



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:10 AM UTC

PDB ID : 2GV9 / pdb_00002gv9
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

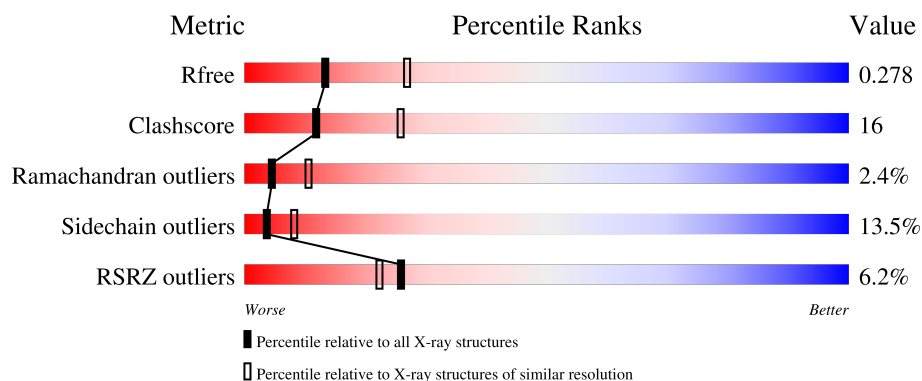
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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}	180053	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (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 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1193	5% 50% 25% 6% • 18%
1	B	1193	6% 59% 21% 6% • 13%

2 Entry composition [i](#)

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 (CCD ID: SO4) (formula: O₄S).

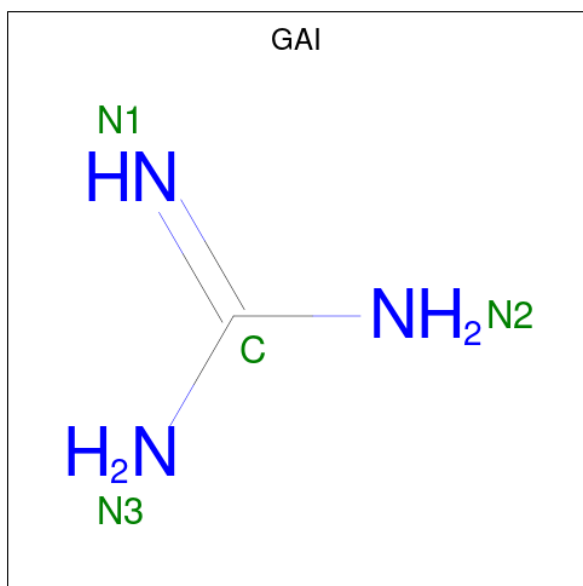


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

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

- Molecule 4 is GUANIDINE (CCD ID: GAI) (formula: CH_5N_3).



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

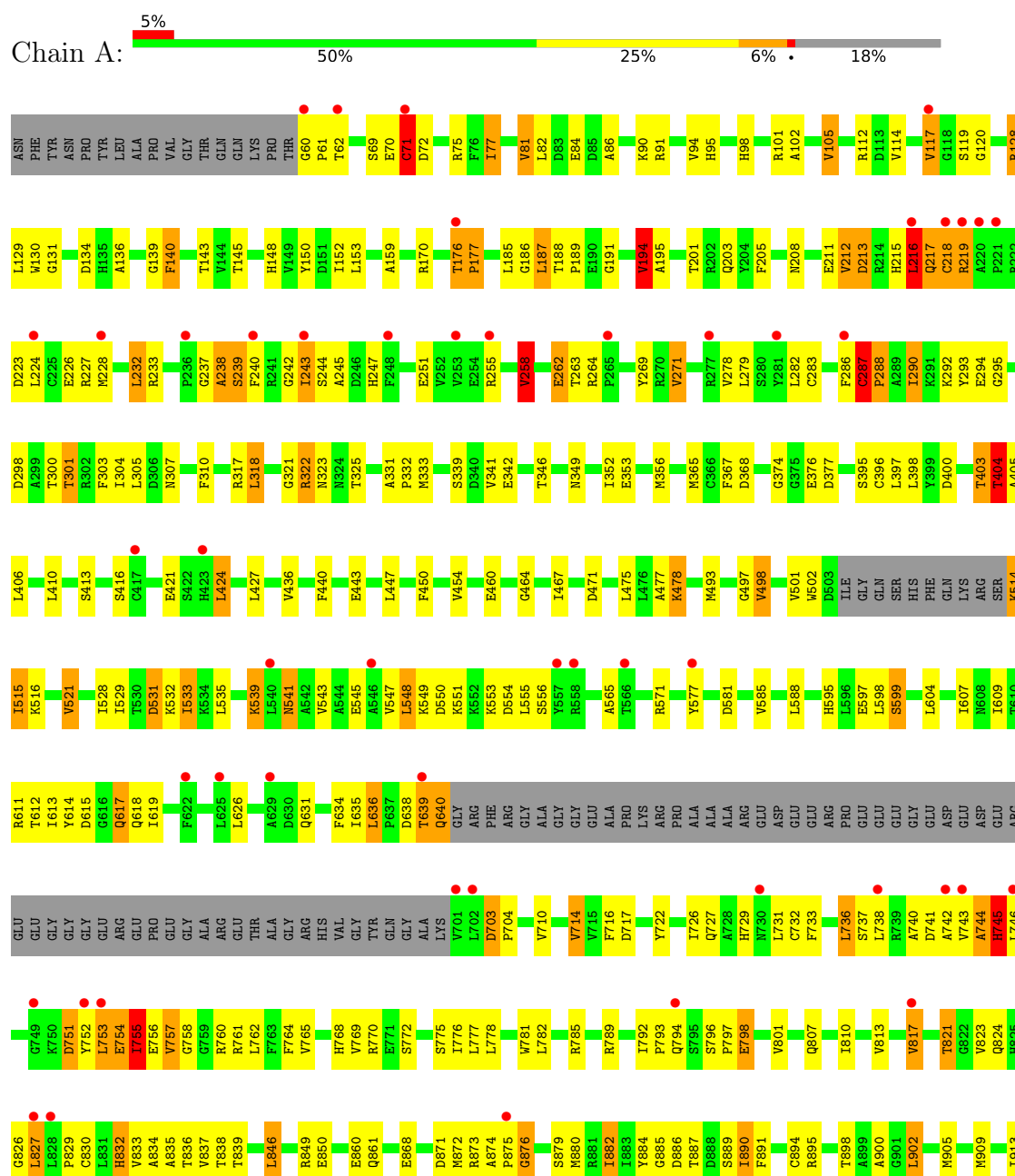
- Molecule 5 is water.

