



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:17 PM UTC

PDB ID : 2ZKU / pdb_00002zku
Title : Structure of hepatitis C virus NS5B polymerase in a new crystal form
Authors : Biswal, B.K.
Deposited on : 2008-03-31
Resolution : 1.95 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

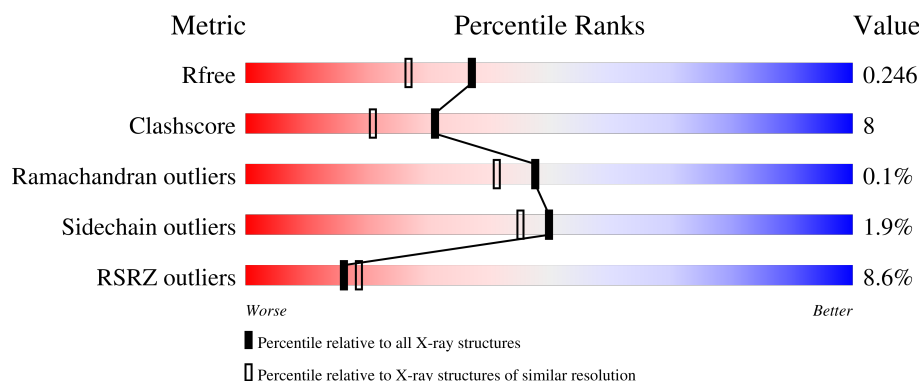
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	576	8% 80% 16% ..
1	B	576	8% 78% 18% ..
1	C	576	9% 75% 22% ..
1	D	576	9% 81% 15% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	4001	-	X	-	-
3	GOL	A	4002	-	X	-	-
3	GOL	A	4004	-	X	-	-
3	GOL	A	4005	-	X	-	-
3	GOL	A	4006	-	X	-	-
3	GOL	B	4003	-	X	-	-
3	GOL	B	4007	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19620 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 Genome polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	562	Total	C	N	O	S	0	0	0
			4372	2758	772	811	31			
1	B	561	Total	C	N	O	S	0	0	0
			4355	2747	768	809	31			
1	C	563	Total	C	N	O	S	0	0	0
			4376	2760	773	812	31			
1	D	558	Total	C	N	O	S	0	0	0
			4340	2738	765	806	31			

There are 24 discrepancies between the modelled and reference sequences:

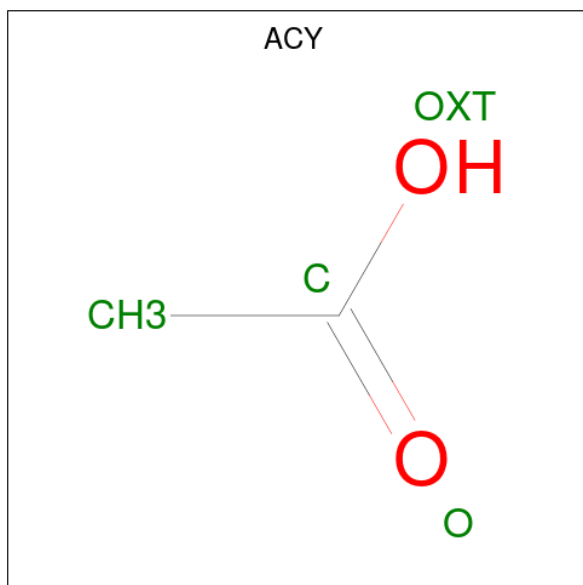
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q99AU2
A	-4	HIS	-	expression tag	UNP Q99AU2
A	-3	HIS	-	expression tag	UNP Q99AU2
A	-2	HIS	-	expression tag	UNP Q99AU2
A	-1	HIS	-	expression tag	UNP Q99AU2
A	0	HIS	-	expression tag	UNP Q99AU2
B	-5	HIS	-	expression tag	UNP Q99AU2
B	-4	HIS	-	expression tag	UNP Q99AU2
B	-3	HIS	-	expression tag	UNP Q99AU2
B	-2	HIS	-	expression tag	UNP Q99AU2
B	-1	HIS	-	expression tag	UNP Q99AU2
B	0	HIS	-	expression tag	UNP Q99AU2
C	-5	HIS	-	expression tag	UNP Q99AU2
C	-4	HIS	-	expression tag	UNP Q99AU2
C	-3	HIS	-	expression tag	UNP Q99AU2
C	-2	HIS	-	expression tag	UNP Q99AU2
C	-1	HIS	-	expression tag	UNP Q99AU2
C	0	HIS	-	expression tag	UNP Q99AU2
D	-5	HIS	-	expression tag	UNP Q99AU2
D	-4	HIS	-	expression tag	UNP Q99AU2
D	-3	HIS	-	expression tag	UNP Q99AU2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	HIS	-	expression tag	UNP Q99AU2
D	-1	HIS	-	expression tag	UNP Q99AU2
D	0	HIS	-	expression tag	UNP Q99AU2

