WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2023 – 06:27 AM EDT

PDB ID	:	2ZKU
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)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	Percentile Ranks	Value
Rfree		0.242
Clashscore		8
Ramachandran outliers		0.1%
Sidechain outliers		1.6%
RSRZ outliers		7.3%

Worse | | *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
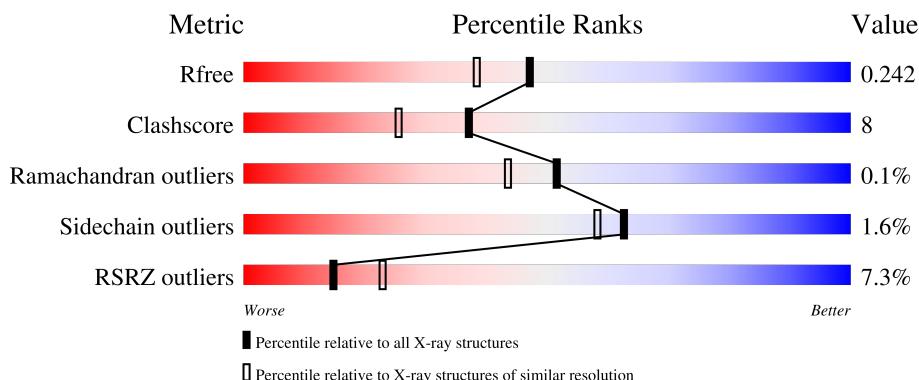
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 <=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	5% / 81% / 15% / ••
1	B	576	6% / 80% / 17% / ••
1	C	576	8% / 78% / 19% / ••
1	D	576	10% / 83% / 13% / ••
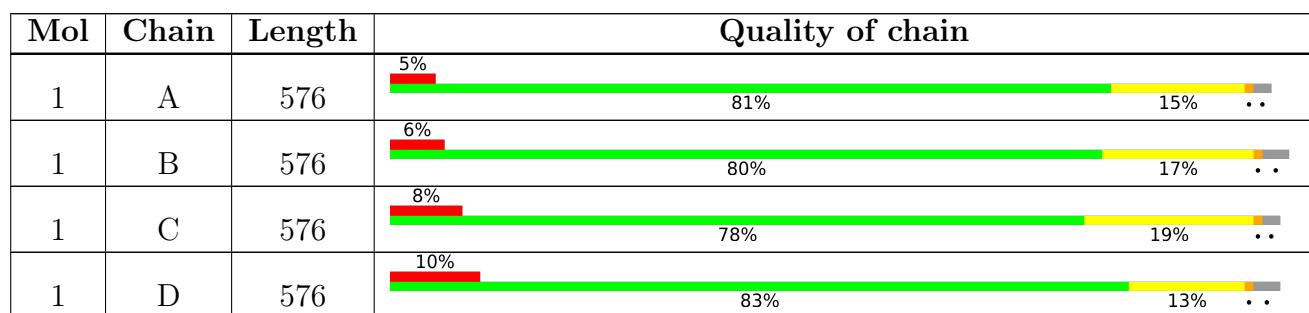
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

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 polyprotein.

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 (three-letter code: ACY) (formula: $C_2H_4O_2$).
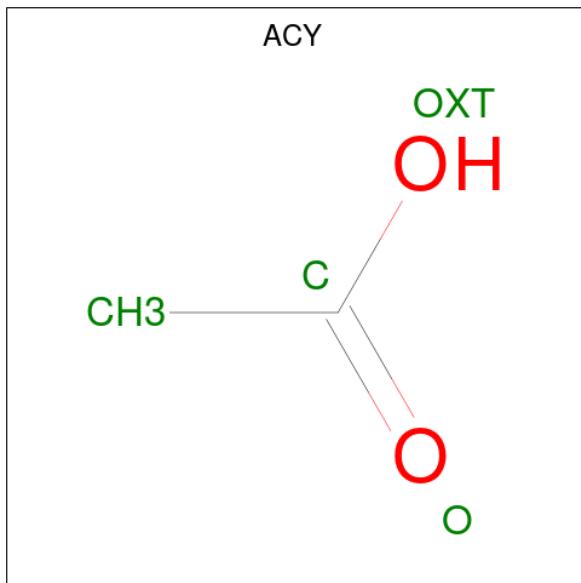
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

C3

OH O3

C1 C2

HO

O1

OH

O2

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

- Molecule 4 is water.