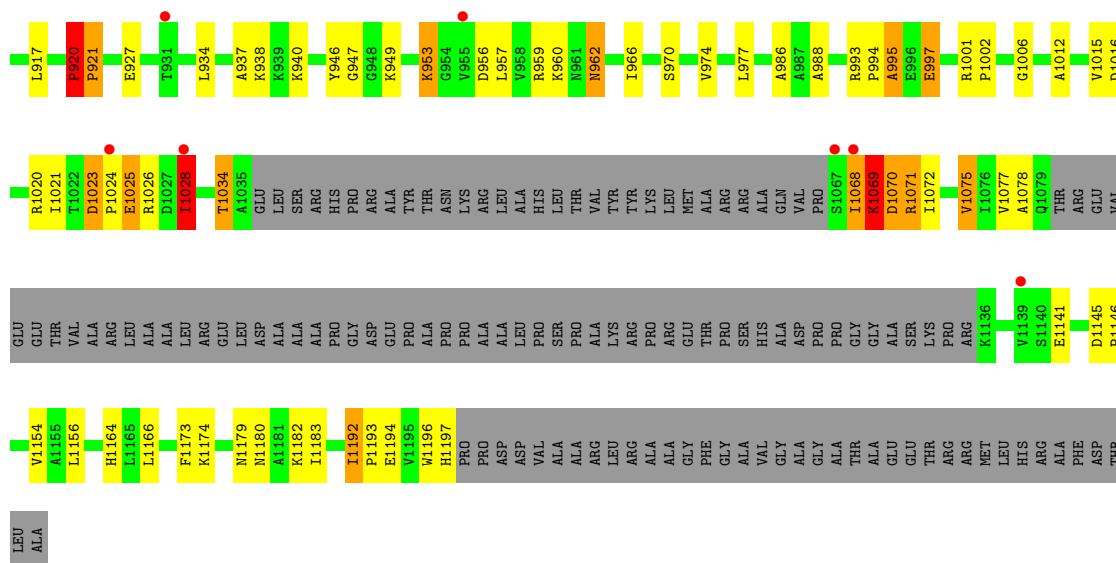
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	33	Total O 33 33	0	0
5	B	54	Total O 54 54	0	0

3 Residue-property plots

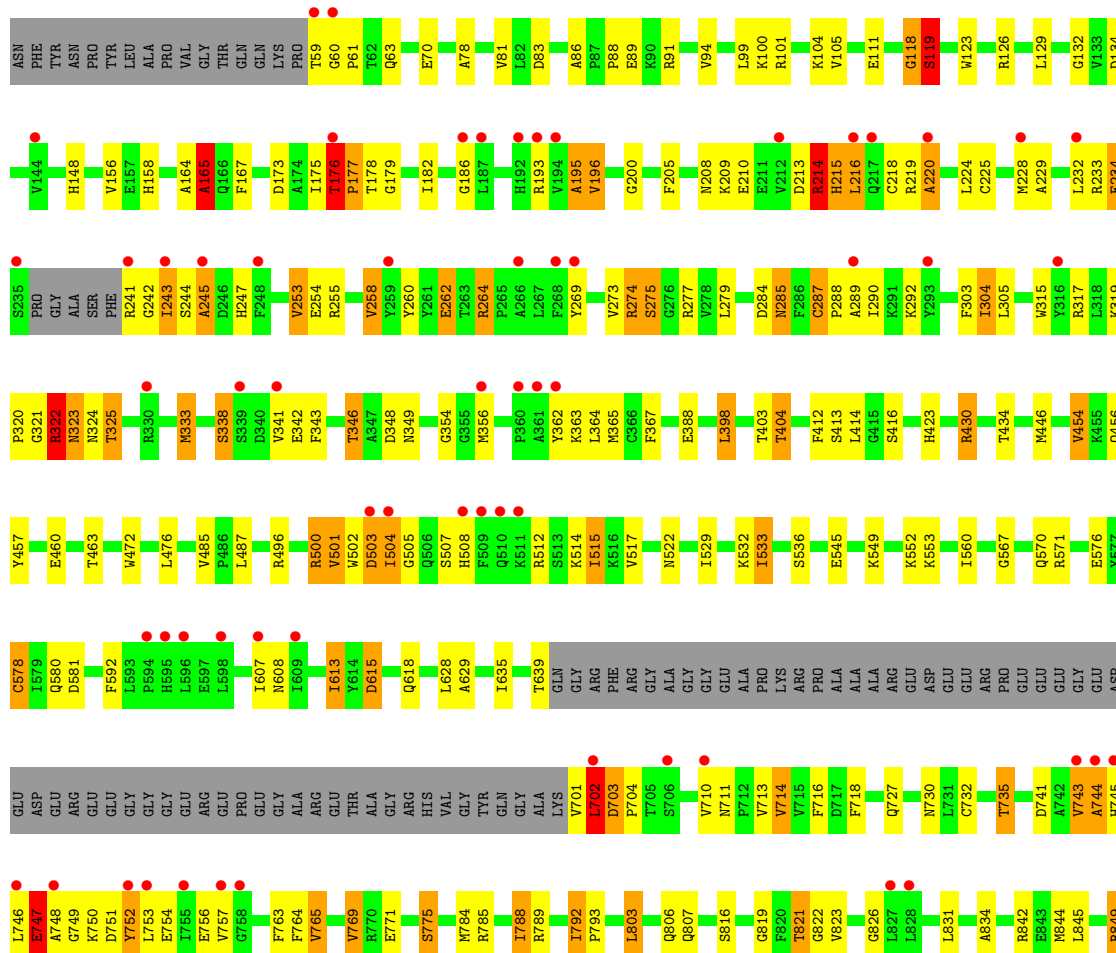
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

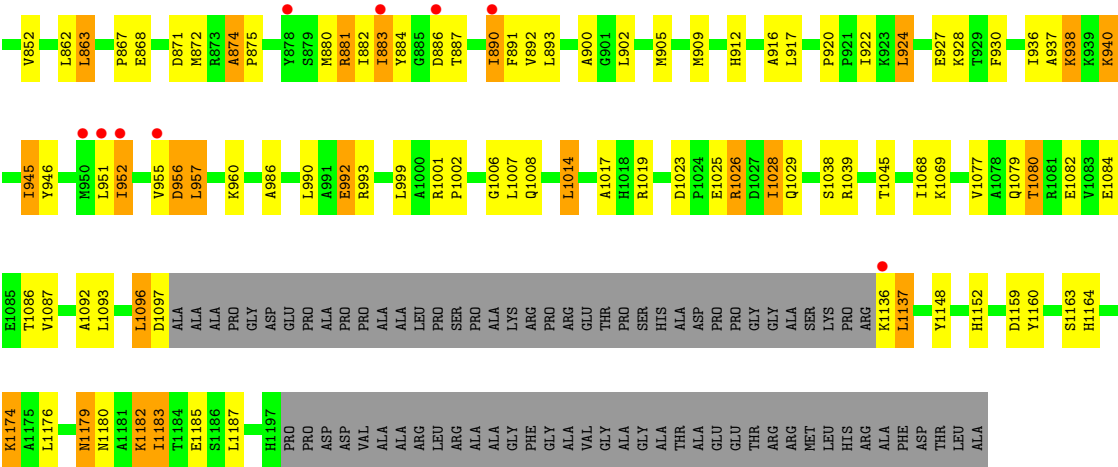
• Molecule 1: DNA polymerase





• Molecule 1: DNA polymerase





4 Data and refinement statistics

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 48.30 – 2.68	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.30-2.68) 99.3 (48.30-2.68)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.222 , 0.281 0.221 , 0.278	Depositor DCC
R_{free} test set	4070 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	67.5	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 65.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HG, SO4, GAI