- Molecule 2 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

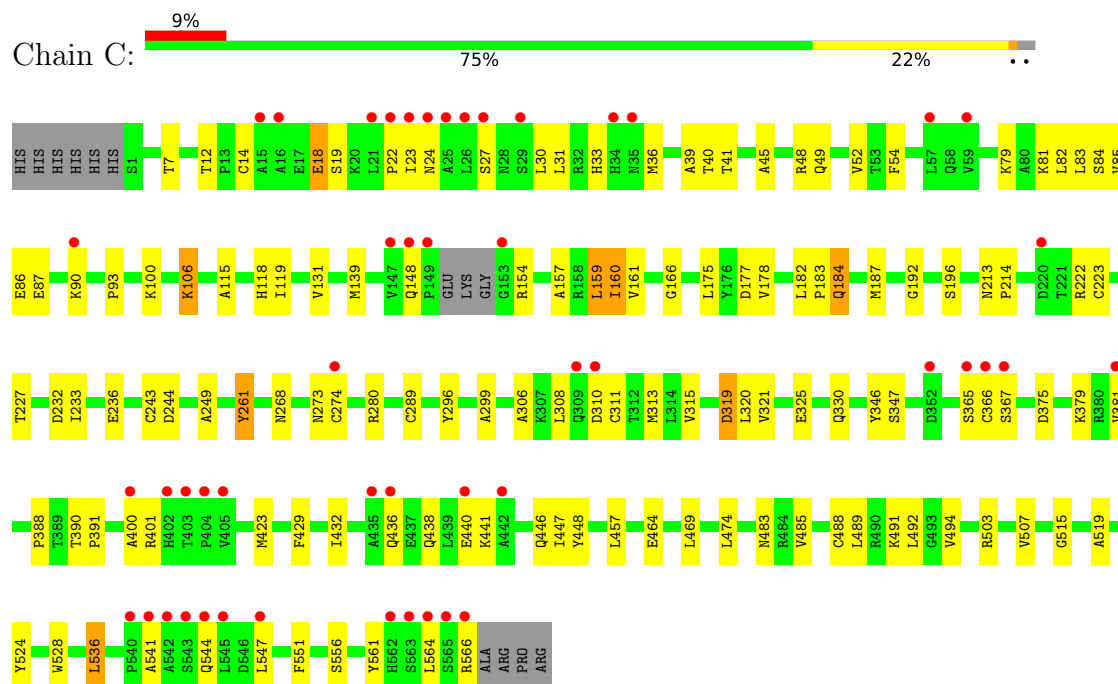


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

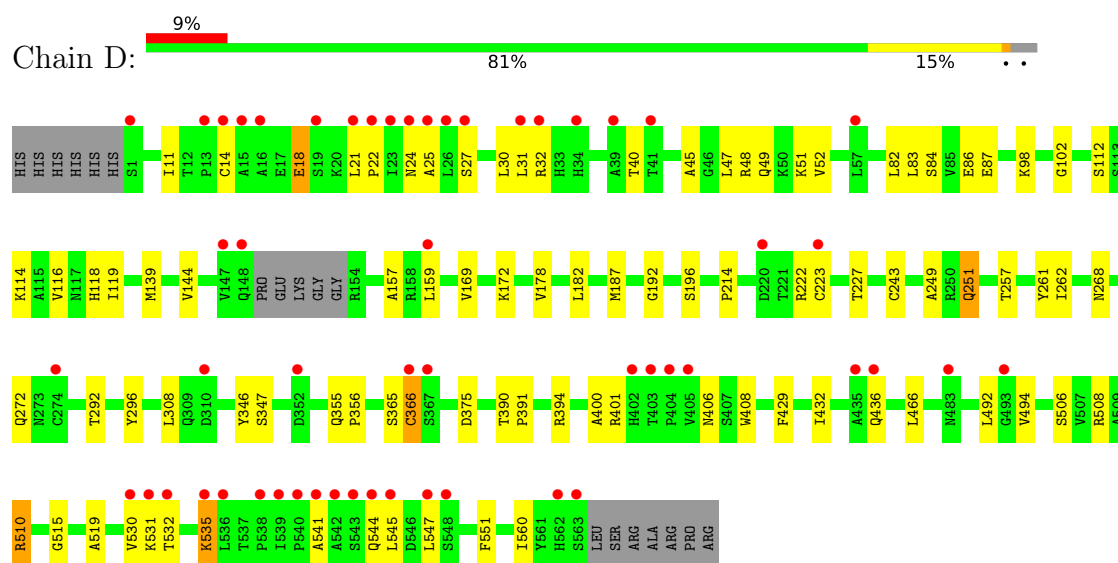
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	559	Total	O	0	0
			559	559		
4	B	551	Total	O	0	0
			551	551		
4	C	526	Total	O	0	0
			526	526		
4	D	471	Total	O	0	0
			471	471		

• Molecule 1: Genome polyprotein



• Molecule 1: Genome polyprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.99Å 102.06Å 251.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.64 – 1.95 45.64 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.0 (45.64-1.95) 97.4 (45.64-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.206 , 0.246 0.205 , 0.246	Depositor DCC
R_{free} test set	9313 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	0.480	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.088 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19620	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.83 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0513e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: ACY, GOL

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	0.38	0/4467	0.85	7/6062 (0.1%)
1	B	0.37	0/4450	0.84	7/6039 (0.1%)
1	C	0.36	0/4471	0.85	11/6067 (0.2%)
1	D	0.36	0/4434	0.83	7/6017 (0.1%)
All	All	0.37	0/17822	0.85	32/24185 (0.1%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	131	VAL	N-CA-C	9.82	120.37	112.12
1	C	196	SER	N-CA-C	-7.31	99.40	110.07
1	A	196	SER	N-CA-C	-6.95	99.93	110.07
1	B	196	SER	N-CA-C	-6.46	100.63	110.07
1	B	192	GLY	N-CA-C	6.45	121.69	113.24
1	C	214	PRO	N-CA-C	6.20	121.23	111.38
1	D	261	TYR	N-CA-C	6.11	117.94	111.28
1	D	196	SER	N-CA-C	-6.07	101.21	110.07
1	A	192	GLY	N-CA-C	6.00	121.10	113.24
1	A	261	TYR	N-CA-C	5.91	117.72	111.28
1	B	261	TYR	N-CA-C	5.91	117.72	111.28
1	D	214	PRO	N-CA-C	5.86	120.69	111.38
1	B	175	LEU	N-CA-C	5.72	122.08	114.12
1	C	261	TYR	N-CA-C	5.70	117.49	111.28
1	C	213	ASN	CA-C-N	5.67	125.58	119.85
1	C	213	ASN	C-N-CA	5.67	125.58	119.85
1	C	175	LEU	N-CA-C	5.67	122.11	113.61
1	C	12	THR	N-CA-C	5.67	117.76	110.39
1	C	429	PHE	N-CA-C	5.47	118.17	111.82
1	D	366	CYS	N-CA-C	-5.43	105.29	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	11	ILE	N-CA-C	-5.42	99.80	107.98
1	A	214	PRO	N-CA-C	5.40	119.97	111.38
1	D	429	PHE	N-CA-C	5.33	118.00	111.82
1	B	214	PRO	N-CA-C	5.30	119.80	111.38
1	A	524	TYR	N-CA-C	5.20	117.74	111.40
1	D	11	ILE	N-CA-C	-5.18	100.15	107.98
1	B	5	THR	N-CA-C	-5.17	100.60	109.24
1	C	192	GLY	N-CA-C	5.16	120.29	113.37
1	C	315	VAL	N-CA-C	5.14	115.31	108.11
1	A	429	PHE	N-CA-C	5.09	116.91	111.36
1	D	192	GLY	N-CA-C	5.08	120.18	113.37
1	A	11	ILE	N-CA-C	-5.01	100.41	107.98

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4372	0	4395	63	0
1	B	4355	0	4372	73	0
1	C	4376	0	4398	92	0
1	D	4340	0	4359	61	0
2	A	8	0	6	0	0
2	B	12	0	9	1	0
2	C	4	0	3	0	0
2	D	4	0	3	0	0
3	A	30	0	20	0	0
3	B	12	0	8	0	0
4	A	559	0	0	5	0
4	B	551	0	0	7	0
4	C	526	0	0	8	0
4	D	471	0	0	4	0
All	All	19620	0	17573	287	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 8.

