1:B:517:VAL:HG23	1.99	0.44
1:A:823:VAL:HG12	1:A:826:GLY:N	2.33	0.44
1:B:822:GLY:O	1:B:831:LEU:HD21	2.17	0.44
1:B:886:ASP:OD1	1:B:887:THR:N	2.51	0.44
1:A:966:ILE:CD1	1:A:1164:HIS:HB3	2.48	0.44
1:A:849:ARG:HG3	1:A:882:ILE:CG2	2.48	0.44
1:B:503:ASP:N	1:B:514:LYS:HG3	2.32	0.44
1:A:714:VAL:CG2	1:A:902:LEU:HD13	2.39	0.43
1:A:403:THR:HG22	1:A:405:ALA:N	2.21	0.43
1:A:977:LEU:HD22	1:A:1173:PHE:HE2	1.82	0.43
1:A:792:ILE:N	1:A:793:PRO:HD2	2.34	0.43
1:A:447:LEU:HD22	1:A:475:LEU:CD2	2.49	0.43
1:A:1077:VAL:CG1	1:A:1078:ALA:N	2.81	0.43
1:A:1023:ASP:C	1:A:1025:GLU:N	2.72	0.43
1:B:210:GLU:O	1:B:214:ARG:NE	2.51	0.43
1:B:703:ASP:HB3	1:B:704:PRO:CD	2.48	0.43
1:B:986:ALA:HB2	1:B:1006:GLY:HA3	2.00	0.43
1:A:833:VAL:O	1:A:837:VAL:HG23	2.19	0.43
1:A:305:LEU:HD12	1:A:626:LEU:CD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1160:TYR:O	1:B:1164:HIS:HD2	2.01	0.43
1:A:533:ILE:HD11	1:A:535:LEU:CD1	2.48	0.43
1:A:416:SER:O	1:A:571:ARG:HD2	2.18	0.43
1:A:467:ILE:HG22	1:A:471:ASP:HB2	2.01	0.43
1:B:277:ARG:HD2	5:B:1289:HOH:O	2.19	0.43
1:B:844:MET:CE	1:B:922:ILE:HD13	2.49	0.43
1:A:216:LEU:HD22	1:A:227:ARG:NH1	2.34	0.43
1:B:882:ILE:CD1	1:B:892:VAL:HG22	2.49	0.43
1:B:319:LYS:HB2	1:B:320:PRO:HD2	1.99	0.43
1:A:946:TYR:CE2	1:B:868:GLU:HG2	2.54	0.42
1:A:528:ILE:O	1:A:531:ASP:HB2	2.19	0.42
1:A:532:LYS:HZ1	1:A:597:GLU:CD	2.22	0.42
1:A:1001:ARG:HB2	1:A:1002:PRO:CD	2.50	0.42
1:A:60:GLY:C	1:A:333:MET:CE	2.88	0.42
1:B:214:ARG:HG3	1:B:214:ARG:HH11	1.84	0.42
1:B:716:PHE:HB3	1:B:924:LEU:HD21	2.00	0.42
1:B:937:ALA:O	1:B:938:LYS:C	2.57	0.42
1:A:205:PHE:CD1	1:A:292:LYS:HE2	2.54	0.42
1:A:740:ALA:O	1:A:743:VAL:CG2	2.67	0.42
1:A:772:SER:O	1:A:775:SER:HB2	2.19	0.42
1:B:176:THR:HB	1:B:177:PRO:HD3	2.02	0.42
1:B:1014:LEU:O	1:B:1017:ALA:HB3	2.20	0.42
1:A:215:HIS:O	1:A:216:LEU:HB2	2.18	0.42
1:B:743:VAL:C	1:B:745:HIS:N	2.70	0.42
1:A:764:PHE:CE1	1:A:836:THR:HG21	2.54	0.42
1:B:788:ILE:HD11	1:B:807:GLN:CB	2.50	0.42
1:A:1077:VAL:HG13	1:A:1154:VAL:HG12	2.00	0.42
1:B:364:LEU:HD11	1:B:463:THR:CG2	2.48	0.42
1:A:81:VAL:HG11	1:A:565:ALA:CB	2.49	0.42
1:B:303:PHE:HD2	1:B:304:ILE:HD12	1.85	0.42
1:A:61:PRO:CA	1:A:333:MET:HE3	2.50	0.42
1:B:1182:LYS:O	1:B:1185:GLU:N	2.52	0.42
1:A:638:ASP:O	1:A:640:GLN:N	2.52	0.42
1:A:797:PRO:O	1:A:801:VAL:HG13	2.20	0.42
1:B:193:ARG:NH1	1:B:338:SER:O	2.52	0.42
1:B:1068:ILE:O	1:B:1069:LYS:HB2	2.20	0.42
1:A:377:ASP:OD1	1:A:377:ASP:C	2.58	0.42
1:B:413:SER:HA	1:B:446:MET:HE1	2.01	0.42
1:B:529:ILE:HD11	1:B:592:PHE:CE1	2.55	0.42