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	0.99	4/7908 (0.1%)	1.22	30/10727 (0.3%)
1	B	1.11	5/8371 (0.1%)	1.13	26/11352 (0.2%)
All	All	1.05	9/16279 (0.1%)	1.18	56/22079 (0.3%)

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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	CYS	CB-SG	8.51	2.09	1.81
1	A	498	VAL	CA-CB	5.79	1.62	1.54
1	A	71	CYS	CA-CB	5.71	1.63	1.53
1	A	921	PRO	N-CA	-5.49	1.40	1.47
1	B	792	ILE	CA-CB	5.27	1.56	1.54
1	B	78	ALA	CA-CB	-5.23	1.46	1.54
1	B	176	THR	CA-CB	-5.11	1.47	1.53
1	B	196	VAL	CA-CB	5.04	1.60	1.54
1	B	262	GLU	CD-OE2	5.02	1.34	1.25

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	920	PRO	CA-C-N	34.73	163.25	119.84
1	A	920	PRO	C-N-CA	34.73	163.25	119.84
1	A	176	THR	CA-C-N	-16.99	101.30	118.97
1	A	176	THR	C-N-CA	-16.99	101.30	118.97
1	B	176	THR	CA-C-N	-12.65	104.03	119.84
1	B	176	THR	C-N-CA	-12.65	104.03	119.84
1	A	920	PRO	C-N-CD	-9.94	84.23	125.00
1	B	218	CYS	N-CA-C	9.66	125.28	108.75
1	A	1068	ILE	CB-CA-C	-9.26	100.03	111.88
1	A	177	PRO	N-CA-C	-8.75	100.96	113.47
1	A	1141	GLU	N-CA-C	-8.57	102.95	112.72
1	A	374	GLY	N-CA-C	-8.29	102.84	112.79
1	A	187	LEU	N-CA-C	7.20	119.68	108.96
1	A	921	PRO	CA-N-CD	-6.80	102.48	112.00
1	B	578	CYS	N-CA-C	6.48	118.88	111.11
1	B	354	GLY	N-CA-C	6.16	119.65	112.50
1	B	485	VAL	CB-CA-C	-6.14	103.72	110.78
1	B	613	ILE	CB-CA-C	-6.12	104.23	111.94
1	B	747	GLU	N-CA-C	6.12	119.63	110.14
1	B	165	ALA	CA-C-N	-6.03	110.03	121.54
1	B	165	ALA	C-N-CA	-6.03	110.03	121.54
1	B	118	GLY	N-CA-C	-5.96	99.05	113.18
1	A	755	ILE	N-CA-C	5.95	117.26	108.45
1	B	936	ILE	CB-CA-C	-5.84	104.91	111.80
1	B	165	ALA	N-CA-C	-5.79	98.46	110.80
1	B	849	ARG	N-CA-C	-5.75	104.70	110.97
1	B	769	VAL	N-CA-C	-5.75	105.51	110.74
1	A	413	SER	N-CA-C	5.73	117.98	108.13
1	A	258	VAL	CB-CA-C	-5.71	104.57	112.04
1	B	367	PHE	N-CA-C	5.67	118.30	109.52
1	A	1028	ILE	N-CA-C	-5.66	104.83	111.00
1	A	937	ALA	N-CA-C	5.64	115.84	107.88
1	A	287	CYS	CA-C-N	-5.62	112.81	119.84
1	A	287	CYS	C-N-CA	-5.62	112.81	119.84
1	B	132	GLY	N-CA-C	5.59	122.97	115.59
1	B	874	ALA	CA-C-N	5.53	126.76	119.84
1	B	874	ALA	C-N-CA	5.53	126.76	119.84
1	A	477	ALA	N-CA-C	-5.53	105.25	111.28
1	B	920	PRO	O-C-N	5.41	123.80	121.31
1	A	239	SER	N-CA-C	-5.41	106.52	113.01
1	A	71	CYS	N-CA-CB	5.38	119.85	110.81
1	B	287	CYS	N-CA-C	5.38	118.26	110.14
1	A	216	LEU	CA-C-N	5.38	131.38	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	LEU	C-N-CA	5.38	131.38	121.70
1	A	838	THR	CB-CA-C	-5.36	102.23	110.81
1	B	258	VAL	CB-CA-C	-5.35	101.57	111.79
1	A	1021	ILE	CB-CA-C	-5.33	105.06	112.04
1	B	200	GLY	N-CA-C	5.20	121.97	115.21
1	A	194	VAL	N-CA-C	5.13	115.87	108.48
1	A	1023	ASP	CB-CA-C	5.12	117.50	109.37
1	B	195	ALA	CA-C-N	-5.05	116.56	123.12
1	B	195	ALA	C-N-CA	-5.05	116.56	123.12
1	B	434	THR	N-CA-C	-5.04	103.30	109.65
1	A	729	HIS	N-CA-C	5.03	118.30	112.97
1	A	331	ALA	CA-C-N	5.01	126.10	119.84
1	A	331	ALA	C-N-CA	5.01	126.10	119.84

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 ⓘ

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	279	0
1	B	8180	0	8181	229	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	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	54	0	0	2	0
All	All	16007	0	15891	504	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 16.