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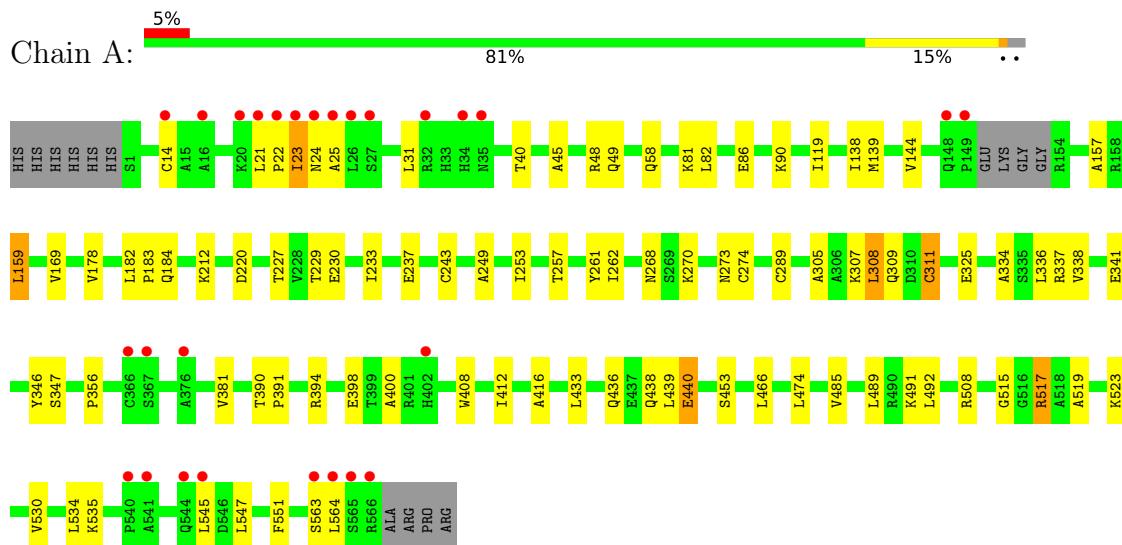
Chain A:

• Molecule 1: Genome polyprotein

Chain B:

• Molecule 1: Genome polyprotein

Chain C:

• Molecule 1: Genome polyprotein

Chain D:
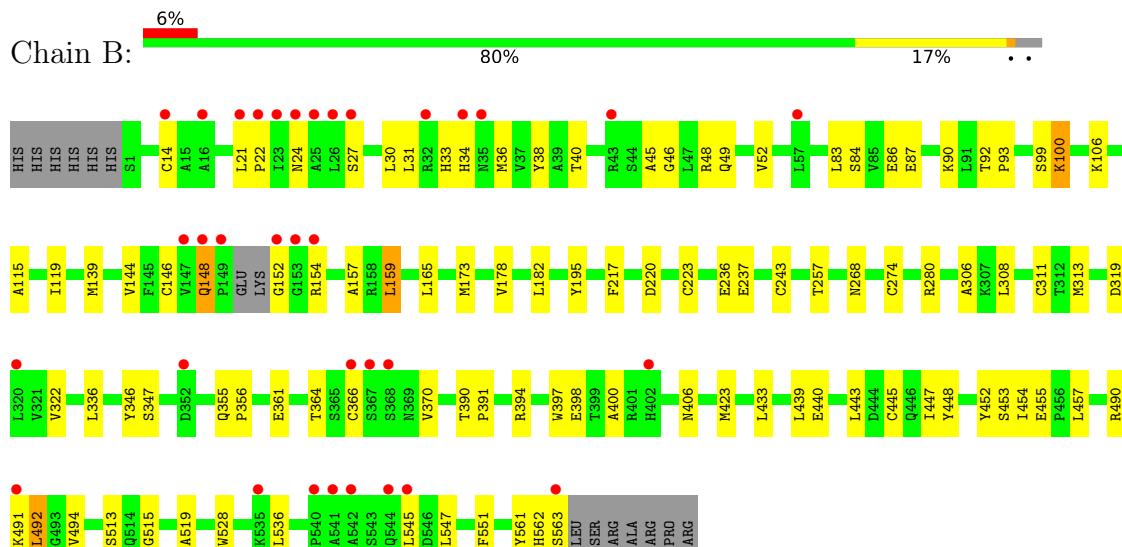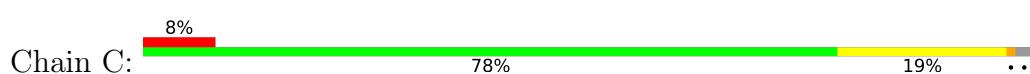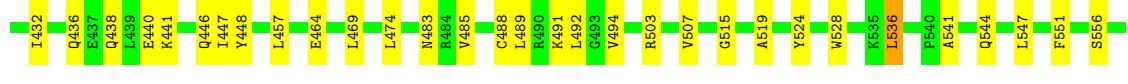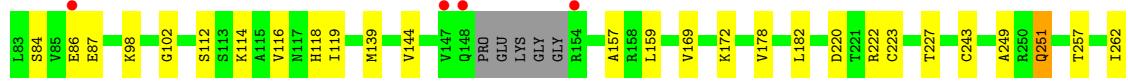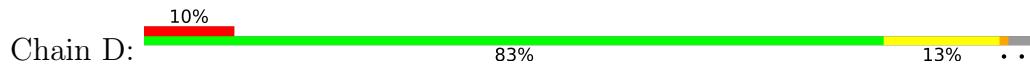
4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.08 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.206 , 0.246 0.201 , 0.242	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)	0.34 , 54.4	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ACY

