



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 04:07 PM EDT

PDB ID : 3EU9 / pdb_00003eu9
Title : The ankyrin repeat domain of Huntingtin interacting protein 14
Authors : Gao, T.; Collins, R.E.; Horton, J.R.; Zhang, R.; Zhang, X.; Cheng, X.
Deposited on : 2008-10-09
Resolution : 1.99 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

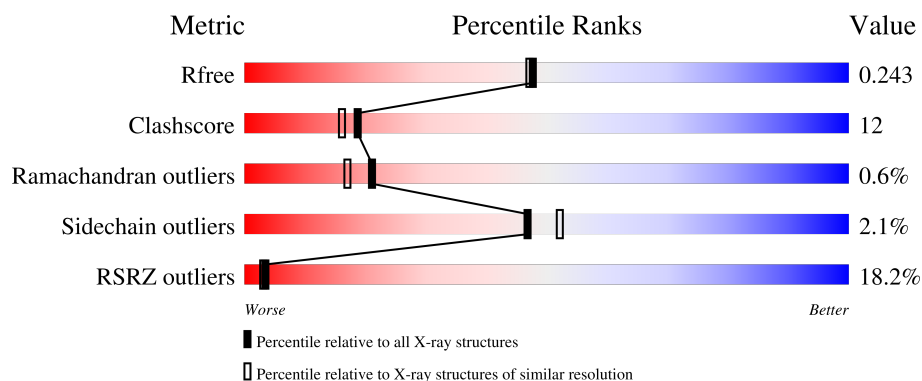
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	240	16% 77% 18% • •
1	B	240	32% 62% 32% • 5%
1	C	240	4% 76% 17% • 6%

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
4	GOL	C	449	-	X	-	-
4	GOL	C	450	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5620 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.

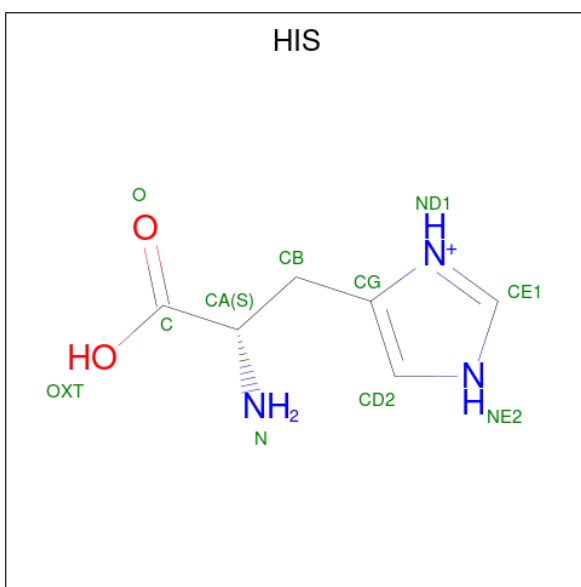
- Molecule 1 is a protein called Huntingtin-interacting protein 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	1	0
			1775	1119	311	335	10			
1	B	227	Total	C	N	O	S	0	0	0
			1696	1069	296	321	10			
1	C	226	Total	C	N	O	S	0	0	0
			1750	1106	312	322	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	49	HIS	-	expression tag	UNP Q8IUH5
A	50	MET	-	expression tag	UNP Q8IUH5
B	49	HIS	-	expression tag	UNP Q8IUH5
B	50	MET	-	expression tag	UNP Q8IUH5
C	49	HIS	-	expression tag	UNP Q8IUH5
C	50	MET	-	expression tag	UNP Q8IUH5

- Molecule 2 is HISTIDINE (CCD ID: HIS) (formula: C₆H₁₀N₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	3	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	137	Total	O	0	0
			137	137		
5	B	65	Total	O	0	0
			65	65		
5	C	140	Total	O	0	0
			140	140		

4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	106.66Å 106.66Å 255.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.27 – 1.99 34.27 – 1.99	Depositor EDS
% Data completeness (in resolution range)	97.5 (34.27-1.99) 97.6 (34.27-1.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.05 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.251 0.215 , 0.243	Depositor DCC
R_{free} test set	3004 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.3	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	0.94	EDS
Total number of atoms	5620	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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: GOL, SO4