All (287) 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:309:GLN:HG3	1:A:325:GLU:HB3	1.45	0.95
1:B:453:SER:HB3	1:B:563:SER:HB2	1.48	0.95
1:C:299:ALA:HB1	1:C:313:MET:HE1	1.56	0.87
1:C:48:ARG:HG2	1:C:159:LEU:HD13	1.61	0.83
1:B:33:HIS:HB2	1:B:36:MET:HE2	1.64	0.80
1:A:82:LEU:HD13	1:A:249:ALA:HB2	1.64	0.80
1:A:453:SER:H	1:A:563:SER:HA	1.47	0.78
1:C:36:MET:HE1	1:C:492:LEU:HA	1.67	0.76
1:A:336:LEU:HD12	1:A:356:PRO:HD3	1.68	0.76
1:A:436:GLN:HB3	1:A:438:GLN:HE21	1.51	0.75
1:A:212:LYS:HG2	1:B:513:SER:O	1.87	0.74
1:C:483:ASN:HB2	4:C:3326:HOH:O	1.87	0.74
1:D:268:ASN:HD21	1:D:272:GLN:HB2	1.53	0.74
1:C:24:ASN:HB3	1:C:27:SER:HB3	1.70	0.73
1:A:453:SER:HB3	1:A:563:SER:HB2	1.70	0.72
1:D:21:LEU:HD12	1:D:22:PRO:HD2	1.71	0.72
1:D:48:ARG:HG2	1:D:159:LEU:HD13	1.69	0.72
1:C:36:MET:HE1	1:C:491:LYS:O	1.89	0.72
1:A:337:ARG:O	1:A:341:GLU:HG3	1.90	0.71
1:B:319:ASP:OD2	1:B:366:CYS:HB2	1.90	0.71
1:C:488:CYS:O	1:C:492:LEU:HD13	1.92	0.70
1:C:160:ILE:HD13	1:C:161:VAL:N	2.06	0.70
1:C:86:GLU:O	1:C:90:LYS:HG3	1.92	0.69
1:C:556:SER:HB3	4:C:3247:HOH:O	1.92	0.69
1:D:268:ASN:ND2	1:D:272:GLN:HB2	2.08	0.69
1:A:305:ALA:O	1:A:307:LYS:HE2	1.91	0.69
1:B:33:HIS:CB	1:B:36:MET:HE2	2.22	0.69
1:C:36:MET:CE	1:C:492:LEU:HA	2.24	0.68
1:A:440:GLU:H	1:A:440:GLU:CD	2.00	0.68
1:C:23:ILE:HD12	1:C:23:ILE:H	1.58	0.67
1:D:119:ILE:HD13	1:D:169:VAL:HG11	1.76	0.67
1:A:381:VAL:HG11	1:A:474:LEU:HD22	1.77	0.67
1:C:381:VAL:HG11	1:C:474:LEU:HD22	1.76	0.67
1:D:346:TYR:O	1:D:347:SER:HB3	1.95	0.66
1:B:182:LEU:HD12	1:B:243:CYS:SG	2.35	0.66
1:C:33:HIS:HB2	1:C:36:MET:HE2	1.77	0.66
1:B:14:CYS:HB2	1:B:139:MET:HE1	1.78	0.66
1:C:19:SER:HA	1:C:39:ALA:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:MET:HE1	1:B:492:LEU:HA	1.77	0.65
1:C:178:VAL:HG23	4:C:3144:HOH:O	1.94	0.65
1:B:36:MET:HE1	1:B:491:LYS:O	1.96	0.65
1:C:106:LYS:HE2	1:C:106:LYS:HA	1.79	0.64
1:C:381:VAL:HG11	1:C:474:LEU:CD2	2.26	0.64
1:B:90:LYS:HG2	4:B:4271:HOH:O	1.96	0.64
1:C:236:GLU:OE1	1:C:280:ARG:NH2	2.22	0.64
1:C:299:ALA:CB	1:C:313:MET:HE1	2.27	0.63
1:B:93:PRO:HG3	1:B:561:TYR:HB2	1.80	0.63
1:A:535:LYS:NZ	1:A:535:LYS:HB3	2.14	0.62
1:B:455:GLU:HB3	4:B:4142:HOH:O	1.98	0.62
1:A:21:LEU:HD12	1:A:22:PRO:HD2	1.80	0.62
1:B:364:THR:HB	2:B:3007:ACY:H2	1.82	0.62
1:D:102:GLY:O	1:D:114:LYS:HE3	2.00	0.62
1:D:535:LYS:HB3	1:D:535:LYS:NZ	2.13	0.62
1:A:325:GLU:HG3	4:A:4395:HOH:O	2.00	0.62
1:B:453:SER:H	1:B:563:SER:HA	1.64	0.61
1:D:390:THR:HB	1:D:391:PRO:HD3	1.81	0.61
1:C:227:THR:HB	1:C:347:SER:O	1.99	0.61
1:B:21:LEU:HD12	1:B:22:PRO:HD2	1.82	0.61
1:B:115:ALA:O	1:B:119:ILE:HG12	2.01	0.61
1:A:517:ARG:HG2	1:A:517:ARG:HH11	1.66	0.61
1:A:48:ARG:HG2	1:A:159:LEU:HD13	1.82	0.60
1:C:23:ILE:HD12	1:C:23:ILE:N	2.15	0.60
1:D:144:VAL:HB	1:D:394:ARG:HG2	1.84	0.60
1:B:336:LEU:HD12	1:B:356:PRO:HG3	1.83	0.60
1:D:182:LEU:C	1:D:182:LEU:HD23	2.26	0.60
1:A:119:ILE:HD13	1:A:169:VAL:HG11	1.84	0.59
1:D:510:ARG:HG2	1:D:510:ARG:HH21	1.66	0.59
1:B:148:GLN:O	1:B:152:GLY:HA2	2.01	0.59
1:A:381:VAL:HG11	1:A:474:LEU:CD2	2.32	0.59
1:A:23:ILE:C	1:A:23:ILE:HD13	2.27	0.59
1:D:506:SER:O	1:D:510:ARG:HD3	2.02	0.59
1:C:33:HIS:CB	1:C:36:MET:HE2	2.33	0.59
1:C:319:ASP:OD2	1:C:366:CYS:HB2	2.03	0.59
1:D:98:LYS:HE3	4:D:3286:HOH:O	2.02	0.59
1:C:182:LEU:HD12	1:C:243:CYS:SG	2.43	0.58
1:D:14:CYS:HB2	1:D:139:MET:HE1	1.85	0.58
1:D:82:LEU:HD13	1:D:249:ALA:HB2	1.86	0.58
1:C:24:ASN:HB3	1:C:27:SER:CB	2.33	0.58
1:A:390:THR:HB	1:A:391:PRO:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:LYS:HG2	4:C:3288:HOH:O	2.02	0.57
1:A:23:ILE:HD13	1:A:24:ASN:N	2.19	0.57
1:B:220:ASP:HB2	4:B:4341:HOH:O	2.05	0.57
1:C:82:LEU:HD13	1:C:249:ALA:HB2	1.87	0.57
1:C:115:ALA:O	1:C:119:ILE:HG12	2.04	0.57
1:B:22:PRO:HG2	1:B:400:ALA:HB1	1.87	0.56
1:C:24:ASN:ND2	1:C:400:ALA:HA	2.21	0.56
1:C:40:THR:HB	1:C:157:ALA:HB2	1.86	0.56
1:C:313:MET:HE2	1:C:320:LEU:HD11	1.87	0.56
1:A:178:VAL:HG23	4:A:4207:HOH:O	2.05	0.56
1:A:436:GLN:CB	1:A:438:GLN:HE21	2.18	0.56
1:D:40:THR:HB	1:D:157:ALA:HB2	1.88	0.56
1:B:31:LEU:HG	1:B:492:LEU:O	2.06	0.56
1:B:45:ALA:O	1:B:49:GLN:HG3	2.06	0.56
1:D:45:ALA:O	1:D:49:GLN:HG3	2.06	0.55
1:D:222:ARG:HH21	1:D:222:ARG:HG3	1.70	0.55
1:A:346:TYR:O	1:A:347:SER:HB3	2.06	0.55
1:A:270:LYS:HD3	4:A:4465:HOH:O	2.07	0.55
1:B:36:MET:CE	1:B:492:LEU:HA	2.36	0.55