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	0.31	0/4467	0.57	0/6062
1	B	0.31	0/4450	0.57	0/6039
1	C	0.30	0/4471	0.57	0/6067
1	D	0.30	0/4434	0.56	0/6017
All	All	0.31	0/17822	0.57	0/24185

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4372	0	4395	61	0
1	B	4355	0	4372	70	0
1	C	4376	0	4398	87	0
1	D	4340	0	4359	56	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	8	0	0
4	A	559	0	0	4	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	272	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 (272) 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:48:ARG:HG2	1:C:159:LEU:HD13	1.61	0.83
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: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: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:C:36:MET:CE	1:C:492:LEU:HA	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:LEU:HD12	1:B:243:CYS:SG	2.35	0.66
1:C:19:SER:HA	1:C:39:ALA:HB3	1.77	0.65
1:C:178:VAL:HG23	4:C:3144:HOH:O	1.94	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:36:MET:HE3	1:B:492:LEU:HA	1.78	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:A:440:GLU:H	1:A:440:GLU:CD	2.00	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: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:D:506:SER:O	1:D:510:ARG:HD3	2.02	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:182:LEU:C	1:D:182:LEU:HD23	2.26	0.55
1:A:23:ILE:HD13	1:A:23:ILE:C	2.27	0.55
1:B:24:ASN:OD1	1:B:27:SER:HB3	2.07	0.54
1:B:346:TYR:O	1:B:347:SER:HB3	2.07	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:B:313:MET:HG2	1:B:322:VAL:HG22	1.89	0.53
1:B:36:MET:HE3	1:B:492:LEU:HD12	1.91	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: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: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
1:B:31:LEU:HD11	1:B:492:LEU:HG	1.92	0.51
1:C:45:ALA:O	1:C:49:GLN:HG3	2.10	0.51
1:C:299:ALA:HB1	1:C:313:MET:CE	2.40	0.51
1:D:31:LEU:HG	1:D:492:LEU:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:MET:HE1	1:C:492:LEU:HA	1.92	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: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:A:24:ASN:HD21	1:A:400:ALA:HB2	1.76	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:C:182:LEU:HD23	1:C:182:LEU:C	2.33	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:C:36:MET:HE3	1:C:492:LEU:HA	1.94	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: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: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
1:C:36:MET:HE1	1:C:491:LYS:O	2.14	0.47
1:C:84:SER:OG	1:C:87:GLU:HG3	2.13	0.47
1:C:299:ALA:HB1	1:C:313:MET:HE2	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:535:LYS:HB3	1:D:535:LYS:HZ2	1.79	0.47
1:A:517:ARG:HG2	1:A:517:ARG:NH1	2.28	0.47
1:A:182:LEU:HD23	1:A:182:LEU:C	2.35	0.46
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:B:40:THR:HB	1:B:157:ALA:HB2	1.96	0.46
1:C:388:PRO:C	1:C:391:PRO:HD2	2.35	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:B:182:LEU:C	1:B:182:LEU:HD23	2.36	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:D:14:CYS:HB2	1:D:139:MET:HE1	1.98	0.45
1:D:365:SER:O	1:D:366:CYS:HB2	2.16	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
1:A:31:LEU:HG	1:A:492:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:14:CYS:HB2	1:B:139:MET:CE	2.48	0.43
1:B:236:GLU:OE2	1:B:280:ARG:NH2	2.46	0.43
1:C:564:LEU:C	1:C:564:LEU:HD13	2.39	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: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: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:A:40:THR:HB	1:A:157:ALA:HB2	2.01	0.42
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:B:33:HIS:HB2	1:B:36:MET:HE1	2.01	0.42
1:A:182:LEU:HB3	1:A:183:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:515:GLY:CA	1:C:519:ALA:HB2	2.50	0.41
1:A:138:ILE:HG23	1:A:138:ILE:O	2.20	0.41
1:A:268:ASN:HB3	1:A:274:CYS:SG	2.60	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
1:A:535:LYS:HB3	1:A:535:LYS:HZ3	1.85	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: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:A:535:LYS:HB3	1:A:535:LYS:HZ2	1.84	0.40
1:B:14:CYS:HB2	1:B:139:MET:HE1	2.02	0.40
1:C:19:SER:HB3	1:C:41:THR:CG2	2.51	0.40
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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	558/576 (97%)	543 (97%)	14 (2%)	1 (0%)	47	38
1	B	557/576 (97%)	543 (98%)	14 (2%)	0	100	100
1	C	559/576 (97%)	547 (98%)	11 (2%)	1 (0%)	47	38
1	D	554/576 (96%)	536 (97%)	17 (3%)	1 (0%)	47	38
All	All	2228/2304 (97%)	2169 (97%)	56 (2%)	3 (0%)	51	43