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	0/1811	0.85	3/2469 (0.1%)
1	B	0.32	0/1731	0.79	1/2365 (0.0%)
1	C	0.38	0/1786	0.86	4/2430 (0.2%)
All	All	0.36	0/5328	0.83	8/7264 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	116	VAL	N-CA-C	6.62	117.32	110.36
1	A	218	ASN	N-CA-C	6.09	119.66	112.72
1	C	218	ASN	N-CA-C	5.93	120.21	112.92
1	A	189	ASN	N-CA-C	-5.54	106.18	113.17
1	B	116	VAL	N-CA-C	5.37	116.00	110.36
1	A	103	ILE	N-CA-C	5.23	115.95	110.62
1	C	60	ASP	N-CA-C	-5.11	104.13	110.41
1	C	222	LYS	N-CA-C	5.10	117.50	111.33

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	1775	0	1707	29	0
1	B	1696	0	1588	68	0
1	C	1750	0	1723	32	0
2	A	10	0	6	1	0
3	A	15	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
4	C	12	0	8	0	0
5	A	137	0	0	2	0
5	B	65	0	0	0	0
5	C	140	0	0	4	0
All	All	5620	0	5032	123	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 12.

All (123) 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:218:ASN:HD21	1:A:250:ASN:H	1.12	0.94
1:B:53:ILE:HG13	1:B:54:ASP:H	1.41	0.86
1:B:192:THR:H	1:B:195:MET:HE3	1.45	0.81
1:B:153:ILE:HD13	1:B:188:GLN:HG2	1.64	0.80
1:B:192:THR:N	1:B:195:MET:HE3	1.99	0.78
1:B:192:THR:HG22	1:B:195:MET:HG3	1.66	0.78
1:B:53:ILE:HG22	1:C:238:THR:HB	1.66	0.76
1:C:218:ASN:HD21	1:C:250:ASN:H	1.35	0.75
1:A:218:ASN:ND2	1:A:250:ASN:H	1.84	0.73
1:A:126:THR:H	1:A:129:HIS:HD2	1.37	0.72
1:B:53:ILE:HG22	1:C:238:THR:CB	2.19	0.72
1:A:240:VAL:HG12	1:A:244:LEU:HD22	1.73	0.70
1:A:262:LEU:HG	1:A:266:LYS:HE3	1.72	0.70
1:B:264:LEU:HD12	1:B:264:LEU:H	1.57	0.70
1:B:157:GLY:O	1:B:187:ASP:HB2	1.94	0.67
1:A:126:THR:H	1:A:129:HIS:CD2	2.12	0.67
1:B:270:ASN:ND2	1:B:273:MET:HE3	2.10	0.66
1:A:71:GLU:H	1:A:71:GLU:CD	2.04	0.65
1:C:218:ASN:ND2	1:C:250:ASN:H	1.96	0.63
1:B:77:VAL:HG21	1:B:108:TYR:CE2	2.34	0.62
1:A:270:ASN:O	1:A:274:ILE:HG13	2.01	0.60
1:A:218:ASN:HD21	1:A:250:ASN:N	1.92	0.60
1:C:275:ASN:O	1:C:279:GLU:HG3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:VAL:HG22	1:C:215:VAL:HG12	1.83	0.59
1:A:183:VAL:HG22	1:A:215:VAL:HG22	1.85	0.58
1:B:264:LEU:HD12	1:B:264:LEU:N	2.18	0.58
1:B:77:VAL:HG21	1:B:108:TYR:HE2	1.69	0.58
1:A:189:ASN:OD1	2:A:322:HIS:N	2.38	0.57