1:B:264:ARG:N	1:B:264:ARG:CD	2.81	0.41
1:B:745:HIS:O	1:B:746:LEU:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1080:THR:CG2	1:B:1082:GLU:H	2.30	0.41
1:B:955:VAL:HG12	1:B:956:ASP:N	2.35	0.41
1:B:711:ASN:HB2	1:B:893:LEU:HD11	2.02	0.41
1:A:150:TYR:CE1	1:A:460:GLU:HB3	2.55	0.41
1:B:244:SER:HA	1:B:247:HIS:CE1	2.54	0.41
1:A:1075:VAL:HG13	1:A:1156:LEU:CD2	2.50	0.41
1:A:554:ASP:HB2	1:A:577:TYR:CZ	2.55	0.41
1:B:1007:LEU:O	1:B:1008:GLN:C	2.59	0.41
1:B:341:VAL:CG1	1:B:343:PHE:CE2	3.03	0.41
1:B:104:LYS:HE3	1:B:111:GLU:OE2	2.19	0.41
1:B:532:LYS:O	1:B:533:ILE:HD13	2.19	0.41
1:A:714:VAL:CG2	1:A:902:LEU:CD1	2.95	0.41
1:A:743:VAL:CG1	1:A:752:TYR:OH	2.68	0.41
1:B:414:LEU:N	1:B:446:MET:HE1	2.34	0.41
1:B:243:ILE:O	1:B:244:SER:OG	2.38	0.41
1:A:615:ASP:OD1	1:A:615:ASP:N	2.53	0.41
1:A:781:TRP:O	1:A:810:ILE:HG21	2.20	0.41
1:B:905:MET:HG2	1:B:909:MET:HE2	2.03	0.41
1:B:255:ARG:HD3	1:B:635:ILE:HG23	2.02	0.41
1:B:476:LEU:HD13	1:B:500:ARG:CG	2.50	0.41
1:A:307:ASN:HB2	1:A:310:PHE:CD2	2.55	0.41
1:A:738:LEU:HD23	1:A:762:LEU:HD22	2.02	0.41
1:B:552:LYS:HD3	1:B:580:GLN:OE1	2.20	0.41
1:B:863:LEU:CD2	1:B:867:PRO:HA	2.50	0.41
1:A:1034:THR:CG2	1:A:1070:ASP:O	2.69	0.41
1:B:753:LEU:HD12	1:B:754:GLU:N	2.36	0.41
1:A:101:ARG:HG3	1:A:102:ALA:O	2.20	0.41
1:A:216:LEU:CA	1:A:217:GLN:HB2	2.47	0.41
1:B:1180:ASN:OD1	1:B:1182:LYS:HG3	2.21	0.41
1:A:247:HIS:N	1:A:247:HIS:CD2	2.89	0.41
1:A:555:LEU:HD22	1:A:577:TYR:CB	2.51	0.41
1:B:916:ALA:O	1:B:917:LEU:HD23	2.21	0.41
1:A:751:ASP:OD1	1:A:751:ASP:N	2.54	0.41
1:A:1174:LYS:CB	1:A:1179:ASN:HA	2.51	0.41
1:A:1166:LEU:HD12	1:A:1166:LEU:HA	1.69	0.41
1:B:792:ILE:HB	1:B:793:PRO:HD3	2.02	0.41
1:B:749:GLY:HA2	1:B:753:LEU:HD21	2.03	0.41
1:A:1194:GLU:HA	1:A:1197:HIS:NE2	2.36	0.41
1:A:213:ASP:OD1	1:A:218:CYS:C	2.60	0.40
1:A:875:PRO:O	1:A:876:GLY:O	2.38	0.40
1:B:748:ALA:O	1:B:752:TYR:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:GLN:H	1:A:617:GLN:CD	2.23	0.40
1:A:871:ASP:HB2	1:B:946:TYR:CD2	2.56	0.40
1:A:84:GLU:OE1	1:A:84:GLU:HA	2.21	0.40
1:A:743:VAL:HG12	1:A:752:TYR:OH	2.21	0.40
1:A:1001:ARG:HE	1:A:1001:ARG:HB2	1.72	0.40
1:A:1075:VAL:HG11	1:A:1156:LEU:HD21	2.03	0.40
1:B:1174:LYS:HZ2	1:B:1179:ASN:HA	1.87	0.40
1:B:986:ALA:HB1	1:B:1007:LEU:HG	2.04	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	971/1193 (81%)	865 (89%)	78 (8%)	28 (3%)	6 13
1	B	1027/1193 (86%)	934 (91%)	73 (7%)	20 (2%)	10 23
All	All	1998/2386 (84%)	1799 (90%)	151 (8%)	48 (2%)	7 17