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 ⓘ

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%)	53	46
1	B	477/491 (97%)	470 (98%)	7 (2%)	65	60
1	C	480/491 (98%)	472 (98%)	8 (2%)	60	55
1	D	476/491 (97%)	471 (99%)	5 (1%)	73	71
All	All	1913/1964 (97%)	1883 (98%)	30 (2%)	62	58

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ILE
1	A	81	LYS
1	A	159	LEU
1	A	184	GLN
1	A	220	ASP
1	A	273	ASN
1	A	308	LEU
1	A	311	CYS
1	A	440	GLU
1	A	517	ARG
1	B	34	HIS
1	B	100	LYS
1	B	148	GLN
1	B	159	LEU
1	B	311	CYS
1	B	492	LEU
1	B	536	LEU
1	C	18	GLU
1	C	106	LYS
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	220	ASP
1	D	251	GLN
1	D	308	LEU
1	D	510	ARG

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

Mol	Chain	Res	Type
1	A	49	GLN
1	A	110	ASN
1	A	184	GLN
1	A	273	ASN
1	A	438	GLN
1	A	544	GLN
1	B	34	HIS
1	B	49	GLN
1	B	184	GLN

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Mol	Chain	Res	Type
1	B	273	ASN
1	B	406	ASN
1	B	438	GLN
1	B	446	GLN
1	B	544	GLN
1	C	49	GLN
1	C	142	ASN
1	C	184	GLN
1	C	273	ASN
1	C	309	GLN
1	C	406	ASN
1	C	436	GLN
1	C	502	HIS
1	D	251	GLN
1	D	273	ASN
1	D	330	GLN
1	D	406	ASN
1	D	411	ASN
1	D	438	GLN
1	D	446	GLN
1	D	461	GLN
1	D	544	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\#|Z| > 2$
3	GOL	A	4005	-	5,5,5	4.41	5 (100%)	5,5,5	1.84	3 (60%)
2	ACY	B	3007	-	3,3,3	0.47	0	3,3,3	1.68	1 (33%)
3	GOL	A	4006	-	5,5,5	4.42	5 (100%)	5,5,5	1.85	3 (60%)
2	ACY	D	3006	-	3,3,3	0.53	0	3,3,3	1.67	1 (33%)
2	ACY	C	3002	-	3,3,3	0.50	0	3,3,3	1.70	1 (33%)
2	ACY	A	3005	-	3,3,3	0.51	0	3,3,3	1.69	1 (33%)
2	ACY	A	3001	-	3,3,3	0.49	0	3,3,3	1.68	1 (33%)
3	GOL	A	4001	-	5,5,5	4.32	5 (100%)	5,5,5	1.84	3 (60%)
3	GOL	A	4004	-	5,5,5	4.41	5 (100%)	5,5,5	1.84	3 (60%)
3	GOL	A	4002	-	5,5,5	4.42	5 (100%)	5,5,5	1.84	3 (60%)
3	GOL	B	4007	-	5,5,5	4.43	5 (100%)	5,5,5	1.85	3 (60%)
2	ACY	B	3004	-	3,3,3	0.52	0	3,3,3	1.68	1 (33%)
2	ACY	B	3003	-	3,3,3	0.51	0	3,3,3	1.65	1 (33%)
3	GOL	B	4003	-	5,5,5	4.37	5 (100%)	5,5,5	1.84	3 (60%)