1:A:245:LEU:HD13	1:A:280:ALA:HB2	1.86	0.57
1:B:274:ILE:O	1:B:278:GLN:HB2	2.06	0.56
1:B:53:ILE:HG23	1:C:272:TRP:CD2	2.41	0.56
1:B:229:LEU:O	1:B:233:VAL:HG23	2.05	0.55
1:B:115:ILE:HB	1:B:118:GLN:HB2	1.87	0.55
1:A:115:ILE:HB	1:A:118:GLN:HB2	1.88	0.54
1:B:153:ILE:CG2	1:B:157:GLY:HA2	2.38	0.54
1:B:255:ASN:C	1:B:257:LYS:H	2.14	0.54
1:A:74:ARG:HG2	1:A:78:GLU:OE1	2.09	0.52
1:C:73:CYS:O	1:C:77:VAL:HG23	2.10	0.52
1:B:110:ILE:HD12	1:B:146:TYR:CD1	2.44	0.52
1:B:187:ASP:C	1:B:189:ASN:H	2.17	0.52
1:B:199:TYR:HB2	1:B:231:TRP:HB3	1.91	0.52
1:B:234:LEU:HD21	1:B:264:LEU:HD23	1.92	0.52
1:B:106:VAL:HG21	1:B:139:MET:SD	2.50	0.52
1:A:166:GLN:HE21	1:A:200:ARG:NH1	2.07	0.51
1:B:221:ASP:O	1:B:225:LYS:HA	2.10	0.51
1:B:237:ASN:O	1:B:241:ILE:HG12	2.11	0.51
1:A:222:LYS:HD2	5:A:412:HOH:O	2.11	0.51
1:C:202:HIS:HE1	5:C:525:HOH:O	1.93	0.51
1:B:264:LEU:H	1:B:264:LEU:CD1	2.22	0.51
1:C:183:VAL:CG2	1:C:215:VAL:HG12	2.41	0.51
1:B:53:ILE:HG13	1:B:54:ASP:N	2.20	0.50
1:B:202:HIS:HA	1:B:237:ASN:ND2	2.27	0.50
1:A:153:ILE:HD12	5:A:372:HOH:O	2.11	0.50
1:B:202:HIS:HA	1:B:237:ASN:HD21	1.76	0.50
1:B:270:ASN:CG	1:B:273:MET:HE3	2.36	0.50
1:B:175:TYR:O	1:B:179:LYS:HG2	2.12	0.49
1:B:53:ILE:HA	1:C:238:THR:HG21	1.94	0.49
1:B:128:LEU:HD11	1:B:140:VAL:HG13	1.95	0.49
1:B:270:ASN:O	1:B:274:ILE:HG13	2.13	0.49
1:C:183:VAL:HG22	1:C:215:VAL:CG1	2.42	0.49
1:C:63:LYS:HD3	1:C:66:GLN:NE2	2.28	0.48
1:A:61:ILE:HG23	1:A:62:VAL:N	2.28	0.47
1:C:188:GLN:HG3	5:C:574:HOH:O	2.13	0.47
1:A:224:HIS:O	1:A:255:ASN:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:ASN:HD21	1:C:250:ASN:N	2.07	0.47
1:B:102:ARG:O	1:B:106:VAL:HG23	2.15	0.47
1:C:74:ARG:O	1:C:78:GLU:HG3	2.14	0.47
1:C:84:ARG:O	1:C:86:PRO:HD3	2.15	0.47
1:C:157:GLY:O	1:C:187:ASP:HB2	2.15	0.47
1:C:108:TYR:O	1:C:112:LYS:HG2	2.15	0.46
1:A:186:MET:SD	1:A:222:LYS:HE3	2.54	0.46
1:B:227:THR:HB	1:B:230:HIS:ND1	2.29	0.46
1:B:227:THR:HG22	1:B:228:ALA:N	2.31	0.46
1:A:175:TYR:O	1:A:179:LYS:HG2	2.16	0.46
1:B:103:ILE:HD13	1:B:139:MET:CE	2.46	0.46
1:B:185:MET:O	1:B:193:PRO:HD3	2.15	0.46
1:B:212:THR:C	1:B:214:ASN:H	2.23	0.46
1:C:106:VAL:HG21	1:C:139:MET:SD	2.55	0.46
1:A:157:GLY:O	1:A:187:ASP:HB2	2.15	0.45