All (504) 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:A:283:CYS:SG	1:A:292:LYS:NZ	2.29	1.05
1:B:702:LEU:O	1:B:702:LEU:HD23	1.54	1.05
1:A:882:ILE:HD13	1:A:882:ILE:C	1.83	1.03
1:B:287:CYS:SG	1:B:290:ILE:HD13	1.98	1.03
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:HE2	1.48	0.94
1:B:852:VAL:HG13	1:B:880:MET:HE2	1.50	0.93
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:1034:THR:HG22	1:A:1070:ASP:C	1.95	0.92
1:A:365:MET:HE2	1:A:396:CYS:SG	2.09	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: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
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:430:ARG:HG2	1:B:430:ARG:HH11	1.46	0.81
1:A:529:ILE:HD13	1:A:543:VAL:HG11	1.63	0.80
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:413:SER:C	1:B:446:MET:CE	2.57	0.78
1:B:872:MET:SD	1:B:905:MET:HE2	2.22	0.78
1:A:367:PHE:HA	1:A:395:SER:O	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:LEU:HD12	1:A:754:GLU:H	1.50	0.77
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:HD13	1:A:882:ILE:O	1.85	0.75
1:A:1023:ASP:HB2	1:A:1025:GLU:HG2	1.69	0.75
1:A:287:CYS:O	1:A:288:PRO:C	2.29	0.74
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:1069:LYS:O	1:A:1070:ASP:C	2.31	0.74
1:A:170:ARG:HH22	1:A:349:ASN:HD21	1.35	0.74
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:472:TRP:HE1	1:B:522:ASN:HD21	1.36	0.73
1:A:727:GLN:HE22	1:A:782:LEU:HD12	1.53	0.73
1:B:472:TRP:HE1	1:B:522:ASN:ND2	1.85	0.73
1:B:872:MET:SD	1:B:905:MET:CE	2.76	0.73
1:A:716:PHE:HB2	1:A:890:ILE:HG22	1.71	0.73
1:B:290:ILE:N	1:B:290:ILE:HD12	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: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:B:905:MET:HG2	1:B:909:MET:HE3	1.73	0.71
1:B:414:LEU:N	1:B:446:MET:CE	2.53	0.71
1:A:228:MET:CE	1:A:282:LEU:HD13	2.20	0.71
1:A:493:MET:HE3	1:A:497:GLY:HA2	1.72	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
1:B:702:LEU:HD13	1:B:849:ARG:NH1	2.07	0.70
1:A:778:LEU:HD11	1:A:817:VAL:HG21	1.73	0.69
1:A:962:ASN:ND2	5:A:1243:HOH:O	2.25	0.69
1:B:765:VAL:HG13	1:B:769:VAL:HB	1.74	0.69
1:B:219:ARG:O	1:B:220:ALA:CB	2.40	0.69
1:B:504:ILE:HD12	1:B:504:ILE:H	1.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:872:MET:CE	1:A:905:MET:HE2	2.22	0.69
1:B:414:LEU:N	1:B:446:MET:HE1	2.08	0.69
1:B:413:SER:C	1:B:446:MET:HE3	2.18	0.68
1:B:164:ALA:C	1:B:165:ALA:O	2.31	0.68
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:A:98:HIS:ND1	5:A:1267:HOH:O	2.25	0.68
1:B:88:PRO:HA	1:B:91:ARG:HD2	1.77	0.67
1:B:123:TRP:HE1	1:B:456:GLN:NE2	1.92	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:882:ILE:C	1:A:882:ILE:CD1	2.61	0.67
1:A:765:VAL:CG1	1:A:769:VAL:HB	2.24	0.66
1:B:61:PRO:N	1:B:333:MET:HE3	2.10	0.66
1:A:541:ASN:H	1:A:541:ASN:ND2	1.94	0.65
1:B:844:MET:HE3	1:B:922:ILE:HD13	1.78	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:A:835:ALA:O	1:A:839:THR:HG23	1.97	0.65
1:B:788:ILE:CD1	1:B:803:LEU:O	2.45	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:852:VAL:CG1	1:B:880:MET:HE2	2.26	0.64
1:B:1080:THR:HG22	1:B:1082:GLU:N	2.13	0.63
1:A:872:MET:SD	1:A:905:MET:HE2	2.37	0.63
1:A:410:LEU:HD23	1:A:436:VAL:HB	1.80	0.63
1:B:413:SER:N	1:B:446:MET:HE2	2.12	0.63
1:A:317:ARG:HD3	5:A:1240:HOH:O	1.99	0.63
1:B:788:ILE:CD1	1:B:807:GLN:HB3	2.28	0.63
1:A:905:MET:CG	1:A:909:MET:HE2	2.26	0.63
1:B:412:PHE:C	1:B:446:MET:HE2	2.24	0.62
1:B:874:ALA:HB1	1:B:875:PRO:HD2	1.80	0.62
1:A:226:GLU:HG3	1:A:245:ALA:HB2	1.81	0.62
1:A:213:ASP:OD1	1:A:219:ARG:HA	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:872:MET:HE1	1:A:905:MET:HE2	1.82	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:A:493:MET:HE3	1:A:497:GLY:CA	2.30	0.61
1:A:228:MET:HE3	1:A:282:LEU:HD22	1.81	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:A:1077:VAL:HG11	1:A:1154:VAL:HG11	1.82	0.60
1:B:242:GLY:O	1:B:243:ILE:HB	2.02	0.60
1:A:61:PRO:HD3	1:A:333:MET:HE1	1.84	0.60
1:B:244:SER:O	1:B:245:ALA:CB	2.50	0.60
1:A:61:PRO:CD	1:A:333:MET:HE1	2.32	0.59
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:159:ALA:HB2	1:A:176:THR:HA	1.84	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: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:414:LEU:N	1:B:446:MET:HE3	2.18	0.58
1:A:986:ALA:HB2	1:A:1006:GLY:HA3	1.84	0.58
1:B:727:GLN:HA	1:B:775:SER:OG	2.04	0.58
1:A:208:ASN:HD22	1:A:211:GLU:H	1.52	0.58
1:B:244:SER:HA	1:B:247:HIS:ND1	2.18	0.58
1:A:321:GLY:O	1:A:323:ASN:N	2.36	0.58
1:B:158:HIS:ND1	1:B:178:THR:HG22	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:832:HIS:O	1:A:836:THR:HG23	2.05	0.57
1:B:225:CYS:HA	1:B:228:MET:CE	2.35	0.57
1:A:216:LEU:HA	1:A:217:GLN:CB	2.34	0.57
1:B:845:LEU:HD22	1:B:890:ILE:HD11	1.86	0.57
1:B:992:GLU:O	1:B:993:ARG:HG3	2.04	0.57
1:B:430:ARG:HG2	1:B:430:ARG:NH1	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:A:176:THR:O	1:A:177:PRO:C	2.37	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:1174:LYS:HZ2	1:B:1174:LYS:HB2	1.70	0.56
1:A:117:VAL:HG12	1:A:130:TRP:CD1	2.40	0.56
1:A:213:ASP:OD1	1:A:219:ARG:CA	2.53	0.56
1:A:1075:VAL:CG1	1:A:1156:LEU:CD2	2.84	0.56
1:B:413:SER:CA	1:B:446:MET:CE	2.83	0.56
1:B:702:LEU:O	1:B:702:LEU:CD2	2.42	0.56
1:A:539:LYS:O	1:A:543:VAL:HG23	2.05	0.56
1:B:702:LEU:HD13	1:B:849:ARG:HH12	1.70	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:O	1:B:515:ILE:CG2	2.53	0.56
1:A:467:ILE:HA	1:A:471:ASP:HB2	1.88	0.55
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:129:LEU:HD21	1:A:332:PRO:O	2.06	0.55
1:A:514:LYS:N	1:A:614:TYR:CD2	2.75	0.55
1:A:785:ARG:O	1:A:789:ARG:HG3	2.07	0.55
1:B:552:LYS:HD2	1:B:553:LYS:O	2.06	0.55
1:A:703:ASP:HB2	1:A:704:PRO:CD	2.37	0.55
1:A:533:ILE:HD13	1:A:547:VAL:HG22	1.88	0.55
1:A:1034:THR:HG22	1:A:1070:ASP:O	2.06	0.55