1:B:24:ASN:OD1	1:B:27:SER:HB3	2.07	0.54
1:C:182:LEU:HD23	1:C:182:LEU:C	2.33	0.54
1:B:144:VAL:HB	1:B:394:ARG:HG2	1.89	0.54
1:A:86:GLU:O	1:A:90:LYS:HD3	2.08	0.53
1:C:541:ALA:HA	1:C:544:GLN:NE2	2.23	0.53
1:A:535:LYS:HB3	1:A:535:LYS:HZ3	1.72	0.53
1:B:313:MET:HG2	1:B:322:VAL:HG22	1.89	0.53
1:B:84:SER:OG	1:B:86:GLU:HG2	2.09	0.53
1:C:346:TYR:O	1:C:347:SER:HB3	2.09	0.53
1:B:178:VAL:HG23	4:B:4253:HOH:O	2.08	0.53
1:B:346:TYR:O	1:B:347:SER:HB3	2.07	0.53
1:C:446:GLN:O	1:C:447:ILE:HD13	2.08	0.53
1:C:515:GLY:HA2	1:C:519:ALA:HB2	1.91	0.53
1:D:14:CYS:HB2	1:D:139:MET:CE	2.39	0.53
1:B:187:MET:HE3	1:B:296:TYR:CD2	2.43	0.53
1:B:545:LEU:HB3	1:B:547:LEU:CD1	2.39	0.53
1:B:84:SER:OG	1:B:87:GLU:HG3	2.10	0.52
1:D:47:LEU:O	1:D:51:LYS:HG3	2.09	0.52
1:B:21:LEU:HD13	1:B:397:TRP:HA	1.91	0.52
1:B:195:TYR:CE1	1:D:531:LYS:HE3	2.43	0.52
1:D:251:GLN:HG3	4:D:3469:HOH:O	2.08	0.52
1:A:144:VAL:HB	1:A:394:ARG:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:LEU:HD11	1:B:492:LEU:HG	1.92	0.51
1:A:182:LEU:HD23	1:A:182:LEU:C	2.35	0.51
1:C:45:ALA:O	1:C:49:GLN:HG3	2.10	0.51
1:D:31:LEU:HG	1:D:492:LEU:O	2.11	0.51
1:C:81:LYS:HD3	1:C:81:LYS:N	2.26	0.51
1:C:438:GLN:OE1	1:C:441:LYS:HD2	2.10	0.51
1:C:388:PRO:C	1:C:391:PRO:HD2	2.35	0.51
1:B:237:GLU:HG3	1:B:257:THR:OG1	2.10	0.51
1:B:100:LYS:HB3	1:B:100:LYS:NZ	2.26	0.51
1:B:515:GLY:HA2	1:B:519:ALA:HB2	1.93	0.51
1:C:432:ILE:HG23	1:C:436:GLN:HE21	1.76	0.51
1:D:545:LEU:HB3	1:D:547:LEU:HD13	1.93	0.50
1:C:306:ALA:HB3	1:C:308:LEU:HD13	1.93	0.50
1:D:118:HIS:HB2	4:D:3146:HOH:O	2.11	0.50
1:D:172:LYS:HE3	1:D:560:ILE:HD13	1.93	0.50
1:B:48:ARG:HG2	1:B:159:LEU:HD13	1.92	0.50
1:C:268:ASN:HB3	1:C:274:CYS:SG	2.52	0.50
1:D:52:VAL:HG12	1:D:223:CYS:SG	2.51	0.50
1:B:182:LEU:C	1:B:182:LEU:HD23	2.36	0.50
1:A:24:ASN:HD21	1:A:400:ALA:HB2	1.76	0.50
1:A:187:MET:HE3	1:A:296:TYR:CD2	2.46	0.50
1:B:433:LEU:HB3	1:B:439:LEU:HD12	1.94	0.50
1:C:18:GLU:HG2	1:C:401:ARG:CZ	2.42	0.49
1:D:466:LEU:HD22	1:D:551:PHE:HE2	1.77	0.49
1:B:394:ARG:O	1:B:398:GLU:HG3	2.12	0.49
1:D:222:ARG:HG3	1:D:222:ARG:NH2	2.28	0.49
1:A:308:LEU:HB3	1:A:311:CYS:SG	2.53	0.49
1:B:406:ASN:ND2	1:B:443:LEU:HB3	2.27	0.49
1:B:83:LEU:HB2	1:B:173:MET:HA	1.95	0.49
1:A:182:LEU:HD12	1:A:243:CYS:SG	2.53	0.49
1:C:440:GLU:HG2	1:C:457:LEU:HD12	1.94	0.49
1:D:187:MET:HE1	1:D:292:THR:HG22	1.92	0.49
1:C:100:LYS:HG3	4:C:3477:HOH:O	2.13	0.48
1:C:330:GLN:OE1	1:C:330:GLN:HA	2.12	0.48
1:C:160:ILE:HD13	1:C:161:VAL:H	1.75	0.48
1:C:503:ARG:O	1:C:507:VAL:HG23	2.13	0.48
1:C:93:PRO:HG3	1:C:561:TYR:HB2	1.96	0.48
1:C:524:TYR:CD2	1:C:536:LEU:HG	2.49	0.48
1:C:14:CYS:HB2	1:C:139:MET:HE1	1.96	0.48
1:B:390:THR:HB	1:B:391:PRO:HD3	1.96	0.48
1:A:523:LYS:HG3	1:A:534:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:564:LEU:C	1:C:564:LEU:HD13	2.39	0.47
1:C:84:SER:OG	1:C:87:GLU:HG3	2.13	0.47
1:A:515:GLY:HA2	1:A:519:ALA:HB2	1.97	0.47
1:A:45:ALA:O	1:A:49:GLN:HG3	2.14	0.47
1:B:21:LEU:CD1	1:B:397:TRP:HA	2.44	0.47
1:C:84:SER:OG	1:C:86:GLU:HG2	2.13	0.47
1:B:268:ASN:HB3	1:B:274:CYS:SG	2.55	0.47
1:B:545:LEU:HB3	1:B:547:LEU:HD13	1.95	0.47
1:C:321:VAL:CG2	1:C:365:SER:OG	2.62	0.47
1:C:544:GLN:HB3	1:C:566:ARG:HD2	1.97	0.47
1:A:545:LEU:HB3	1:A:547:LEU:HD13	1.97	0.47
1:A:517:ARG:HG2	1:A:517:ARG:NH1	2.28	0.47
1:A:508:ARG:CZ	1:A:530:VAL:HG11	2.45	0.46
1:B:562:HIS:O	1:B:563:SER:CB	2.62	0.46
1:C:187:MET:HE3	1:C:296:TYR:CD2	2.50	0.46
1:B:40:THR:HB	1:B:157:ALA:HB2	1.96	0.46
1:D:178:VAL:HG23	4:D:3089:HOH:O	2.15	0.46
1:C:464:GLU:HG3	1:C:469:LEU:HD23	1.98	0.46
1:D:24:ASN:HD21	1:D:27:SER:HB2	1.81	0.46
1:A:545:LEU:HB3	1:A:547:LEU:CD1	2.45	0.46
1:B:423:MET:HA	1:B:528:TRP:CZ2	2.50	0.46
1:C:366:CYS:O	1:C:367:SER:HB2	2.16	0.46
1:B:99:SER:HB2	1:B:165:LEU:HB3	1.98	0.45
1:D:257:THR:O	1:D:262:ILE:HG23	2.16	0.45
1:B:52:VAL:HG12	1:B:223:CYS:SG	2.56	0.45
1:C:52:VAL:HG12	1:C:223:CYS:SG	2.57	0.45
1:D:22:PRO:HG2	1:D:400:ALA:HB1	1.97	0.45
1:D:182:LEU:HD12	1:D:243:CYS:SG	2.55	0.45
1:D:535:LYS:HB3	1:D:535:LYS:HZ2	1.81	0.45
1:B:440:GLU:HG2	1:B:457:LEU:HD12	1.99	0.45
1:A:183:PRO:HG3	1:A:289:CYS:SG	2.57	0.45
1:B:106:LYS:HD2	1:B:106:LYS:N	2.32	0.45
1:C:448:TYR:CE2	1:C:551:PHE:HD1	2.35	0.45
1:C:23:ILE:H	1:C:23:ILE:CD1	2.26	0.45
1:C:119:ILE:CD1	1:C:166:GLY:HA2	2.47	0.45
1:D:18:GLU:HG2	1:D:401:ARG:CZ	2.47	0.45
