



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 04:45 AM GMT

PDB ID : 1UHG
Title : Crystal Structure of S-Ovalbumin At 1.9 Angstrom Resolution
Authors : Yamasaki, M.; Takahashi, N.; Hirose, M.
Deposited on : 2003-07-03
Resolution : 1.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

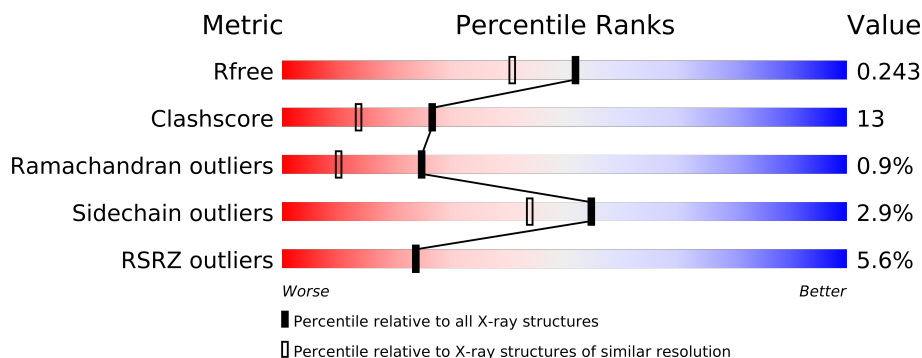
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.90 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}	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	385	
1	B	385	
1	C	385	
1	D	385	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	SO4	B	1401	-	X
4	SO4	B	1402	-	X
4	SO4	C	2401	-	X
4	SO4	D	3401	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12910 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Ovalbumin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	P	S	0	0	0
			2987	1891	496	576	2	22			
1	B	385	Total	C	N	O	P	S	0	0	0
			3001	1901	499	578	1	22			
1	C	374	Total	C	N	O	P	S	0	0	0
			2933	1865	488	558		22			
1	D	385	Total	C	N	O	P	S	0	0	0
			3005	1901	499	581	2	22			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	SEP	SER	MODIFIED RESIDUE	UNP P01012
A	164	DSN	SER	MODIFIED RESIDUE	UNP P01012
A	236	DSN	SER	MODIFIED RESIDUE	UNP P01012
A	320	DSN	SER	MODIFIED RESIDUE	UNP P01012
A	344	SEP	SER	MODIFIED RESIDUE	UNP P01012
B	68	SEP	SER	MODIFIED RESIDUE	UNP P01012
B	164	DSN	SER	MODIFIED RESIDUE	UNP P01012
B	236	DSN	SER	MODIFIED RESIDUE	UNP P01012
B	320	DSN	SER	MODIFIED RESIDUE	UNP P01012
B	344	SEP	SER	MODIFIED RESIDUE	UNP P01012
C	68	SEP	SER	MODIFIED RESIDUE	UNP P01012
C	164	DSN	SER	MODIFIED RESIDUE	UNP P01012
C	236	DSN	SER	MODIFIED RESIDUE	UNP P01012
C	320	DSN	SER	MODIFIED RESIDUE	UNP P01012
C	344	SEP	SER	MODIFIED RESIDUE	UNP P01012
D	68	SEP	SER	MODIFIED RESIDUE	UNP P01012
D	164	DSN	SER	MODIFIED RESIDUE	UNP P01012
D	236	DSN	SER	MODIFIED RESIDUE	UNP P01012
D	320	DSN	SER	MODIFIED RESIDUE	UNP P01012
D	344	SEP	SER	MODIFIED RESIDUE	UNP P01012

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		
2	C	2	Total	C	N	O	0	0
			28	16	2	10		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	SEP	SER	MODIFIED RESIDUE	UNP P01012
A	164	DSN	SER	MODIFIED RESIDUE	UNP P01012
A	236	DSN	SER	MODIFIED RESIDUE	UNP P01012
A	320	DSN	SER	MODIFIED RESIDUE	UNP P01012
A	344	SEP	SER	MODIFIED RESIDUE	UNP P01012