1:B:515:ILE:O	1:B:515:ILE:HG22	2.07	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:152:ILE:HG21	1:A:300:THR:HG23	1.89	0.54
1:A:223:ASP:O	1:A:227:ARG:HG3	2.06	0.54
1:B:321:GLY:HA3	1:B:325:THR:HG22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:ARG:HB3	1:B:323:ASN:ND2	2.21	0.54
1:A:703:ASP:HB2	1:A:704:PRO:HD3	1.88	0.54
1:A:879:SER:HB3	1:A:895:ARG:HB2	1.88	0.54
1:B:743:VAL:O	1:B:744:ALA:C	2.51	0.54
1:B:1182:LYS:O	1:B:1183:ILE:C	2.51	0.54
1:A:397:LEU:HD13	1:A:406:LEU:HD21	1.90	0.54
1:A:611:ARG:HG2	1:A:615:ASP:OD2	2.08	0.53
1:A:1012:ALA:O	1:A:1016:ASP:HB2	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:A:237:GLY:O	1:A:238:ALA:HB3	2.07	0.53
1:A:1028:ILE:H	1:A:1028:ILE:HD12	1.73	0.53
1:B:883:ILE:O	1:B:883:ILE:HD12	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:732:CYS:SG	1:A:733:PHE:N	2.81	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: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:A:1075:VAL:HG11	1:A:1156:LEU:CD2	2.39	0.52
1:B:423:HIS:ND1	1:B:576:GLU:HG3	2.24	0.52
1:A:464:GLY:HA2	1:A:585:VAL:HG11	1.91	0.52
1:A:994:PRO:HD2	1:A:997:GLU:HG3	1.91	0.52
1:B:403:THR:O	1:B:404:THR:CB	2.51	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:B:905:MET:HG2	1:B:909:MET:CE	2.38	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:212:VAL:CG2	1:A:290:ILE:HG21	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:913:ILE:HG23	1:A:917:LEU:HD12	1.91	0.51
1:A:1028:ILE:HD12	1:A:1028:ILE:N	2.26	0.51
1:B:254:GLU:O	1:B:255:ARG:HG2	2.11	0.51
1:B:284:ASP:C	1:B:285:ASN:OD1	2.53	0.51
1:B:868:GLU:O	1:B:872:MET:HE3	2.10	0.51
1:B:325:THR:HG23	1:B:349:ASN:HD21	1.75	0.51
1:B:765:VAL:CG1	1:B:769:VAL:HB	2.40	0.51
1:B:126:ARG:HH22	1:B:460:GLU:CD	2.19	0.51
1:B:315:TRP:CG	1:B:356:MET:HG2	2.45	0.51
1:A:203:GLN:NE2	1:A:279:LEU:CD2	2.74	0.51
1:B:165:ALA:HB1	1:B:167:PHE:CE2	2.45	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:1068:ILE:HA	5:A:1256:HOH:O	2.11	0.50
1:A:205:PHE:CE2	1:A:271:VAL:HG22	2.46	0.50
1:B:552:LYS:NZ	1:B:581:ASP:OD1	2.42	0.50
1:B:930:PHE:CE2	1:B:945:ILE:CD1	2.95	0.50
1:A:293:TYR:HB3	1:A:635:ILE:HG21	1.92	0.50
1:B:999:LEU:HD23	1:B:1187:LEU:CD2	2.39	0.50
1:A:994:PRO:O	1:A:995:ALA:C	2.55	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:188:THR:HB	1:A:189:PRO:HD2	1.93	0.49
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:B:1148:TYR:CE1	1:B:1152:HIS:CE1	3.00	0.49
1:A:846:LEU:O	1:A:850:GLU:HG3	2.12	0.49
1:B:819:GLY:O	1:B:823:VAL:HG23	2.13	0.49
1:B:1159:ASP:O	1:B:1163:SER:HB2	2.12	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:A:239:SER:O	1:A:240:PHE:C	2.56	0.49
1:A:532:LYS:NZ	1:A:597:GLU:OE1	2.46	0.49
1:A:884:TYR:HB3	1:A:891:PHE:HB2	1.94	0.49
1:B:225:CYS:HA	1:B:228:MET:HE2	1.94	0.49
1:A:139:GLY:O	1:A:140:PHE:C	2.56	0.49
1:A:874:ALA:HB1	1:A:875:PRO:CD	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ARG:O	1:B:216:LEU:N	2.46	0.49
1:B:290:ILE:N	1:B:290:ILE:CD1	2.74	0.49
1:B:784:MET:O	1:B:788:ILE:HG23	2.12	0.49
1:A:61:PRO:N	1:A:333:MET:CE	2.76	0.49
1:B:404:THR:O	1:B:404:THR:CG2	2.61	0.49
1:B:61:PRO:CD	1:B:333:MET:HE3	2.43	0.48
1:A:832:HIS:ND1	1:A:832:HIS:N	2.60	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:205:PHE:HD2	1:B:279:LEU:HD11	1.77	0.48
1:B:323:ASN:HD22	1:B:323:ASN:N	2.11	0.48
1:B:821:THR:HG22	1:B:834:ALA:HB2	1.95	0.48
1:A:450:PHE:O	1:A:454:VAL:HG23	2.13	0.48
1:A:521:VAL:HG11	1:A:609:ILE:HD13	1.95	0.48
1:A:604:LEU:HD23	1:A:813:VAL:HG21	1.95	0.48
1:A:872:MET:CE	1:A:905:MET:CE	2.89	0.48
1:A:1023:ASP:C	1:A:1025:GLU:N	2.72	0.48
1:A:1075:VAL:CG1	1:A:1156:LEU:HD23	2.43	0.48
1:B:718:PHE:HE1	1:B:845:LEU:HD23	1.79	0.48
1:A:443:GLU:OE2	1:A:478:LYS:NZ	2.46	0.48
1:A:736:LEU:HG	1:A:737:SER:N	2.28	0.48
1:B:129:LEU:HD23	1:B:134:ASP:HA	1.94	0.48
1:B:173:ASP:O	1:B:176:THR:OG1	2.32	0.48
1:A:303:PHE:O	1:A:307:ASN:ND2	2.41	0.47
1:B:404:THR:O	1:B:404:THR:HG23	2.14	0.47
1:A:744:ALA:HB3	1:A:746:LEU:HG	1.96	0.47
1:B:1026:ARG:NH1	1:B:1028:ILE:HD12	2.29	0.47
1:A:233:ARG:NH1	1:A:243:ILE:HD11	2.29	0.47
1:B:244:SER:O	1:B:245:ALA:HB3	2.14	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:A:60:GLY:C	1:A:333:MET:CE	2.88	0.47
1:B:229:ALA:HB1	1:B:244:SER:HB2	1.96	0.47
1:A:886:ASP:OD1	1:A:887:THR:N	2.48	0.47
1:B:60:GLY:C	1:B:333:MET:HE3	2.38	0.47
1:B:325:THR:CG2	1:B:349:ASN:HD21	2.27	0.47
1:B:416:SER:O	1:B:571:ARG:HD2	2.14	0.47
1:B:703:ASP:CB	1:B:704:PRO:CD	2.93	0.47
1:B:937:ALA:O	1:B:938:LYS:C	2.57	0.47
1:B:1001:ARG:HD3	1:B:1002:PRO:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:LEU:CD1	1:A:626:LEU:HD23	2.45	0.47
1:A:940:LYS:HA	1:A:953:LYS:O	2.15	0.47
1:A:1025:GLU:OE2	1:A:1025:GLU:HA	2.14	0.47
1:B:213:ASP:OD1	1:B:269:TYR:OH	2.33	0.47
1:B:264:ARG:H	1:B:264:ARG:CD	2.24	0.47
1:A:244:SER:HB3	1:A:247:HIS:NE2	2.29	0.46
1:A:1192:ILE:HD13	1:A:1196:TRP:HB2	1.96	0.46
1:A:555:LEU:HD13	1:A:577:TYR:CD1	2.50	0.46
1:A:607:ILE:HD13	1:A:619:ILE:HG23	1.97	0.46
1:B:785:ARG:O	1:B:789:ARG:HG3	2.15	0.46
1:B:502:TRP:CE2	1:B:512:ARG:HG3	2.51	0.46
1:B:747:GLU:HG3	1:B:752:TYR:CD2	2.50	0.46
1:B:1007:LEU:O	1:B:1008:GLN:C	2.59	0.46
1:A:239:SER:O	1:A:242:GLY:N	2.47	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:A:1194:GLU:HA	1:A:1197:HIS:CD2	2.50	0.46
1:B:315:TRP:CD2	1:B:356:MET:HG2	2.51	0.46
1:A:72:ASP:O	1:A:101:ARG:N	2.49	0.46
1:A:377:ASP:C	1:A:377:ASP:OD1	2.58	0.46
1:A:548:LEU:HD21	1:A:588:LEU:HD23	1.97	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:743:VAL:C	1:B:745:HIS:N	2.70	0.46
1:B:745:HIS:O	1:B:746:LEU:C	2.58	0.46
1:B:414:LEU:H	1:B:446:MET:HE1	1.80	0.46
1:B:732:CYS:HB3	1:B:735:THR:HB	1.97	0.46
1:B:784:MET:HE3	1:B:784:MET:HB2	1.78	0.46
1:B:1079:GLN:NE2	1:B:1137:LEU:HB2	2.31	0.46
1:A:60:GLY:N	1:A:333:MET:HE2	2.32	0.45
1:A:595:HIS:O	1:A:599:SER:OG	2.31	0.45