1:B:153:ILE:HG21	1:B:157:GLY:HA2	1.97	0.45
1:B:55:ASP:OD2	1:B:58:THR:HG23	2.17	0.45
1:B:209:LEU:O	1:B:212:THR:HB	2.15	0.45
1:B:260:SER:O	1:B:262:LEU:N	2.50	0.44
1:A:98:ALA:HA	1:A:139:MET:HE3	2.00	0.44
1:B:154:ASP:OD1	1:B:156:GLU:N	2.45	0.44
1:B:77:VAL:HG21	1:B:108:TYR:OH	2.17	0.44
1:B:240:VAL:O	1:B:244:LEU:HD13	2.18	0.44
1:B:204:VAL:HA	1:B:243:LEU:HD11	1.99	0.44
1:A:166:GLN:HB2	1:A:200:ARG:HD3	2.00	0.43
1:B:103:ILE:HD13	1:B:139:MET:HE2	2.00	0.43
1:B:77:VAL:CG2	1:B:108:TYR:OH	2.67	0.43
1:C:267:GLN:HG3	5:C:543:HOH:O	2.18	0.43
1:A:224:HIS:O	1:A:225:LYS:HB2	2.19	0.43
1:A:106:VAL:HG21	1:A:139:MET:SD	2.59	0.42
1:B:54:ASP:O	1:B:55:ASP:HB3	2.19	0.42
1:B:184:ASP:OD1	1:B:215:VAL:HG23	2.19	0.42
1:B:254:GLN:HA	1:B:259:GLU:O	2.20	0.42
1:B:261:ALA:HA	1:B:264:LEU:HD13	2.01	0.42
1:B:137:LEU:O	1:B:141:VAL:HG23	2.19	0.42
1:C:224:HIS:O	1:C:255:ASN:HB2	2.19	0.42
1:C:115:ILE:HB	1:C:118:GLN:HB2	2.00	0.42
1:B:108:TYR:OH	1:B:112:LYS:HE3	2.20	0.42
1:B:255:ASN:C	1:B:257:LYS:N	2.78	0.42
1:C:266:LYS:HA	1:C:274:ILE:HD11	2.01	0.41
1:B:53:ILE:HG22	1:C:238:THR:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:ASP:C	1:B:189:ASN:N	2.78	0.41
1:B:106:VAL:O	1:B:110:ILE:HG13	2.19	0.41
1:A:237:ASN:O	1:A:241:ILE:HG13	2.21	0.41
1:C:60:ASP:OD1	1:C:60:ASP:C	2.64	0.41
1:B:74:ARG:O	1:B:77:VAL:HG22	2.21	0.41
1:C:123:LEU:O	1:C:124:ASN:C	2.64	0.41
1:A:253:ALA:O	1:A:260:SER:HA	2.21	0.41
1:A:254:GLN:HA	1:A:259:GLU:O	2.20	0.41
1:B:53:ILE:HG23	1:C:272:TRP:CE2	2.56	0.41
1:C:142:GLN:HE21	1:C:142:GLN:HA	1.85	0.41
1:C:174:ALA:HB2	1:C:209:LEU:HD21	2.03	0.41
1:B:254:GLN:HA	1:B:260:SER:HA	2.03	0.41
1:C:84:ARG:HD2	5:C:578:HOH:O	2.21	0.41
1:B:169:HIS:O	1:B:173:VAL:HG23	2.21	0.40
1:B:180:GLY:O	1:B:181:GLN:C	2.65	0.40
1:B:220:GLY:HA2	1:B:226:ASN:O	2.21	0.40
1:B:77:VAL:HG23	1:B:78:GLU:N	2.37	0.40
1:C:204:VAL:HG11	1:C:208:ARG:NH1	2.37	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	231/240 (96%)	227 (98%)	4 (2%)	0	100	100
1	B	225/240 (94%)	202 (90%)	19 (8%)	4 (2%)	6	3
1	C	224/240 (93%)	220 (98%)	4 (2%)	0	100	100
All	All	680/720 (94%)	649 (95%)	27 (4%)	4 (1%)	21	17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	223	TYR
1	B	261	ALA
1	B	55	ASP
1	B	256	ILE