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	SER
1	A	217	GLN
1	A	322	ARG
1	A	376	GLU
1	A	531	ASP
1	A	639	THR
1	A	745	HIS
1	A	921	PRO
1	A	938	LYS
1	A	1069	LYS

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Mol	Chain	Res	Type
1	A	1070	ASP
1	A	1071	ARG
1	B	119	SER
1	B	215	HIS
1	B	220	ALA
1	B	243	ILE
1	B	245	ALA
1	B	1137	LEU
1	A	120	GLY
1	A	404	THR
1	A	757	VAL
1	B	275	SER
1	B	322	ARG
1	B	702	LEU
1	B	741	ASP
1	B	900	ALA
1	B	938	LYS
1	A	216	LEU
1	A	742	ALA
1	A	830	CYS
1	B	177	PRO
1	B	234	GLU
1	B	288	PRO
1	B	744	ALA
1	A	140	PHE
1	A	287	CYS
1	B	165	ALA
1	A	112	ARG
1	A	876	GLY
1	A	995	ALA
1	B	505	GLY
1	B	1096	LEU
1	A	238	ALA
1	A	1024	PRO
1	B	260	TYR
1	A	131	GLY
1	A	288	PRO
1	A	920	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	814/971 (84%)	718 (88%)	96 (12%)	6 14
1	B	862/971 (89%)	770 (89%)	92 (11%)	8 17
All	All	1676/1942 (86%)	1488 (89%)	188 (11%)	7 16

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	SER
1	A	70	GLU
1	A	71	CYS
1	A	75	ARG
1	A	81	VAL
1	A	90	LYS
1	A	117	VAL
1	A	128	ARG
1	A	143	THR
1	A	145	THR
1	A	194	VAL
1	A	213	ASP
1	A	218	CYS
1	A	219	ARG
1	A	224	LEU
1	A	251	GLU
1	A	255	ARG
1	A	258	VAL
1	A	264	ARG
1	A	271	VAL
1	A	301	THR
1	A	304	ILE
1	A	318	LEU
1	A	319	LYS
1	A	325	THR
1	A	339	SER
1	A	368	ASP

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Mol	Chain	Res	Type
1	A	386	HIS
1	A	388	GLU
1	A	404	THR
1	A	421	GLU
1	A	424	LEU
1	A	478	LYS
1	A	492	ARG
1	A	498	VAL
1	A	502	TRP
1	A	515	ILE
1	A	516	LYS
1	A	531	ASP
1	A	533	ILE
1	A	539	LYS
1	A	541	ASN
1	A	545	GLU
1	A	548	LEU
1	A	549	LYS
1	A	550	ASP
1	A	551	LYS
1	A	552	LYS
1	A	553	LYS
1	A	556	SER
1	A	581	ASP
1	A	599	SER
1	A	613	ILE
1	A	615	ASP
1	A	617	GLN
1	A	636	LEU
1	A	640	GLN
1	A	714	VAL
1	A	717	ASP
1	A	736	LEU
1	A	739	ARG
1	A	751	ASP
1	A	753	LEU
1	A	754	GLU
1	A	755	ILE
1	A	756	GLU
1	A	760	ARG
1	A	770	ARG
1	A	796	SER