1:A:872:MET:HE1	1:A:902:LEU:HA	1.98	0.45
1:A:153:LEU:HD11	1:A:185:LEU:HD11	1.97	0.45
1:A:1180:ASN:ND2	1:A:1183:ILE:CD1	2.79	0.45
1:A:86:ALA:HB1	1:A:91:ARG:HD2	1.98	0.45
1:B:175:ILE:HG22	1:B:179:GLY:HA3	1.98	0.45
1:A:1145:ASP:OD2	1:A:1146:PRO:HD2	2.16	0.45
1:B:195:ALA:HB3	1:B:342:GLU:HG2	1.98	0.45
1:A:533:ILE:HD11	1:A:535:LEU:HD11	1.98	0.45
1:B:253:VAL:CG1	1:B:255:ARG:HG3	2.45	0.45
1:B:615:ASP:OD2	1:B:615:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:617:GLN:CD	1:A:617:GLN:H	2.23	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:232:LEU:HD11	1:A:278:VAL:HG13	1.98	0.45
1:A:598:LEU:O	1:A:599:SER:C	2.60	0.45
1:A:885:GLY:HA2	1:A:890:ILE:HD12	1.99	0.45
1:A:117:VAL:HG11	1:A:130:TRP:CG	2.52	0.45
1:A:757:VAL:HG12	1:A:758:GLY:N	2.32	0.45
1:B:765:VAL:HG21	1:B:769:VAL:HG11	1.99	0.45
1:A:244:SER:HB3	1:A:247:HIS:CD2	2.52	0.44
1:A:213:ASP:OD1	1:A:218:CYS:C	2.60	0.44
1:A:541:ASN:ND2	1:A:541:ASN:N	2.64	0.44
1:B:99:LEU:CD2	1:B:101:ARG:NH1	2.79	0.44
1:A:77:ILE:HA	1:A:95:HIS:O	2.18	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:B:822:GLY:HA2	1:B:831:LEU:HD23	1.99	0.44
1:A:744:ALA:O	1:A:745:HIS:C	2.61	0.44
1:A:977:LEU:HD22	1:A:1173:PHE:CE2	2.52	0.44
1:A:1072:ILE:O	1:A:1072:ILE:HG22	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: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:B:999:LEU:CD2	1:B:1187:LEU:HD21	2.43	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:B:912:HIS:C	1:B:912:HIS:CD2	2.95	0.44
1:A:318:LEU:HA	1:A:349:ASN:O	2.18	0.44
1:A:823:VAL:HG12	1:A:826:GLY:N	2.33	0.44
1:A:966:ILE:CD1	1:A:1164:HIS:HB3	2.48	0.44
1:B:515:ILE:HD13	1:B:517:VAL:HG23	1.99	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:321:GLY:O	1:A:322:ARG:C	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:THR:HG22	1:A:405:ALA:N	2.21	0.43
1:A:792:ILE:N	1:A:793:PRO:HD2	2.34	0.43
1:A:977:LEU:HD22	1:A:1173:PHE:HE2	1.82	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:61:PRO:N	1:A:333:MET:HE1	2.32	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:B:628:LEU:O	1:B:629:ALA:C	2.61	0.43
1:A:305:LEU:HD12	1:A:626:LEU:CD2	2.48	0.43
1:B:289:ALA:C	1:B:290:ILE:HD12	2.44	0.43
1:B:1160:TYR:O	1:B:1164:HIS:HD2	2.01	0.43
1:A:416:SER:O	1:A:571:ARG:HD2	2.18	0.43
1:A:533:ILE:HD11	1:A:535:LEU:CD1	2.48	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:A:216:LEU:HD22	1:A:227:ARG:NH1	2.34	0.43
1:B:319:LYS:HB2	1:B:320:PRO:HD2	1.99	0.43
1:B:882:ILE:CD1	1:B:892:VAL:HG22	2.49	0.43
1:A:528:ILE:O	1:A:531:ASP:HB2	2.19	0.42
1:A:946:TYR:CE2	1:B:868:GLU:HG2	2.54	0.42
1:A:807:GLN:C	1:A:807:GLN:CD	2.87	0.42
1:A:776:ILE:O	1:A:777:LEU:C	2.60	0.42
1:A:1001:ARG:HB2	1:A:1002:PRO:CD	2.50	0.42
1:A:396:CYS:C	1:A:397:LEU:HD23	2.44	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: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:A:794:GLN:OE1	1:B:771:GLU:CD	2.62	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:764:PHE:CE1	1:A:836:THR:HG21	2.54	0.42
1:A:1077:VAL:HG13	1:A:1154:VAL:HG12	2.00	0.42
1:B:788:ILE:HD11	1:B:807:GLN:CB	2.50	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:B:364:LEU:HD11	1:B:463:THR:CG2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:ASP:O	1:A:640:GLN:N	2.52	0.42
1:A:880:MET:HE2	1:A:894:CYS:SG	2.59	0.42
1:B:1182:LYS:O	1:B:1185:GLU:N	2.52	0.42
1:A:215:HIS:O	1:A:216:LEU:HB2	2.18	0.42
1:A:797:PRO:O	1:A:801:VAL:HG13	2.20	0.42
1:A:1192:ILE:HD12	1:A:1192:ILE:C	2.45	0.42
1:B:193:ARG:NH1	1:B:338:SER:O	2.52	0.42
1:B:1026:ARG:HD2	1:B:1026:ARG:C	2.44	0.42
1:B:1068:ILE:O	1:B:1069:LYS:HB2	2.20	0.42
1:B:529:ILE:HD11	1:B:592:PHE:CE1	2.55	0.42
1:B:1028:ILE:O	1:B:1029:GLN:C	2.63	0.42
1:A:150:TYR:CE1	1:A:460:GLU:HB3	2.55	0.41
1:A:872:MET:SD	1:A:905:MET:CE	3.05	0.41
1:B:264:ARG:N	1:B:264:ARG:CD	2.81	0.41
1:B:711:ASN:HB2	1:B:893:LEU:HD11	2.02	0.41
1:B:1080:THR:CG2	1:B:1082:GLU:H	2.30	0.41
1:A:554:ASP:HB2	1:A:577:TYR:CZ	2.55	0.41
1:A:1075:VAL:HG13	1:A:1156:LEU:CD2	2.50	0.41
1:B:104:LYS:HE3	1:B:111:GLU:OE2	2.19	0.41
1:B:244:SER:HA	1:B:247:HIS:CE1	2.54	0.41
1:B:341:VAL:CG1	1:B:343:PHE:CE2	3.03	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:365:MET:HE1	1:B:454:VAL:HG22	2.02	0.41
1:A:615:ASP:N	1:A:615:ASP:OD1	2.53	0.41
1:A:781:TRP:O	1:A:810:ILE:HG21	2.20	0.41
1:B:243:ILE:O	1:B:244:SER:OG	2.38	0.41
1:A:213:ASP:CG	1:A:219:ARG:HA	2.45	0.41
1:A:307:ASN:HB2	1:A:310:PHE:CD2	2.55	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:738:LEU:HD23	1:A:762:LEU:HD22	2.02	0.41
1:A:754:GLU:C	1:A:755:ILE:HG12	2.45	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:101:ARG:HG3	1:A:102:ALA:O	2.20	0.41
1:A:262:GLU:O	1:A:263:THR:C	2.63	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:247:HIS:CD2	1:A:247:HIS:N	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:LEU:C	1:A:398:LEU:HD23	2.46	0.41
1:A:555:LEU:HD22	1:A:577:TYR:CB	2.51	0.41
1:A:751:ASP:OD1	1:A:751:ASP:N	2.54	0.41
1:A:1034:THR:CG2	1:A:1070:ASP:C	2.79	0.41
1:A:1166:LEU:HD12	1:A:1166:LEU:HA	1.69	0.41
1:A:1174:LYS:CB	1:A:1179:ASN:HA	2.51	0.41
1:B:792:ILE:HB	1:B:793:PRO:HD3	2.02	0.41
1:B:916:ALA:O	1:B:917:LEU:HD23	2.21	0.41
1:B:1180:ASN:OD1	1:B:1182:LYS:HG3	2.21	0.41
1:A:1194:GLU:HA	1:A:1197:HIS:NE2	2.36	0.41
1:B:749:GLY:HA2	1:B:753:LEU:HD21	2.03	0.41
1:A:875:PRO:O	1:A:876:GLY:O	2.38	0.40
1:B:955:VAL:HG12	1:B:956:ASP:N	2.35	0.40
1:A:871:ASP:HB2	1:B:946:TYR:CD2	2.56	0.40
1:B:748:ALA:O	1:B:752:TYR:HB2	2.22	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:HB2	1:A:1001:ARG:HE	1.72	0.40
1:A:1075:VAL:HG11	1:A:1156:LEU:HD21	2.03	0.40
1:B:844:MET:CE	1:B:922:ILE:HD13	2.49	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%)	3	8
1	B	1027/1193 (86%)	934 (91%)	73 (7%)	20 (2%)	6	15
All	All	1998/2386 (84%)	1799 (90%)	151 (8%)	48 (2%)	4	10