B	68	SEP	SER	MODIFIED RESIDUE	UNP P01012
B	164	DSN	SER	MODIFIED RESIDUE	UNP P01012
B	236	DSN	SER	MODIFIED RESIDUE	UNP P01012
B	320	DSN	SER	MODIFIED RESIDUE	UNP P01012
B	344	SEP	SER	MODIFIED RESIDUE	UNP P01012
C	68	SEP	SER	MODIFIED RESIDUE	UNP P01012
C	164	DSN	SER	MODIFIED RESIDUE	UNP P01012
C	236	DSN	SER	MODIFIED RESIDUE	UNP P01012
C	320	DSN	SER	MODIFIED RESIDUE	UNP P01012
C	344	SEP	SER	MODIFIED RESIDUE	UNP P01012

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	218	Total	O	0	0
			218	218		
5	B	219	Total	O	0	0
			219	219		
5	C	206	Total	O	0	0
			206	206		
5	D	208	Total	O	0	0
			208	208		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.65Å 70.91Å 83.39Å 87.24° 71.73° 75.95°	Depositor
Resolution (Å)	14.89 – 1.90 29.25 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.1 (14.89-1.90) 94.7 (29.25-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 1.80Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.196 , 0.247 0.193 , 0.243	Depositor DCC
R_{free} test set	10051 reflections (11.18%)	DCC
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 48.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 116048 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12910	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DSN, SO4, NAG, SEP

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	0.51	1/2999 (0.0%)	0.70	0/4043
1	B	0.49	0/3018	0.69	0/4070
1	C	0.51	0/2960	0.69	0/3991
1	D	0.52	0/3018	0.69	2/4070 (0.0%)
All	All	0.51	1/11995 (0.0%)	0.69	2/16174 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	1	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	367	CYS	CB-SG	-5.30	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	183	LEU	CA-CB-CG	5.35	127.60	115.30
1	D	216	LEU	CA-CB-CG	5.34	127.58	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	164	DSN	CA

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2987	0	2964	81	0
1	B	3001	0	2978	85	0
1	C	2933	0	2924	84	0
1	D	3005	0	2979	80	0
2	A	28	0	25	1	0
2	B	28	0	25	0	0
2	C	28	0	25	2	0
3	D	14	0	13	3	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	C	5	0	0	0	0
4	D	10	0	0	0	0
5	A	218	0	0	10	0
5	B	219	0	0	3	0
5	C	206	0	0	1	0
5	D	208	0	0	6	0
All	All	12910	0	11933	316	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (316) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:99:PHE:CZ	1:C:178:ILE:HD11	1.92	1.04