1:D:510:ARG:HG2	1:D:510:ARG:NH2	2.32	0.45
1:C:423:MET:HA	1:C:528:TRP:CZ2	2.52	0.45
1:C:30:LEU:O	1:C:494:VAL:HG22	2.16	0.44
1:A:398:GLU:OE1	1:A:408:TRP:HD1	2.01	0.44
1:B:30:LEU:O	1:B:494:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LEU:HG	1:A:492:LEU:O	2.17	0.44
1:A:230:GLU:HB3	1:A:262:ILE:HD11	1.99	0.44
1:D:227:THR:HB	1:D:347:SER:O	2.18	0.44
1:D:365:SER:O	1:D:366:CYS:HB2	2.16	0.44
1:C:31:LEU:C	1:C:31:LEU:HD23	2.43	0.44
1:C:390:THR:HB	1:C:391:PRO:HD3	2.00	0.44
1:D:515:GLY:HA2	1:D:519:ALA:HB2	2.00	0.44
1:D:406:ASN:HD22	1:D:408:TRP:HE1	1.65	0.44
1:A:249:ALA:O	1:A:253:ILE:HG13	2.18	0.43
1:D:187:MET:HE3	1:D:296:TYR:CD2	2.53	0.43
1:A:227:THR:HB	1:A:347:SER:O	2.18	0.43
1:B:440:GLU:HG2	1:B:457:LEU:CD1	2.48	0.43
1:C:492:LEU:HD12	1:C:492:LEU:N	2.34	0.43
1:A:485:VAL:O	1:A:489:LEU:HG	2.18	0.43
1:A:14:CYS:HB2	1:A:139:MET:HE1	1.99	0.43
1:D:187:MET:HE1	1:D:292:THR:CG2	2.48	0.43
1:B:236:GLU:OE2	1:B:280:ARG:NH2	2.46	0.43
1:A:412:ILE:O	1:A:416:ALA:HB2	2.19	0.43
1:B:217:PHE:CD2	1:B:336:LEU:HD21	2.53	0.43
1:C:183:PRO:HG3	1:C:289:CYS:SG	2.59	0.43
1:B:447:ILE:HB	1:B:452:TYR:CE2	2.54	0.43
1:D:24:ASN:OD1	1:D:27:SER:HB3	2.18	0.43
1:A:237:GLU:HG3	1:A:257:THR:OG1	2.19	0.42
1:B:14:CYS:HB2	1:B:139:MET:CE	2.48	0.42
1:C:233:ILE:HD13	1:C:261:TYR:O	2.19	0.42
1:A:233:ILE:HD13	1:A:261:TYR:O	2.19	0.42
1:C:48:ARG:CG	1:C:159:LEU:HD13	2.38	0.42
1:D:508:ARG:CZ	1:D:530:VAL:HG11	2.50	0.42
1:A:564:LEU:HD12	4:A:4498:HOH:O	2.19	0.42
1:B:361:GLU:HG2	1:B:370:VAL:O	2.19	0.42
1:B:448:TYR:CE2	1:B:551:PHE:HD1	2.37	0.42
1:C:7:THR:HG21	1:C:273:ASN:ND2	2.33	0.42
1:C:106:LYS:HA	1:C:106:LYS:CE	2.49	0.42
1:C:148:GLN:HG3	1:C:148:GLN:O	2.19	0.42
1:A:466:LEU:HD22	1:A:551:PHE:HE2	1.85	0.42
1:B:306:ALA:HB3	1:B:308:LEU:HD13	2.02	0.42
1:D:375:ASP:OD1	1:D:375:ASP:C	2.62	0.42
1:C:310:ASP:HB3	1:C:325:GLU:HG2	2.02	0.42
1:C:184:GLN:HB2	4:C:3110:HOH:O	2.20	0.42
1:D:541:ALA:HA	1:D:544:GLN:CD	2.44	0.42
1:A:40:THR:HB	1:A:157:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:GLU:HG2	1:D:87:GLU:N	2.35	0.42
1:B:146:CYS:SG	1:B:492:LEU:HD11	2.60	0.42
1:B:491:LYS:HE3	1:B:492:LEU:HD13	2.00	0.42
1:C:22:PRO:HD3	1:C:401:ARG:NH2	2.34	0.42
1:C:118:HIS:HB2	4:C:3280:HOH:O	2.20	0.42
1:A:182:LEU:HB3	1:A:183:PRO:HD3	2.02	0.41
1:C:346:TYR:O	1:C:347:SER:CB	2.68	0.41
1:D:432:ILE:O	1:D:436:GLN:HG3	2.20	0.41
1:A:72:LYS:NZ	4:A:4291:HOH:O	2.54	0.41
1:C:515:GLY:CA	1:C:519:ALA:HB2	2.50	0.41
1:A:268:ASN:HB3	1:A:274:CYS:SG	2.60	0.41
1:A:388:PRO:C	1:A:391:PRO:HD2	2.45	0.41
4:B:4338:HOH:O	1:D:532:THR:HG23	2.19	0.41
1:C:81:LYS:HE2	1:C:177:ASP:OD2	2.20	0.41
1:D:30:LEU:O	1:D:494:VAL:HG13	2.21	0.41
1:D:346:TYR:O	1:D:347:SER:CB	2.66	0.41
1:C:432:ILE:CG2	1:C:436:GLN:HE21	2.33	0.41
1:D:355:GLN:HA	1:D:356:PRO:HD3	1.97	0.41
1:B:38:TYR:CB	1:B:154:ARG:HH21	2.33	0.41
1:D:84:SER:OG	1:D:86:GLU:HG2	2.20	0.41
1:D:112:SER:O	1:D:116:VAL:HG23	2.20	0.41
1:B:445:CYS:SG	1:B:454:ILE:HD12	2.61	0.41
1:B:490:ARG:NH1	4:B:4424:HOH:O	2.52	0.41
1:A:14:CYS:HB2	1:A:139:MET:CE	2.51	0.41
1:A:58:GLN:HG3	1:A:229:THR:HG21	2.02	0.41
1:A:433:LEU:HB3	1:A:439:LEU:HD23	2.01	0.41
1:A:491:LYS:HE3	1:A:492:LEU:HD11	2.03	0.41
4:B:4338:HOH:O	1:D:531:LYS:HE2	2.20	0.41
1:C:232:ASP:O	1:C:236:GLU:HG3	2.21	0.41
1:C:375:ASP:OD2	1:C:379:LYS:HB3	2.21	0.41
1:C:541:ALA:O	1:C:544:GLN:HB2	2.21	0.41
1:B:355:GLN:HA	1:B:356:PRO:HD3	1.93	0.41
1:A:334:ALA:O	1:A:338:VAL:HG23	2.21	0.40
1:B:46:GLY:HA2	1:B:49:GLN:HE21	1.86	0.40
1:C:54:PHE:CE2	1:C:222:ARG:NH1	2.89	0.40
1:C:79:LYS:HA	1:C:244:ASP:HB3	2.03	0.40
1:C:485:VAL:O	1:C:489:LEU:HG	2.21	0.40
1:B:236:GLU:CD	1:B:280:ARG:HH22	2.30	0.40
1:C:85:VAL:HG23	4:C:3502:HOH:O	2.20	0.40
1:D:466:LEU:HD22	1:D:551:PHE:CE2	2.56	0.40
1:C:19:SER:HB3	1:C:41:THR:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:ARG:HH11	1:D:32:ARG:HG2	1.87	0.40
1:B:92:THR:HA	1:B:93:PRO:HD3	1.95	0.40
1:D:18:GLU:HG2	1:D:401:ARG:NH2	2.36	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	558/576 (97%)	543 (97%)	14 (2%)	1 (0%)	43	36
1	B	557/576 (97%)	543 (98%)	14 (2%)	0	100	100
1	C	559/576 (97%)	547 (98%)	11 (2%)	1 (0%)	43	36
1	D	554/576 (96%)	536 (97%)	17 (3%)	1 (0%)	43	36
All	All	2228/2304 (97%)	2169 (97%)	56 (2%)	3 (0%)	48	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	154	ARG
1	D	25	ALA
1	A	25	ALA