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Mol	Chain	Res	Type
1	A	798	GLU
1	A	807	GLN
1	A	821	THR
1	A	824	GLN
1	A	827	LEU
1	A	832	HIS
1	A	846	LEU
1	A	860	GLU
1	A	861	GLN
1	A	873	ARG
1	A	881	ARG
1	A	882	ILE
1	A	902	LEU
1	A	934	LEU
1	A	953	LYS
1	A	956	ASP
1	A	959	ARG
1	A	962	ASN
1	A	970	SER
1	A	974	VAL
1	A	993	ARG
1	A	997	GLU
1	A	1020	ARG
1	A	1025	GLU
1	A	1069	LYS
1	A	1182	LYS
1	A	1192	ILE
1	B	59	THR
1	B	70	GLU
1	B	81	VAL
1	B	94	VAL
1	B	101	ARG
1	B	119	SER
1	B	170	ARG
1	B	176	THR
1	B	182	ILE
1	B	196	VAL
1	B	208	ASN
1	B	214	ARG
1	B	215	HIS
1	B	216	LEU
1	B	222	ARG

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Mol	Chain	Res	Type
1	B	224	LEU
1	B	232	LEU
1	B	241	ARG
1	B	253	VAL
1	B	258	VAL
1	B	262	GLU
1	B	264	ARG
1	B	285	ASN
1	B	292	LYS
1	B	317	ARG
1	B	322	ARG
1	B	324	ASN
1	B	325	THR
1	B	338	SER
1	B	346	THR
1	B	398	LEU
1	B	404	THR
1	B	430	ARG
1	B	471	ASP
1	B	500	ARG
1	B	501	VAL
1	B	503	ASP
1	B	507	SER
1	B	508	HIS
1	B	515	ILE
1	B	536	SER
1	B	552	LYS
1	B	570	GLN
1	B	580	GLN
1	B	607	ILE
1	B	608	ASN
1	B	613	ILE
1	B	639	THR
1	B	702	LEU
1	B	703	ASP
1	B	710	VAL
1	B	714	VAL
1	B	735	THR
1	B	743	VAL
1	B	747	GLU
1	B	750	LYS
1	B	751	ASP

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Mol	Chain	Res	Type
1	B	752	TYR
1	B	756	GLU
1	B	757	VAL
1	B	765	VAL
1	B	775	SER
1	B	788	ILE
1	B	803	LEU
1	B	806	GLN
1	B	816	SER
1	B	821	THR
1	B	849	ARG
1	B	862	LEU
1	B	863	LEU
1	B	871	ASP
1	B	881	ARG
1	B	924	LEU
1	B	927	GLU
1	B	940	LYS
1	B	945	ILE
1	B	951	LEU
1	B	956	ASP
1	B	957	LEU
1	B	960	LYS
1	B	1014	LEU
1	B	1019	ARG
1	B	1025	GLU
1	B	1026	ARG
1	B	1028	ILE
1	B	1038	SER
1	B	1039	ARG
1	B	1086	THR
1	B	1093	LEU
1	B	1136	LYS
1	B	1174	LYS
1	B	1182	LYS

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

Mol	Chain	Res	Type
1	A	203	GLN
1	A	208	ASN
1	A	247	HIS

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Mol	Chain	Res	Type
1	A	324	ASN
1	A	349	ASN
1	A	423	HIS
1	A	494	ASN
1	A	541	ASN
1	A	595	HIS
1	A	727	GLN
1	A	768	HIS
1	A	824	GLN
1	A	1018	HIS
1	A	1152	HIS
1	B	148	HIS
1	B	203	GLN
1	B	323	ASN
1	B	456	GLN
1	B	494	ASN
1	B	506	GLN
1	B	522	ASN
1	B	618	GLN
1	B	787	GLN
1	B	824	GLN
1	B	1079	GLN
1	B	1164	HIS
1	B	1179	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\#\|Z\| > 2$
2	SO4	B	1236	-	4,4,4	0.22	0	6,6,6	0.31	0
2	SO4	B	1237	-	4,4,4	0.12	0	6,6,6	0.35	0
4	GAI	B	1239	-	0,3,3	0.00	-	0,3,3	0.00	-