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
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

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Mol	Chain	Res	Type
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 ⓘ

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%)	699 (86%)	115 (14%)	3	7
1	B	862/971 (89%)	750 (87%)	112 (13%)	4	9
All	All	1676/1942 (86%)	1449 (86%)	227 (14%)	4	8

All (227) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	THR
1	A	69	SER
1	A	70	GLU
1	A	71	CYS
1	A	75	ARG
1	A	77	ILE
1	A	81	VAL
1	A	82	LEU
1	A	90	LYS
1	A	94	VAL
1	A	105	VAL
1	A	117	VAL
1	A	128	ARG
1	A	143	THR
1	A	145	THR
1	A	194	VAL
1	A	201	THR

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Mol	Chain	Res	Type
1	A	212	VAL
1	A	213	ASP
1	A	218	CYS
1	A	219	ARG
1	A	224	LEU
1	A	232	LEU
1	A	243	ILE
1	A	251	GLU
1	A	255	ARG
1	A	258	VAL
1	A	262	GLU
1	A	264	ARG
1	A	271	VAL
1	A	290	ILE
1	A	301	THR
1	A	304	ILE
1	A	318	LEU
1	A	325	THR
1	A	339	SER
1	A	352	ILE
1	A	368	ASP
1	A	403	THR
1	A	404	THR
1	A	421	GLU
1	A	424	LEU
1	A	427	LEU
1	A	478	LYS
1	A	498	VAL
1	A	502	TRP
1	A	515	ILE
1	A	516	LYS
1	A	521	VAL
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	553	LYS
1	A	556	SER

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Mol	Chain	Res	Type
1	A	581	ASP
1	A	599	SER
1	A	613	ILE
1	A	617	GLN
1	A	631	GLN
1	A	636	LEU
1	A	639	THR
1	A	640	GLN
1	A	714	VAL
1	A	717	ASP
1	A	736	LEU
1	A	745	HIS
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	768	HIS
1	A	770	ARG
1	A	796	SER
1	A	798	GLU
1	A	817	VAL
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	868	GLU
1	A	873	ARG
1	A	882	ILE
1	A	890	ILE
1	A	902	LEU
1	A	934	LEU
1	A	949	LYS
1	A	953	LYS
1	A	956	ASP
1	A	957	LEU
1	A	959	ARG
1	A	960	LYS

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Mol	Chain	Res	Type
1	A	962	ASN
1	A	970	SER
1	A	974	VAL
1	A	993	ARG
1	A	997	GLU
1	A	1015	VAL
1	A	1020	ARG
1	A	1025	GLU
1	A	1028	ILE
1	A	1034	THR
1	A	1069	LYS
1	A	1075	VAL
1	A	1182	LYS
1	A	1192	ILE
1	B	59	THR
1	B	70	GLU
1	B	81	VAL
1	B	89	GLU
1	B	94	VAL
1	B	100	LYS
1	B	105	VAL
1	B	119	SER
1	B	156	VAL
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	224	LEU
1	B	232	LEU
1	B	233	ARG
1	B	234	GLU
1	B	241	ARG
1	B	253	VAL
1	B	258	VAL
1	B	262	GLU
1	B	264	ARG
1	B	274	ARG
1	B	285	ASN
1	B	292	LYS