1:C:8:MET:HE3	1:C:376:VAL:HG21	1.50	0.93
1:B:199:ARG:HG2	1:B:249:VAL:HG21	1.54	0.89
1:D:162:GLN:NE2	1:D:162:GLN:H	1.72	0.86
1:B:100:SER:O	1:B:178:ILE:HD12	1.76	0.85
1:D:178:ILE:HD13	1:D:378:PHE:HE1	1.40	0.84
1:A:43:LEU:HD13	1:A:120:CYS:SG	2.17	0.84
1:D:312:LEU:HD12	1:D:321:LEU:HD22	1.61	0.81
1:B:286:LYS:HG3	1:B:333:GLU:HG2	1.63	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:218:ARG:HH21	1:A:273:MET:HB2	1.45	0.80
1:A:100:SER:O	1:A:178:ILE:HD12	1.82	0.80
1:C:199:ARG:HD3	1:C:199:ARG:N	1.99	0.78
1:C:278:ILE:HG22	1:C:356:GLU:HG2	1.65	0.77
1:B:8:MET:HG2	1:B:376:VAL:HG23	1.66	0.77
1:B:58:ARG:HB3	1:B:61:LYS:NZ	2.00	0.76
1:B:69:ILE:HG12	1:B:79:VAL:HG12	1.67	0.76
1:B:110:ARG:HD3	1:B:110:ARG:C	2.07	0.74
1:B:108:GLU:OE1	1:B:110:ARG:HG3	1.86	0.74
1:D:172:MET:CE	1:D:321:LEU:HD21	2.17	0.73
1:C:122:LYS:NZ	1:C:123:GLU:HB2	2.04	0.72
1:D:341:VAL:HG22	5:D:4145:HOH:O	1.89	0.72
1:C:220:ALA:HB3	1:C:229:ILE:CG2	2.21	0.71
1:B:286:LYS:HE3	1:B:333:GLU:CD	2.11	0.70
1:B:58:ARG:HB3	1:B:61:LYS:HZ1	1.57	0.69
1:C:162:GLN:HE22	1:C:165:SER:HB3	1.57	0.69
1:A:114:LEU:HD23	1:A:116:GLU:H	1.58	0.69
1:B:8:MET:HG2	1:B:376:VAL:CG2	2.23	0.69
1:D:325:GLN:HE22	3:D:386:NAG:H82	1.58	0.69
1:A:325:GLN:HE22	2:A:386:NAG:HN2	1.39	0.69
1:D:43:LEU:HD13	1:D:120:CYS:SG	2.34	0.68
1:A:122:LYS:HD3	1:A:122:LYS:O	1.93	0.68
1:D:178:ILE:HD11	1:D:330:ALA:HB1	1.74	0.67
1:C:1:GLY:HA3	1:C:61:LYS:HD3	1.76	0.67
1:A:254:GLN:HE21	1:A:254:GLN:C	1.98	0.67
1:C:91:THR:O	1:D:93:PRO:HG2	1.94	0.67
1:C:99:PHE:CE1	1:C:178:ILE:HD11	2.30	0.67
1:D:178:ILE:HD13	1:D:378:PHE:CE1	2.28	0.67
1:D:162:GLN:CD	1:D:162:GLN:H	1.97	0.66
1:D:178:ILE:HD11	1:D:330:ALA:CB	2.25	0.66
1:B:1:GLY:N	1:B:61:LYS:HD2	2.11	0.66
1:A:163:PRO:HD3	1:C:75:THR:HG21	1.79	0.65
1:B:199:ARG:HH21	1:B:204:GLU:C	2.00	0.64
1:B:72:GLN:O	1:B:79:VAL:HG11	1.98	0.64
1:C:214:ILE:C	1:C:214:ILE:HD13	2.18	0.64
1:D:142:ARG:HG3	1:D:166:VAL:HG22	1.80	0.63
1:D:66:GLY:O	1:D:69:ILE:HG22	1.98	0.63
1:D:172:MET:HE1	1:D:321:LEU:HD21	1.79	0.63
1:D:178:ILE:O	1:D:178:ILE:HD12	1.98	0.63
1:D:74:GLY:HA3	5:D:2082:HOH:O	1.98	0.63
1:A:117:TYR:O	1:A:120:CYS:HB3	1.98	0.63
1:C:122:LYS:HD3	1:C:123:GLU:N	2.14	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:264:LEU:C	1:C:264:LEU:HD13	2.18	0.62
1:B:116:GLU:CD	1:B:116:GLU:H	2.03	0.62