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	SO4	B	1236	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1237	-	-	0/0/0/0	0/0/0/0
4	GAI	B	1239	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	981/1193 (82%)	0.54	83 (8%)	13	10	41, 61, 88, 104	0
1	B	1035/1193 (86%)	0.47	39 (3%)	44	43	39, 60, 85, 99	0
All	All	2016/2386 (84%)	0.50	122 (6%)	25	23	39, 60, 87, 104	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	742	ALA	8.1
1	B	509	PHE	7.3
1	B	217	GLN	6.4
1	B	228	MET	5.7
1	B	744	ALA	5.6
1	A	752	TYR	5.6
1	A	281	TYR	5.6
1	A	240	PHE	5.6
1	A	233	ARG	5.4
1	A	286	PHE	5.4
1	B	745	HIS	5.4
1	B	212	VAL	5.3
1	A	794	GLN	5.0
1	B	269	TYR	4.9
1	A	731	LEU	4.6
1	B	503	ASP	4.5
1	A	291	LYS	4.5
1	A	769	VAL	4.3
1	B	504	ILE	4.2
1	B	286	PHE	4.1
1	A	824	GLN	4.0
1	A	733	PHE	3.9
1	B	231	ALA	3.9
1	B	233	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	117	VAL	3.8
1	A	592	PHE	3.8
1	A	215	HIS	3.7
1	A	726	ILE	3.6
1	A	625	LEU	3.6
1	A	747	GLU	3.6
1	A	739	ARG	3.6
1	B	289	ALA	3.6
1	B	763	PHE	3.5
1	A	261	TYR	3.5
1	A	243	ILE	3.5
1	A	725	ILE	3.5
1	A	831	LEU	3.4
1	A	746	LEU	3.4
1	B	285	ASN	3.4
1	A	765	VAL	3.3
1	B	878	TYR	3.3
1	A	216	LEU	3.2
1	B	288	PRO	3.2
1	A	938	LYS	3.2
1	A	289	ALA	3.2
1	B	743	VAL	3.2
1	A	547	VAL	3.1
1	B	215	HIS	3.1
1	B	224	LEU	3.1
1	B	232	LEU	3.0
1	A	224	LEU	3.0
1	A	800	ALA	3.0
1	A	730	ASN	2.9
1	A	770	ARG	2.9
1	A	282	LEU	2.8
1	A	288	PRO	2.8
1	A	756	GLU	2.8
1	A	71	CYS	2.8
1	A	133	VAL	2.7
1	B	281	TYR	2.7
1	A	750	LYS	2.7
1	B	293	TYR	2.7
1	A	263	THR	2.7
1	A	283	CYS	2.6
1	A	1137	LEU	2.6
1	B	318	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	743	VAL	2.6
1	A	140	PHE	2.6
1	A	259	TYR	2.6
1	A	552	LYS	2.6
1	A	152	ILE	2.6
1	A	817	VAL	2.6
1	B	507	SER	2.6
1	A	60	GLY	2.5
1	A	196	VAL	2.5
1	A	577	TYR	2.5
1	A	242	GLY	2.5
1	A	622	PHE	2.5
1	A	219	ARG	2.5
1	A	721	LEU	2.4
1	A	1136	LYS	2.4
1	A	1138	LEU	2.4
1	A	835	ALA	2.4
1	A	745	HIS	2.4
1	B	138	ALA	2.3
1	A	234	GLU	2.3
1	A	287	CYS	2.3
1	B	510	GLN	2.3
1	A	548	LEU	2.3
1	B	214	ARG	2.3
1	A	427	LEU	2.3
1	A	1162	PHE	2.3
1	A	89	GLU	2.3
1	A	628	LEU	2.3
1	B	1137	LEU	2.2
1	B	227	ARG	2.2
1	A	285	ASN	2.2
1	B	176	THR	2.2
1	A	764	PHE	2.2
1	A	1022	THR	2.2
1	A	553	LYS	2.2
1	A	228	MET	2.2
1	A	252	VAL	2.2
1	B	210	GLU	2.2
1	A	136	ALA	2.2
1	A	266	ALA	2.2
1	A	540	LEU	2.2
1	A	558	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	729	HIS	2.2
1	B	266	ALA	2.2
1	B	1083	VAL	2.1
1	A	207	MET	2.1
1	A	232	LEU	2.1
1	A	717	ASP	2.1
1	A	734	SER	2.1
1	B	508	HIS	2.1
1	B	1152	HIS	2.1
1	A	1142	LEU	2.1
1	A	1026	ARG	2.1
1	B	890	ILE	2.0
1	B	752	TYR	2.0
1	B	1090	LEU	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, 95^{th} 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
2	SO4	B	1236	5/5	0.96	0.12	-2.32	86,89,90,91	0
4	GAI	B	1239	4/4	0.98	0.14	-2.90	41,41,42,42	0
3	HG	B	1238	1/1	0.97	0.03	-	142,142,142,142	0
2	SO4	B	1237	5/5	0.85	0.17	-	111,112,112,113	0

6.5 Other polymers (i)

There are no such residues in this entry.