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	480/491 (98%)	470 (98%)	10 (2%)	47	41
1	B	477/491 (97%)	467 (98%)	10 (2%)	47	41
1	C	480/491 (98%)	470 (98%)	10 (2%)	47	41
1	D	476/491 (97%)	470 (99%)	6 (1%)	61	58
All	All	1913/1964 (97%)	1877 (98%)	36 (2%)	50	45

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ILE
1	A	81	LYS
1	A	83	LEU
1	A	159	LEU
1	A	184	GLN
1	A	220	ASP
1	A	308	LEU
1	A	311	CYS
1	A	440	GLU
1	A	535	LYS
1	B	34	HIS
1	B	81	LYS
1	B	100	LYS
1	B	106	LYS
1	B	148	GLN
1	B	159	LEU
1	B	308	LEU
1	B	311	CYS
1	B	492	LEU
1	B	536	LEU
1	C	18	GLU
1	C	83	LEU
1	C	106	LYS
1	C	159	LEU
1	C	160	ILE
1	C	184	GLN
1	C	311	CYS
1	C	319	ASP
1	C	536	LEU
1	C	547	LEU
1	D	18	GLU
1	D	83	LEU
1	D	251	GLN

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Mol	Chain	Res	Type
1	D	308	LEU
1	D	510	ARG
1	D	535	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	95	HIS
1	A	110	ASN
1	A	184	GLN
1	A	273	ASN
1	A	355	GLN
1	A	406	ASN
1	A	438	GLN
1	A	446	GLN
1	A	514	GLN
1	A	544	GLN
1	B	34	HIS
1	B	49	GLN
1	B	63	HIS
1	B	184	GLN
1	B	273	ASN
1	B	406	ASN
1	B	436	GLN
1	B	438	GLN
1	B	446	GLN
1	B	514	GLN
1	B	544	GLN
1	C	49	GLN
1	C	117	ASN
1	C	142	ASN
1	C	184	GLN
1	C	273	ASN
1	C	309	GLN
1	C	436	GLN
1	C	514	GLN
1	C	562	HIS
1	D	273	ASN
1	D	330	GLN
1	D	411	ASN
1	D	436	GLN