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	A	4005	-	-	4/4/4/4	-
3	GOL	A	4006	-	-	4/4/4/4	-
3	GOL	A	4004	-	-	4/4/4/4	-
3	GOL	A	4001	-	-	4/4/4/4	-
3	GOL	A	4002	-	-	4/4/4/4	-
3	GOL	B	4007	-	-	4/4/4/4	-
3	GOL	B	4003	-	-	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	-7.14	1.22	1.51
3	A	4005	GOL	C3-C2	-7.11	1.22	1.51
3	A	4004	GOL	C3-C2	-7.08	1.22	1.51
3	B	4007	GOL	C3-C2	-6.97	1.23	1.51
3	B	4003	GOL	C3-C2	-6.96	1.23	1.51
3	A	4006	GOL	C3-C2	-6.95	1.23	1.51
3	A	4001	GOL	C3-C2	-6.93	1.23	1.51
3	B	4007	GOL	O1-C1	4.66	1.62	1.42
3	A	4006	GOL	O1-C1	4.60	1.61	1.42
3	B	4003	GOL	O1-C1	4.49	1.61	1.42
3	A	4001	GOL	O1-C1	4.47	1.61	1.42
3	A	4004	GOL	O1-C1	4.47	1.61	1.42
3	A	4005	GOL	O1-C1	4.46	1.61	1.42
3	A	4002	GOL	O1-C1	4.37	1.60	1.42
3	A	4001	GOL	O3-C3	3.72	1.58	1.42
3	A	4004	GOL	O3-C3	3.72	1.58	1.42
3	B	4003	GOL	O3-C3	3.67	1.57	1.42
3	A	4006	GOL	O3-C3	3.65	1.57	1.42
3	B	4007	GOL	O3-C3	3.65	1.57	1.42
3	A	4002	GOL	O3-C3	3.62	1.57	1.42
3	A	4005	GOL	O3-C3	3.53	1.57	1.42
3	B	4007	GOL	O2-C2	-2.84	1.34	1.43
3	A	4006	GOL	O2-C2	-2.82	1.35	1.43
3	A	4002	GOL	O2-C2	-2.81	1.35	1.43
3	A	4005	GOL	O2-C2	-2.77	1.35	1.43
3	A	4004	GOL	O2-C2	-2.65	1.35	1.43
3	A	4005	GOL	C1-C2	-2.62	1.41	1.51
3	B	4003	GOL	O2-C2	-2.61	1.35	1.43
3	A	4002	GOL	C1-C2	-2.60	1.41	1.51
3	A	4006	GOL	C1-C2	-2.60	1.41	1.51
3	B	4003	GOL	C1-C2	-2.57	1.41	1.51
3	B	4007	GOL	C1-C2	-2.55	1.41	1.51
3	A	4004	GOL	C1-C2	-2.53	1.41	1.51
3	A	4001	GOL	C1-C2	-2.47	1.41	1.51
3	A	4001	GOL	O2-C2	-2.33	1.36	1.43