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	182/200 (91%)	177 (97%)	5 (3%)	39	42
1	B	167/200 (84%)	165 (99%)	2 (1%)	63	70
1	C	182/200 (91%)	178 (98%)	4 (2%)	45	50
All	All	531/600 (88%)	520 (98%)	11 (2%)	47	52

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	GLU
1	A	94	LEU
1	A	101	ASN
1	A	229	LEU
1	A	244	LEU
1	B	94	LEU
1	B	101	ASN
1	C	101	ASN
1	C	137	LEU
1	C	142	GLN
1	C	214	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	90	ASN
1	A	101	ASN

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Mol	Chain	Res	Type
1	A	118	GLN
1	A	129	HIS
1	A	166	GLN
1	A	189	ASN
1	A	218	ASN
1	A	254	GLN
1	A	276	HIS
1	B	66	GLN
1	B	90	ASN
1	B	101	ASN
1	B	118	GLN
1	B	134	GLN
1	B	136	HIS
1	B	275	ASN
1	C	66	GLN
1	C	101	ASN
1	C	134	GLN
1	C	214	ASN
1	C	218	ASN
1	C	254	GLN
1	C	275	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	SO4	C	451	-	4,4,4	0.35	0	6,6,6	0.08	0
2	HIS	A	322	-	9,10,11	0.50	0	8,12,14	0.98	0
3	SO4	B	322	-	4,4,4	0.37	0	6,6,6	0.08	0
4	GOL	C	450	-	5,5,5	4.81	5 (100%)	5,5,5	6.06	3 (60%)
3	SO4	A	323	-	4,4,4	0.35	0	6,6,6	0.10	0
3	SO4	C	452	-	4,4,4	0.36	0	6,6,6	0.09	0
3	SO4	A	324	-	4,4,4	0.38	0	6,6,6	0.08	0
4	GOL	C	449	-	5,5,5	4.75	5 (100%)	5,5,5	6.05	3 (60%)
3	SO4	A	325	-	4,4,4	0.34	0	6,6,6	0.10	0
3	SO4	B	323	-	4,4,4	0.36	0	6,6,6	0.08	0

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
4	GOL	C	449	-	-	3/4/4/4	-
4	GOL	C	450	-	-	4/4/4/4	-
2	HIS	A	322	-	-	0/5/6/8	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	450	GOL	C3-C2	-8.20	1.20	1.51
4	C	449	GOL	C3-C2	-7.92	1.21	1.51
4	C	449	GOL	O1-C1	4.62	1.61	1.42
4	C	450	GOL	O1-C1	4.61	1.61	1.42
4	C	449	GOL	O3-C3	3.46	1.56	1.42
4	C	450	GOL	O3-C3	3.19	1.55	1.42
4	C	450	GOL	C1-C2	-2.93	1.40	1.51
4	C	449	GOL	C1-C2	-2.92	1.40	1.51
4	C	449	GOL	O2-C2	-2.88	1.35	1.43
4	C	450	GOL	O2-C2	-2.85	1.35	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	449	GOL	O3-C3-C2	11.07	160.23	110.38
4	C	450	GOL	O3-C3-C2	11.07	160.23	110.38
4	C	449	GOL	O2-C2-C3	6.88	137.66	109.18
4	C	450	GOL	O2-C2-C3	6.88	137.65	109.18
4	C	450	GOL	O1-C1-C2	3.58	126.48	110.38
4	C	449	GOL	O1-C1-C2	3.46	125.93	110.38

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	450	GOL	C1-C2-C3-O3
4	C	449	GOL	O1-C1-C2-C3
4	C	449	GOL	O1-C1-C2-O2
4	C	450	GOL	O1-C1-C2-O2
4	C	449	GOL	O2-C2-C3-O3
4	C	450	GOL	O2-C2-C3-O3
4	C	450	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	322	HIS	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	232/240 (96%)	0.85	38 (16%) 4 4	18, 33, 62, 68	1 (0%)
1	B	227/240 (94%)	1.74	77 (33%) 1 1	28, 52, 79, 83	0
1	C	226/240 (94%)	0.33	10 (4%) 39 38	18, 28, 53, 64	0
All	All	685/720 (95%)	0.97	125 (18%) 3 3	18, 37, 72, 83	1 (0%)