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Mol	Chain	Res	Type
1	D	438	GLN
1	D	446	GLN
1	D	461	GLN
1	D	544	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 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	ACY	A	3001	-	3,3,3	0.52	0	3,3,3	1.65	1 (33%)
3	GOL	B	4007	-	5,5,5	4.65	5 (100%)	5,5,5	1.95	3 (60%)
2	ACY	B	3004	-	3,3,3	0.56	0	3,3,3	1.65	1 (33%)
3	GOL	A	4001	-	5,5,5	4.54	5 (100%)	5,5,5	1.94	3 (60%)
3	GOL	A	4006	-	5,5,5	4.64	5 (100%)	5,5,5	1.95	3 (60%)
2	ACY	B	3007	-	3,3,3	0.51	0	3,3,3	1.65	1 (33%)
3	GOL	A	4004	-	5,5,5	4.64	5 (100%)	5,5,5	1.94	3 (60%)
3	GOL	B	4003	-	5,5,5	4.60	5 (100%)	5,5,5	1.94	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACY	B	3003	-	3,3,3	0.55	0	3,3,3	1.63	1 (33%)
3	GOL	A	4005	-	5,5,5	4.65	5 (100%)	5,5,5	1.94	3 (60%)
2	ACY	D	3006	-	3,3,3	0.57	0	3,3,3	1.64	1 (33%)
2	ACY	C	3002	-	3,3,3	0.54	0	3,3,3	1.67	1 (33%)
3	GOL	A	4002	-	5,5,5	4.66	5 (100%)	5,5,5	1.94	3 (60%)
2	ACY	A	3005	-	3,3,3	0.55	0	3,3,3	1.66	1 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	4007	-	-	4/4/4/4	-
3	GOL	A	4001	-	-	4/4/4/4	-
3	GOL	A	4006	-	-	4/4/4/4	-
3	GOL	A	4004	-	-	4/4/4/4	-
3	GOL	B	4003	-	-	4/4/4/4	-
3	GOL	A	4005	-	-	4/4/4/4	-
3	GOL	A	4002	-	-	4/4/4/4	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4002	GOL	C3-C2	-7.72	1.22	1.51
3	A	4005	GOL	C3-C2	-7.69	1.22	1.51
3	A	4004	GOL	C3-C2	-7.65	1.22	1.51
3	B	4007	GOL	C3-C2	-7.53	1.23	1.51
3	B	4003	GOL	C3-C2	-7.53	1.23	1.51
3	A	4006	GOL	C3-C2	-7.52	1.23	1.51
3	A	4001	GOL	C3-C2	-7.49	1.23	1.51
3	B	4007	GOL	O1-C1	4.68	1.62	1.42
3	A	4006	GOL	O1-C1	4.62	1.61	1.42
3	B	4003	GOL	O1-C1	4.51	1.61	1.42
3	A	4001	GOL	O1-C1	4.49	1.61	1.42
3	A	4004	GOL	O1-C1	4.49	1.61	1.42
3	A	4005	GOL	O1-C1	4.48	1.61	1.42
3	A	4002	GOL	O1-C1	4.39	1.60	1.42
3	A	4001	GOL	O3-C3	3.74	1.58	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4004	GOL	O3-C3	3.73	1.58	1.42
3	B	4003	GOL	O3-C3	3.69	1.57	1.42
3	A	4006	GOL	O3-C3	3.67	1.57	1.42
3	B	4007	GOL	O3-C3	3.66	1.57	1.42
3	A	4002	GOL	O3-C3	3.63	1.57	1.42
3	A	4005	GOL	O3-C3	3.55	1.57	1.42
3	B	4007	GOL	O2-C2	-2.91	1.34	1.43
3	A	4006	GOL	O2-C2	-2.89	1.35	1.43
3	A	4002	GOL	O2-C2	-2.88	1.35	1.43
3	A	4005	GOL	C1-C2	-2.84	1.41	1.51
3	A	4005	GOL	O2-C2	-2.84	1.35	1.43
3	A	4002	GOL	C1-C2	-2.83	1.41	1.51
3	A	4006	GOL	C1-C2	-2.82	1.41	1.51
3	B	4003	GOL	C1-C2	-2.79	1.41	1.51
3	B	4007	GOL	C1-C2	-2.77	1.41	1.51
3	A	4004	GOL	C1-C2	-2.74	1.41	1.51
3	A	4004	GOL	O2-C2	-2.71	1.35	1.43
3	A	4001	GOL	C1-C2	-2.68	1.41	1.51
3	B	4003	GOL	O2-C2	-2.67	1.35	1.43
3	A	4001	GOL	O2-C2	-2.39	1.36	1.43

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4006	GOL	C3-C2-C1	2.73	121.80	111.80
3	B	4007	GOL	C3-C2-C1	2.69	121.67	111.80
3	A	4001	GOL	O2-C2-C1	2.66	120.18	109.18
3	A	4005	GOL	C3-C2-C1	2.64	121.46	111.80
3	B	4003	GOL	C3-C2-C1	2.60	121.33	111.80
3	A	4002	GOL	C3-C2-C1	2.58	121.27	111.80
3	A	4002	GOL	O2-C2-C1	2.58	119.84	109.18
3	A	4004	GOL	O2-C2-C1	2.55	119.73	109.18
3	A	4004	GOL	C3-C2-C1	2.53	121.09	111.80
3	A	4005	GOL	O2-C2-C1	2.49	119.48	109.18
3	B	4003	GOL	O2-C2-C1	2.49	119.47	109.18
3	B	4007	GOL	O2-C2-C1	2.43	119.24	109.18
3	A	4001	GOL	C3-C2-C1	2.41	120.65	111.80
3	A	4001	GOL	O2-C2-C3	2.41	119.14	109.18
3	B	4003	GOL	O2-C2-C3	2.40	119.13	109.18
3	A	4004	GOL	O2-C2-C3	2.39	119.09	109.18
3	A	4006	GOL	O2-C2-C1	2.39	119.08	109.18
3	A	4006	GOL	O2-C2-C3	2.39	119.06	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	4007	GOL	O2-C2-C3	2.38	119.05	109.18
3	A	4005	GOL	O2-C2-C3	2.37	118.99	109.18
3	A	4002	GOL	O2-C2-C3	2.34	118.88	109.18
2	C	3002	ACY	O-C-CH3	-2.30	113.10	122.53
2	A	3005	ACY	O-C-CH3	-2.28	113.18	122.53
2	A	3001	ACY	O-C-CH3	-2.27	113.20	122.53
2	B	3007	ACY	O-C-CH3	-2.27	113.21	122.53
2	B	3004	ACY	O-C-CH3	-2.26	113.24	122.53
2	D	3006	ACY	O-C-CH3	-2.25	113.30	122.53
2	B	3003	ACY	O-C-CH3	-2.23	113.36	122.53

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	4001	GOL	O1-C1-C2-C3
3	A	4004	GOL	O1-C1-C2-C3
3	A	4005	GOL	O1-C1-C2-C3
3	A	4006	GOL	O1-C1-C2-C3
3	B	4003	GOL	O1-C1-C2-C3
3	B	4007	GOL	O1-C1-C2-C3
3	A	4001	GOL	C1-C2-C3-O3
3	A	4002	GOL	O1-C1-C2-C3
3	A	4002	GOL	C1-C2-C3-O3
3	A	4004	GOL	C1-C2-C3-O3
3	A	4005	GOL	C1-C2-C3-O3
3	A	4006	GOL	C1-C2-C3-O3
3	B	4003	GOL	C1-C2-C3-O3
3	B	4007	GOL	C1-C2-C3-O3
3	A	4001	GOL	O2-C2-C3-O3
3	A	4002	GOL	O2-C2-C3-O3
3	A	4004	GOL	O2-C2-C3-O3
3	A	4005	GOL	O2-C2-C3-O3
3	A	4006	GOL	O2-C2-C3-O3
3	B	4003	GOL	O2-C2-C3-O3
3	B	4007	GOL	O2-C2-C3-O3
3	A	4001	GOL	O1-C1-C2-O2
3	A	4002	GOL	O1-C1-C2-O2
3	A	4004	GOL	O1-C1-C2-O2
3	A	4005	GOL	O1-C1-C2-O2
3	A	4006	GOL	O1-C1-C2-O2
3	B	4003	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	B	4007	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3007	ACY	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	562/576 (97%)	0.41	44 (7%)	19	22	16, 28, 53, 75	0
1	B	561/576 (97%)	0.52	46 (8%)	17	20	17, 29, 57, 81	0
1	C	563/576 (97%)	0.53	49 (8%)	16	18	16, 30, 56, 79	0
1	D	558/576 (96%)	0.72	54 (9%)	13	15	16, 33, 63, 85	0
All	All	2244/2304 (97%)	0.55	193 (8%)	16	19	16, 30, 57, 85	0