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Mol	Chain	Res	Type
1	B	304	ILE
1	B	305	LEU
1	B	317	ARG
1	B	322	ARG
1	B	323	ASN
1	B	324	ASN
1	B	325	THR
1	B	333	MET
1	B	338	SER
1	B	346	THR
1	B	388	GLU
1	B	398	LEU
1	B	404	THR
1	B	430	ARG
1	B	454	VAL
1	B	500	ARG
1	B	501	VAL
1	B	503	ASP
1	B	504	ILE
1	B	507	SER
1	B	508	HIS
1	B	515	ILE
1	B	533	ILE
1	B	536	SER
1	B	560	ILE
1	B	570	GLN
1	B	578	CYS
1	B	607	ILE
1	B	608	ASN
1	B	613	ILE
1	B	615	ASP
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
1	B	752	TYR

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Mol	Chain	Res	Type
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	862	LEU
1	B	863	LEU
1	B	871	ASP
1	B	881	ARG
1	B	883	ILE
1	B	890	ILE
1	B	924	LEU
1	B	927	GLU
1	B	940	LYS
1	B	945	ILE
1	B	951	LEU
1	B	952	ILE
1	B	956	ASP
1	B	957	LEU
1	B	960	LYS
1	B	992	GLU
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	1045	THR
1	B	1077	VAL
1	B	1080	THR
1	B	1086	THR
1	B	1093	LEU
1	B	1136	LYS
1	B	1174	LYS
1	B	1179	ASN
1	B	1182	LYS
1	B	1183	ILE

Sometimes 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
1	A	349	ASN
1	A	408	HIS
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	806	GLN
1	A	1152	HIS
1	A	1164	HIS
1	A	1179	ASN
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	510	GLN
1	B	522	ASN
1	B	618	GLN
1	B	787	GLN
1	B	824	GLN
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	GAI	B	1239	-	3,3,3	0.80	0	3,3,3	0.25	0
2	SO4	B	1236	-	4,4,4	0.33	0	6,6,6	0.36	0
2	SO4	B	1237	-	4,4,4	0.25	0	6,6,6	0.35	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, 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	981/1193 (82%)	0.58	56 (5%)	29	25	41, 61, 88, 104	0
1	B	1035/1193 (86%)	0.53	70 (6%)	23	20	39, 60, 85, 99	0
All	All	2016/2386 (84%)	0.55	126 (6%)	26	22	39, 60, 87, 104	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	509	PHE	5.6
1	A	236	PRO	4.5
1	A	742	ALA	4.5
1	B	212	VAL	4.5
1	A	752	TYR	4.3
1	A	240	PHE	3.9
1	A	286	PHE	3.9
1	B	745	HIS	3.6
1	A	220	ALA	3.6
1	B	753	LEU	3.6
1	B	243	ILE	3.6
1	B	828	LEU	3.5
1	A	417	CYS	3.4
1	B	269	TYR	3.4
1	B	59	THR	3.4
1	A	117	VAL	3.3
1	B	217	GLN	3.3
1	B	232	LEU	3.2
1	B	187	LEU	3.1
1	B	235	SER	3.1
1	B	710	VAL	3.1
1	B	744	ALA	3.0
1	B	341	VAL	3.0
1	B	293	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	71	CYS	2.9
1	B	503	ASP	2.9
1	A	794	GLN	2.9
1	B	339	SER	2.9
1	B	755	ILE	2.9
1	B	508	HIS	2.9
1	B	827	LEU	2.8
1	A	1068	ILE	2.8
1	B	510	GLN	2.7
1	B	883	ILE	2.7
1	A	753	LEU	2.7
1	B	220	ALA	2.7
1	B	266	ALA	2.7
1	A	221	PRO	2.7
1	A	1024	PRO	2.7
1	B	607	ILE	2.7
1	B	890	ILE	2.7
1	A	827	LEU	2.7
1	B	216	LEU	2.7
1	B	504	ILE	2.7
1	B	702	LEU	2.7
1	B	362	TYR	2.6
1	A	746	LEU	2.6
1	A	955	VAL	2.6
1	A	1139	VAL	2.6
1	A	1028	ILE	2.6
1	A	60	GLY	2.6
1	B	360	PRO	2.6
1	B	757	VAL	2.6
1	B	241	ARG	2.5
1	B	1136	LYS	2.5
1	B	194	VAL	2.5
1	B	228	MET	2.5
1	B	743	VAL	2.5
1	B	955	VAL	2.5
1	A	248	PHE	2.5
1	B	746	LEU	2.5
1	B	952	ILE	2.4
1	B	361	ALA	2.4
1	B	176	THR	2.4
1	B	594	PRO	2.4
1	A	701	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	281	TYR	2.4
1	A	540	LEU	2.4
1	A	265	PRO	2.4
1	B	245	ALA	2.4
1	B	248	PHE	2.4
1	B	60	GLY	2.3
1	A	219	ARG	2.3
1	A	253	VAL	2.3
1	A	828	LEU	2.3
1	A	557	TYR	2.3
1	A	176	THR	2.3
1	A	577	TYR	2.3
1	A	218	CYS	2.2
1	B	192	HIS	2.2
1	A	228	MET	2.2
1	A	255	ARG	2.2
1	B	951	LEU	2.2
1	A	243	ILE	2.2
1	A	875	PRO	2.2
1	A	702	LEU	2.2
1	B	268	PHE	2.2
1	A	62	THR	2.2
1	A	730	ASN	2.2
1	A	749	GLY	2.2
1	B	186	GLY	2.2
1	A	1067	SER	2.2
1	A	743	VAL	2.2
1	B	193	ARG	2.2
1	A	625	LEU	2.2
1	A	423	HIS	2.2
1	B	609	ILE	2.2
1	A	622	PHE	2.2
1	A	931	THR	2.1
1	B	316	TYR	2.1
1	B	758	GLY	2.1
1	A	817	VAL	2.1
1	B	748	ALA	2.1
1	A	639	THR	2.1
1	B	356	MET	2.1
1	B	259	TYR	2.1
1	B	144	VAL	2.1
1	B	706	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	289	ALA	2.1
1	A	277	ARG	2.1
1	B	511	LYS	2.1
1	A	216	LEU	2.1
1	B	598	LEU	2.1
1	A	558	ARG	2.1
1	B	330	ARG	2.1
1	A	224	LEU	2.1
1	B	595	HIS	2.1
1	B	878	TYR	2.1
1	A	738	LEU	2.0
1	B	752	TYR	2.0
1	A	546	ALA	2.0
1	A	629	ALA	2.0
1	B	886	ASP	2.0
1	A	566	THR	2.0
1	B	950	MET	2.0
1	B	596	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	SO4	B	1237	5/5	0.73	0.10	111,112,112,113	0
2	SO4	B	1236	5/5	0.85	0.17	86,89,90,91	0
4	GAI	B	1239	4/4	0.97	0.07	41,41,42,42	0
3	HG	B	1238	1/1	0.98	0.13	142,142,142,142	0

6.5 Other polymers [i](#)

There are no such residues in this entry.