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	53	ILE	6.8
1	B	223	TYR	5.9
1	A	272	TRP	5.5
1	B	219	LEU	5.2
1	C	59	TRP	4.9
1	B	277	LEU	4.8
1	C	284	LYS	4.8
1	A	277	LEU	4.7
1	B	262	LEU	4.2
1	A	280	ALA	4.2
1	B	261	ALA	4.2
1	B	153	ILE	4.2
1	A	269	LYS	4.1
1	B	228	ALA	4.1
1	B	246	GLU	4.0
1	B	54	ASP	4.0
1	A	274	ILE	3.9
1	B	267	GLN	3.8
1	B	253	ALA	3.8
1	B	204	VAL	3.8
1	B	217	VAL	3.7
1	A	271	VAL	3.6
1	A	215	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	231	TRP	3.5
1	A	262	LEU	3.5
1	B	263	ASP	3.5
1	B	245	LEU	3.4
1	B	251	VAL	3.4
1	B	227	THR	3.4
1	B	244	LEU	3.3
1	B	259	GLU	3.3
1	A	278	GLN	3.3
1	A	256	ILE	3.3
1	B	190	GLY	3.3
1	C	79	ALA	3.2
1	A	245	LEU	3.2
1	B	274	ILE	3.2
1	B	122	ASP	3.2
1	A	50	MET	3.1
1	B	271	VAL	3.1
1	B	247	ALA	3.1
1	B	264	LEU	3.1
1	B	224	HIS	3.0
1	B	260	SER	3.0
1	B	178	ALA	2.9
1	B	197	ALA	2.9
1	C	283	ALA	2.9
1	A	281	ARG	2.9
1	B	258	GLY	2.9
1	B	279	GLU	2.9
1	B	265	ALA	2.8
1	A	71	GLU	2.8
1	B	256	ILE	2.8
1	B	229	LEU	2.8
1	B	254	GLN	2.8
1	B	215	VAL	2.8
1	B	177	ILE	2.8
1	A	275	ASN	2.7
1	B	158	CYS	2.7
1	A	276	HIS	2.7
1	A	236	GLY	2.7
1	A	273	MET	2.7
1	A	261	ALA	2.7
1	B	241	ILE	2.7
1	A	279	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	62	VAL	2.7
1	B	157	GLY	2.6
1	B	242	SER	2.6
1	A	264	LEU	2.6
1	B	77	VAL	2.6
1	A	242	SER	2.6
1	A	79	ALA	2.5
1	B	192	THR	2.5
1	C	76	LEU	2.5
1	A	57	SER	2.5
1	A	202	HIS	2.5
1	B	124	ASN	2.5
1	B	276	HIS	2.5
1	A	59	TRP	2.5
1	A	265	ALA	2.5
1	B	255	ASN	2.4
1	B	148	ALA	2.4
1	B	183	VAL	2.4
1	B	218	ASN	2.4
1	B	252	ASP	2.4
1	C	86	PRO	2.4
1	B	222	LYS	2.4
1	B	119	LEU	2.3
1	B	243	LEU	2.3
1	B	225	LYS	2.3
1	C	77	VAL	2.3
1	B	143	LEU	2.3
1	B	176	LEU	2.3
1	B	272	TRP	2.3
1	B	186	MET	2.3
1	B	180	GLY	2.3
1	B	55	ASP	2.3
1	A	235	ALA	2.2
1	B	57	SER	2.2
1	B	208	ARG	2.2
1	A	62	VAL	2.2
1	A	241	ILE	2.2
1	A	84	ARG	2.2
1	B	185	MET	2.2
1	A	249	ALA	2.2
1	B	115	ILE	2.1
1	B	278	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	239	THR	2.1
1	B	220	GLY	2.1
1	B	198	ALA	2.1
1	B	235	ALA	2.1
1	B	146	TYR	2.1
1	A	260	SER	2.1
1	C	82	ASP	2.1
1	A	200	ARG	2.1
1	B	151	SER	2.1
1	A	224	HIS	2.1
1	A	214	ASN	2.1
1	B	104	ASP	2.1
1	C	256	ILE	2.0
1	A	67	TYR	2.0
1	B	160	CYS	2.0
1	B	234	LEU	2.0
1	B	273	MET	2.0
1	B	189	ASN	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(Å ²)	Q<0.9
3	SO4	A	324	5/5	0.66	0.15	108,108,108,108	0
3	SO4	A	325	5/5	0.68	0.17	93,93,93,93	0
2	HIS	A	322	10/11	0.70	0.21	60,60,60,61	0
3	SO4	B	322	5/5	0.71	0.17	88,89,89,89	0
3	SO4	B	323	5/5	0.73	0.14	98,98,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	C	449	6/6	0.77	0.15	57,58,59,59	0
4	GOL	C	450	6/6	0.80	0.15	44,46,47,48	0
3	SO4	C	451	5/5	0.84	0.12	87,87,88,88	0
3	SO4	C	452	5/5	0.86	0.12	83,83,84,84	0
3	SO4	A	323	5/5	0.88	0.15	51,52,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.