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	25	ALA	6.6
1	B	26	LEU	6.1
1	A	23	ILE	6.1
1	B	23	ILE	6.0
1	C	23	ILE	5.3
1	C	404	PRO	4.8
1	D	23	ILE	4.7
1	D	542	ALA	4.6
1	B	149	PRO	4.3
1	A	563	SER	4.3
1	A	564	LEU	4.3
1	D	22	PRO	4.2
1	C	26	LEU	4.2
1	D	545	LEU	4.2
1	C	366	CYS	4.2
1	D	26	LEU	4.2
1	B	545	LEU	4.1
1	A	367	SER	4.1
1	D	536	LEU	4.1
1	A	149	PRO	4.0
1	A	21	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	25	ALA	4.0
1	D	563	SER	4.0
1	A	26	LEU	3.9
1	C	22	PRO	3.9
1	C	149	PRO	3.9
1	A	24	ASN	3.9
1	A	25	ALA	3.9
1	B	367	SER	3.8
1	C	27	SER	3.8
1	D	547	LEU	3.7
1	A	148	GLN	3.7
1	D	24	ASN	3.7
1	D	25	ALA	3.7
1	B	542	ALA	3.6
1	D	531	LYS	3.6
1	B	366	CYS	3.6
1	B	22	PRO	3.6
1	C	220	ASP	3.5
1	B	152	GLY	3.5
1	B	402	HIS	3.5
1	C	365	SER	3.5
1	B	368	SER	3.5
1	A	402	HIS	3.4
1	B	24	ASN	3.4
1	C	21	LEU	3.4
1	A	566	ARG	3.4
1	A	22	PRO	3.4
1	A	548	SER	3.3
1	D	540	PRO	3.3
1	D	57	LEU	3.3
1	B	404	PRO	3.2
1	A	565	SER	3.2
1	D	493	GLY	3.2
1	A	366	CYS	3.2
1	D	352	ASP	3.2
1	A	545	LEU	3.2
1	B	21	LEU	3.2
1	D	539	ILE	3.1
1	D	530	VAL	3.1
1	B	403	THR	3.1
1	B	16	ALA	3.1
1	D	39	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	34	HIS	3.1
1	A	542	ALA	3.0
1	C	402	HIS	3.0
1	A	543	SER	2.9
1	D	544	GLN	2.9
1	C	566	ARG	2.9
1	B	543	SER	2.9
1	D	31	LEU	2.9
1	B	154	ARG	2.9
1	D	220	ASP	2.9
1	D	532	THR	2.8
1	B	148	GLN	2.8
1	D	366	CYS	2.8
1	B	513	SER	2.8
1	D	21	LEU	2.8
1	D	562	HIS	2.8
1	C	16	ALA	2.8
1	C	367	SER	2.8
1	A	404	PRO	2.8
1	B	147	VAL	2.8
1	D	147	VAL	2.7
1	B	541	ALA	2.7
1	C	542	ALA	2.7
1	A	549	GLY	2.7
1	C	274	CYS	2.7
1	B	563	SER	2.7
1	D	32	ARG	2.6
1	B	532	THR	2.6
1	C	540	PRO	2.6
1	C	147	VAL	2.6
1	A	220	ASP	2.6
1	A	539	ILE	2.6
1	B	544	GLN	2.6
1	D	402	HIS	2.6
1	A	57	LEU	2.6
1	A	435	ALA	2.6
1	C	403	THR	2.6
1	A	540	PRO	2.5
1	B	540	PRO	2.5
1	A	352	ASP	2.5
1	C	153	GLY	2.5
1	D	535	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	548	SER	2.5
1	A	403	THR	2.5
1	C	24	ASN	2.5
1	C	148	GLN	2.5
1	C	381	VAL	2.5
1	C	352	ASP	2.5
1	B	274	CYS	2.4
1	B	536	LEU	2.4
1	D	159	LEU	2.4
1	C	435	ALA	2.4
1	D	16	ALA	2.4
1	C	440	GLU	2.4
1	D	403	THR	2.4
1	A	405	VAL	2.4
1	D	405	VAL	2.4
1	D	148	GLN	2.4
1	B	15	ALA	2.4
1	C	310	ASP	2.3
1	D	15	ALA	2.3
1	D	14	CYS	2.3
1	A	438	GLN	2.3
1	A	547	LEU	2.3
1	C	547	LEU	2.3
1	C	562	HIS	2.3
1	C	541	ALA	2.3
1	D	13	PRO	2.3
1	C	544	GLN	2.3
1	A	14	CYS	2.3
1	B	547	LEU	2.3
1	C	564	LEU	2.3
1	A	532	THR	2.3
1	D	404	PRO	2.3
1	B	220	ASP	2.3
1	A	355	GLN	2.3
1	B	14	CYS	2.3
1	D	483	ASN	2.3
1	C	57	LEU	2.3
1	C	545	LEU	2.3
1	D	41	THR	2.3
1	A	513	SER	2.2
1	D	548	SER	2.2
1	A	35	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	19	SER	2.2
1	B	153	GLY	2.2
1	B	352	ASP	2.2
1	D	274	CYS	2.2
1	C	543	SER	2.2
1	D	367	SER	2.2
1	C	15	ALA	2.2
1	C	442	ALA	2.2
1	A	379	LYS	2.2
1	B	86	GLU	2.2
1	A	530	VAL	2.2
1	D	223	CYS	2.2
1	A	378	GLY	2.2
1	B	549	GLY	2.2
1	D	538	PRO	2.2
1	C	35	ASN	2.1
1	C	309	GLN	2.1
1	D	436	GLN	2.1
1	C	59	VAL	2.1
1	B	27	SER	2.1
1	D	19	SER	2.1
1	B	562	HIS	2.1
1	C	29	SER	2.1
1	C	405	VAL	2.1
1	C	34	HIS	2.1
1	B	310	ASP	2.1
1	B	539	ILE	2.1
1	D	310	ASP	2.1
1	B	365	SER	2.1
1	C	563	SER	2.1
1	D	543	SER	2.1
1	A	440	GLU	2.1
1	A	381	VAL	2.1
1	A	544	GLN	2.1
1	B	57	LEU	2.1
1	D	435	ALA	2.1
1	D	541	ALA	2.1
1	C	90	LYS	2.0
1	C	565	SER	2.0
1	D	1	SER	2.0
1	D	27	SER	2.0
1	B	550	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	400	ALA	2.0
1	A	365	SER	2.0
1	A	351	GLY	2.0
1	C	436	GLN	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	ACY	C	3002	4/4	0.66	0.24	57,58,59,59	0
2	ACY	D	3006	4/4	0.72	0.18	69,70,70,70	0
2	ACY	A	3001	4/4	0.73	0.16	57,57,58,59	0
2	ACY	B	3007	4/4	0.74	0.21	54,57,57,57	0
3	GOL	A	4005	6/6	0.77	0.17	43,52,56,56	0
3	GOL	B	4003	6/6	0.77	0.17	51,52,55,57	0
3	GOL	B	4007	6/6	0.79	0.17	62,64,66,67	0
3	GOL	A	4004	6/6	0.80	0.16	47,49,50,50	0
2	ACY	A	3005	4/4	0.81	0.15	53,55,55,56	0
3	GOL	A	4006	6/6	0.82	0.20	68,70,71,71	0
3	GOL	A	4002	6/6	0.83	0.15	39,48,49,51	0
3	GOL	A	4001	6/6	0.83	0.14	32,40,43,46	0
2	ACY	B	3003	4/4	0.84	0.19	68,69,69,70	0
2	ACY	B	3004	4/4	0.85	0.13	73,73,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.