1:A:142:ARG:NH1	1:A:163:PRO:HD3	2.15	0.62
1:D:321:LEU:HD23	1:D:322:LYS:N	2.15	0.62
1:B:12:PHE:O	1:B:16:LYS:HD3	1.99	0.62
1:C:99:PHE:CZ	1:C:178:ILE:CD1	2.77	0.62
1:B:168:SER:OG	1:B:169:GLN:NE2	2.33	0.61
1:B:163:PRO:HG2	1:D:119:GLN:HG3	1.82	0.61
2:C:387:NAG:H3	2:C:387:NAG:O7	2.00	0.61
1:A:109:GLU:OE2	1:A:133:ASN:HB2	2.01	0.61
1:A:214:ILE:HG21	1:A:350:ASP:HB3	1.83	0.61
1:B:48:SER:O	1:B:52:GLN:HG3	2.00	0.60
1:B:58:ARG:CB	1:B:61:LYS:HZ1	2.13	0.60
1:C:214:ILE:HD13	1:C:215:GLY:N	2.16	0.60
1:A:129:LEU:HD13	1:A:129:LEU:C	2.22	0.60
1:D:79:VAL:HB	1:D:124:LEU:HD11	1.84	0.60
1:A:47:ASP:O	1:A:51:THR:HG23	2.02	0.59
1:C:162:GLN:NE2	1:C:165:SER:HB3	2.18	0.59
1:A:126:ARG:NH2	5:A:1212:HOH:O	2.35	0.59
1:A:198:PHE:O	1:A:205:SER:HB2	2.02	0.59
1:D:200:VAL:HG23	1:D:201:THR:HG23	1.85	0.59
1:C:57:VAL:O	1:C:57:VAL:HG12	2.03	0.59
1:B:64:GLY:HA2	1:B:69:ILE:HD13	1.84	0.59
1:B:58:ARG:HB2	5:B:2107:HOH:O	2.03	0.59
1:C:8:MET:HG2	1:C:376:VAL:CG2	2.33	0.58
1:C:244:LEU:HD12	1:C:244:LEU:N	2.18	0.58
1:C:199:ARG:H	1:C:199:ARG:HD3	1.68	0.58
3:D:386:NAG:H83	3:D:386:NAG:O3	2.03	0.57
1:A:230:LEU:HD21	1:A:232:LEU:HD21	1.85	0.57
1:B:199:ARG:HG2	1:B:249:VAL:CG2	2.30	0.57
1:B:110:ARG:HD2	1:B:111:TYR:CD1	2.38	0.57
1:C:220:ALA:HB2	1:C:273:MET:HG2	1.87	0.57
1:A:58:ARG:HB2	5:A:1238:HOH:O	2.04	0.57
1:B:218:ARG:HG2	1:B:275:GLU:HG2	1.86	0.57
1:D:316:SER:HB3	1:D:321:LEU:HD12	1.85	0.57
1:D:172:MET:HE3	5:D:4144:HOH:O	2.05	0.57
1:D:75:THR:O	1:D:77:VAL:N	2.39	0.56
1:B:1:GLY:H1	1:B:61:LYS:HD2	1.70	0.56
1:C:8:MET:HG2	1:C:376:VAL:HG23	1.88	0.56
1:D:101:LEU:HD13	1:D:178:ILE:CG2	2.36	0.56
1:A:114:LEU:CD2	1:A:116:GLU:HB3	2.36	0.56
1:B:381:ARG:HD3	1:B:383:VAL:HG13	1.88	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:110:ARG:HG2	1:B:135:GLN:OE1	2.07	0.55
1:D:219:VAL:HG22	1:D:220:ALA:N	2.21	0.55
1:C:271:ASN:N	1:C:271:ASN:HD22	2.04	0.55
1:D:132:ILE:HD11	1:D:141:ALA:HA	1.88	0.55
1:A:174:LEU:HG	5:A:1178:HOH:O	2.06	0.55
1:A:122:LYS:HD3	1:A:122:LYS:C	2.27	0.54
1:C:91:THR:O	1:D:93:PRO:CG	2.55	0.54
1:B:79:VAL:CG2	1:B:124:LEU:HD21	2.38	0.54
1:B:227:MET:HE3	1:B:229:ILE:HG13	1.89	0.54
1:A:341:VAL:HG22	1:A:342:VAL:N	2.21	0.54
1:D:155:GLY:O	1:D:158:ARG:NH2	2.36	0.54
1:A:137:ALA:HB1	1:A:140:GLN:HB3	1.90	0.54
1:B:54:ASN:OD1	1:B:60:ASP:HB3	2.07	0.54
1:C:229:ILE:HD11	1:C:242:LEU:HB3	1.90	0.53
1:A:114:LEU:HD23	1:A:116:GLU:N	2.24	0.53