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	4006	GOL	C3-C2-C1	2.60	121.80	111.70
3	B	4007	GOL	C3-C2-C1	2.56	121.67	111.70
3	A	4001	GOL	O2-C2-C1	2.51	120.18	109.12
3	A	4005	GOL	C3-C2-C1	2.51	121.46	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	4003	GOL	C3-C2-C1	2.48	121.33	111.70
3	A	4002	GOL	C3-C2-C1	2.46	121.27	111.70
3	A	4002	GOL	O2-C2-C1	2.43	119.84	109.12
3	A	4004	GOL	C3-C2-C1	2.41	121.09	111.70
3	A	4004	GOL	O2-C2-C1	2.41	119.73	109.12
2	C	3002	ACY	O-C-CH3	-2.37	113.10	122.33
2	A	3005	ACY	O-C-CH3	-2.35	113.18	122.33
3	A	4005	GOL	O2-C2-C1	2.35	119.48	109.12
3	B	4003	GOL	O2-C2-C1	2.35	119.47	109.12
2	A	3001	ACY	O-C-CH3	-2.34	113.20	122.33
2	B	3007	ACY	O-C-CH3	-2.34	113.21	122.33
2	B	3004	ACY	O-C-CH3	-2.33	113.24	122.33
2	D	3006	ACY	O-C-CH3	-2.32	113.30	122.33
2	B	3003	ACY	O-C-CH3	-2.30	113.36	122.33
3	A	4001	GOL	C3-C2-C1	2.30	120.65	111.70
3	B	4007	GOL	O2-C2-C1	2.30	119.24	109.12
3	A	4001	GOL	O2-C2-C3	2.27	119.14	109.12
3	B	4003	GOL	O2-C2-C3	2.27	119.13	109.12
3	A	4004	GOL	O2-C2-C3	2.26	119.09	109.12
3	A	4006	GOL	O2-C2-C1	2.26	119.08	109.12
3	A	4006	GOL	O2-C2-C3	2.26	119.06	109.12
3	B	4007	GOL	O2-C2-C3	2.25	119.05	109.12
3	A	4005	GOL	O2-C2-C3	2.24	118.99	109.12
3	A	4002	GOL	O2-C2-C3	2.22	118.88	109.12

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	4002	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	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

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Mol	Chain	Res	Type	Atoms
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
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(Å²)	Q<0.9
1	A	562/576 (97%)	0.40	27 (4%)	30	40	16, 28, 53, 75	0
1	B	561/576 (97%)	0.46	34 (6%)	21	29	17, 29, 57, 81	0
1	C	563/576 (97%)	0.55	47 (8%)	11	17	16, 30, 56, 79	0
1	D	558/576 (96%)	0.66	55 (9%)	7	12	16, 33, 63, 85	0
All	All	2244/2304 (97%)	0.52	163 (7%)	15	23	16, 30, 57, 85	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	23	ILE	14.0
1	B	23	ILE	13.9
1	D	23	ILE	10.6
1	A	23	ILE	10.2
1	B	25	ALA	7.7
1	A	25	ALA	5.7
1	D	25	ALA	5.6
1	B	152	GLY	5.4
1	C	25	ALA	5.3
1	C	566	ARG	5.2
1	D	57	LEU	4.9
1	D	32	ARG	4.8
1	A	566	ARG	4.7
1	D	16	ALA	4.6
1	B	27	SER	4.5
1	D	545	LEU	4.5
1	C	57	LEU	4.4
1	B	26	LEU	4.4
1	D	14	CYS	4.4
1	C	16	ALA	4.3
1	C	153	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	148	GLN	4.2
1	A	564	LEU	4.1
1	C	34	HIS	4.1
1	A	149	PRO	4.1
1	D	544	GLN	4.1
1	C	26	LEU	4.0
1	B	14	CYS	3.9
1	D	27	SER	3.9
1	D	10	LEU	3.9
1	C	541	ALA	3.8
1	B	545	LEU	3.8
1	D	26	LEU	3.8
1	A	565	SER	3.8
1	A	402	HIS	3.8
1	A	563	SER	3.7
1	D	563	SER	3.7
1	A	148	GLN	3.7
1	A	24	ASN	3.7
1	D	24	ASN	3.7
1	C	366	CYS	3.7
1	D	50	LYS	3.7
1	D	31	LEU	3.6
1	D	34	HIS	3.6
1	C	10	LEU	3.6
1	D	21	LEU	3.6
1	B	541	ALA	3.6
1	C	43	ARG	3.6
1	D	43	ARG	3.6
1	D	147	VAL	3.5
1	C	15	ALA	3.5
1	A	14	CYS	3.5
1	B	402	HIS	3.4
1	A	34	HIS	3.4
1	C	149	PRO	3.3
1	A	26	LEU	3.3
1	C	564	LEU	3.2
1	B	153	GLY	3.2
1	D	39	ALA	3.2
1	A	541	ALA	3.2
1	C	35	ASN	3.1
1	D	535	LYS	3.1
1	B	24	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	35	ASN	3.1
1	C	565	SER	3.1
1	A	16	ALA	3.1
1	C	14	CYS	3.0
1	A	544	GLN	3.0
1	C	540	PRO	3.0
1	C	148	GLN	3.0
1	D	402	HIS	2.9
1	B	544	GLN	2.9
1	C	18	GLU	2.9
1	C	404	PRO	2.9
1	D	47	LEU	2.9
1	D	15	ALA	2.9
1	A	366	CYS	2.8
1	A	32	ARG	2.8
1	D	493	GLY	2.8
1	B	21	LEU	2.7
1	C	21	LEU	2.7
1	C	544	GLN	2.7
1	D	20	LYS	2.7
1	D	401	ARG	2.7
1	C	7	THR	2.7
1	B	22	PRO	2.7
1	C	47	LEU	2.6
1	D	53	THR	2.6
1	D	148	GLN	2.6
1	A	545	LEU	2.6
1	C	367	SER	2.6
1	A	27	SER	2.6
1	B	540	PRO	2.6
1	D	51	LYS	2.6
1	B	147	VAL	2.6
1	A	35	ASN	2.6
1	D	5	THR	2.6
1	C	402	HIS	2.5
1	C	24	ASN	2.5
1	D	274	CYS	2.5
1	D	11	ILE	2.5
1	D	541	ALA	2.5
1	C	32	ARG	2.5
1	D	41	THR	2.5
1	B	34	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	59	VAL	2.5
1	A	22	PRO	2.4
1	B	149	PRO	2.4
1	B	35	ASN	2.4
1	B	32	ARG	2.4
1	D	272	GLN	2.4
1	C	28	ASN	2.4
1	C	293	LEU	2.4
1	D	540	PRO	2.4
1	D	543	SER	2.4
1	D	154	ARG	2.4
1	B	57	LEU	2.4
1	B	368	SER	2.4
1	B	366	CYS	2.3
1	C	20	LYS	2.3
1	D	29	SER	2.3
1	D	18	GLU	2.3
1	B	542	ALA	2.3
1	B	43	ARG	2.3
1	C	29	SER	2.3
1	B	563	SER	2.3
1	D	320	LEU	2.3
1	D	448	TYR	2.3
1	D	6	TRP	2.3
1	D	28	ASN	2.3
1	B	154	ARG	2.3
1	B	16	ALA	2.2
1	A	367	SER	2.2
1	C	154	ARG	2.2
1	C	289	CYS	2.2
1	C	9	ALA	2.2
1	D	19	SER	2.2
1	B	535	LYS	2.2
1	D	9	ALA	2.2
1	D	86	GLU	2.2
1	C	36	MET	2.2
1	D	553	ALA	2.2
1	B	352	ASP	2.2
1	C	352	ASP	2.1
1	C	22	PRO	2.1
1	C	147	VAL	2.1
1	D	7	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	376	ALA	2.1
1	A	20	LYS	2.1
1	C	321	VAL	2.1
1	B	367	SER	2.1
1	C	563	SER	2.1
1	D	352	ASP	2.1
1	C	317	GLY	2.1
1	C	222	ARG	2.1
1	C	535	LYS	2.1
1	A	540	PRO	2.1
1	D	22	PRO	2.0
1	B	320	LEU	2.0
1	C	220	ASP	2.0
1	B	491	LYS	2.0
1	D	321	VAL	2.0
1	A	21	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	B	4007	6/6	0.61	0.36	62,64,66,67	0
2	ACY	D	3006	4/4	0.65	0.18	69,70,70,70	0
2	ACY	C	3002	4/4	0.67	0.25	57,58,59,59	0
3	GOL	B	4003	6/6	0.74	0.20	51,52,55,57	0
2	ACY	B	3007	4/4	0.77	0.28	54,57,57,57	0
3	GOL	A	4004	6/6	0.78	0.20	47,49,50,50	0
2	ACY	A	3001	4/4	0.79	0.18	57,57,58,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	A	4006	6/6	0.79	0.26	68,70,71,71	0
3	GOL	A	4001	6/6	0.80	0.21	32,40,43,46	0
2	ACY	B	3003	4/4	0.82	0.24	68,69,69,70	0
3	GOL	A	4002	6/6	0.83	0.21	39,48,49,51	0
3	GOL	A	4005	6/6	0.86	0.26	43,52,56,56	0
2	ACY	A	3005	4/4	0.88	0.17	53,55,55,56	0
2	ACY	B	3004	4/4	0.92	0.10	73,73,73,73	0

6.5 Other polymers (i)

There are no such residues in this entry.