1:A:13:ASP:OD2	1:A:58:ARG:NH2	2.37	0.53
1:C:311:ASN:C	1:C:311:ASN:HD22	2.11	0.53
1:A:214:ILE:HG12	1:A:279:LYS:HG2	1.90	0.53
1:A:108:GLU:OE1	1:A:135:GLN:HG3	2.07	0.53
1:A:114:LEU:HD21	1:A:116:GLU:HB3	1.89	0.53
1:D:150:GLU:HG3	1:D:155:GLY:HA2	1.89	0.53
1:B:79:VAL:HG23	1:B:124:LEU:CD2	2.38	0.53
1:A:218:ARG:HD3	5:A:1173:HOH:O	2.09	0.53
1:B:79:VAL:HG23	1:B:124:LEU:HD21	1.90	0.53
1:D:178:ILE:CD1	1:D:378:PHE:HE1	2.17	0.52
1:B:60:ASP:O	1:B:61:LYS:HB3	2.09	0.52
1:D:172:MET:HE2	1:D:321:LEU:HD21	1.89	0.52
1:A:77:VAL:O	1:A:77:VAL:HG12	2.10	0.52
1:C:162:GLN:H	1:C:162:GLN:NE2	2.07	0.52
1:A:8:MET:HG3	1:A:376:VAL:HG23	1.91	0.52
1:A:189:LYS:HE2	1:A:341:VAL:HG21	1.92	0.52
1:C:189:LYS:NZ	1:D:140:GLN:HG3	2.25	0.52
1:C:311:ASN:HD22	1:C:313:SER:H	1.58	0.51
1:C:119:GLN:O	1:C:122:LYS:HD3	2.10	0.51
1:A:108:GLU:HB3	1:A:111:TYR:HD1	1.75	0.51
1:B:255:LEU:O	1:B:258:ILE:HD13	2.10	0.51
1:C:199:ARG:NH2	1:C:361:ASP:OD2	2.44	0.51
1:D:335:ASN:C	1:D:335:ASN:HD22	2.13	0.51
1:D:36:SER:HA	1:D:83:LEU:HD21	1.91	0.51
1:A:138:ALA:HB1	1:A:166:VAL:HG12	1.93	0.51
1:C:260:ASN:OD1	1:C:262:GLU:HB2	2.10	0.51
1:A:84:ARG:NE	1:A:124:LEU:O	2.44	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:77:VAL:O	1:B:77:VAL:HG22	2.10	0.51
1:B:58:ARG:CG	1:B:61:LYS:HZ1	2.23	0.51
1:B:110:ARG:HD3	1:B:111:TYR:N	2.26	0.51
1:A:73:CYS:SG	1:A:124:LEU:HD12	2.51	0.50
1:A:373:THR:O	1:A:374:ASN:HB2	2.10	0.50
1:A:199:ARG:N	1:A:199:ARG:HD2	2.26	0.50
1:A:77:VAL:HG23	5:A:1239:HOH:O	2.11	0.50
1:C:68:SEP:O	1:C:72:GLN:HG3	2.11	0.50
1:A:88:ASN:HB3	5:A:1250:HOH:O	2.10	0.50
1:D:162:GLN:NE2	1:D:162:GLN:N	2.53	0.50
1:C:122:LYS:HZ2	1:C:123:GLU:HB2	1.74	0.50
1:B:114:LEU:HB3	1:B:116:GLU:OE1	2.12	0.50
1:B:16:LYS:N	1:B:16:LYS:HD2	2.26	0.50
1:C:61:LYS:HG2	1:C:61:LYS:O	2.11	0.50
1:B:57:VAL:O	1:B:58:ARG:HB2	2.12	0.49
1:B:65:PHE:CE1	1:B:80:HIS:HA	2.47	0.49
1:C:229:ILE:HD12	1:C:243:VAL:O	2.13	0.49
1:C:122:LYS:HZ3	1:C:123:GLU:HB2	1.77	0.49
1:B:58:ARG:HG3	1:B:61:LYS:HZ1	1.77	0.49
1:A:108:GLU:OE2	1:A:110:ARG:N	2.37	0.49
1:B:381:ARG:HD3	1:B:383:VAL:CG1	2.43	0.49
1:D:187:ALA:HB2	1:D:338:GLY:CA	2.43	0.49
1:C:189:LYS:NZ	1:D:140:GLN:CG	2.76	0.48
1:D:83:LEU:O	1:D:87:LEU:HD23	2.12	0.48
1:D:187:ALA:HB2	1:D:338:GLY:HA3	1.94	0.48
1:A:214:ILE:HG21	1:A:350:ASP:CB	2.43	0.48
1:C:12:PHE:O	1:C:16:LYS:HG2	2.14	0.48
1:B:187:ALA:HB2	1:B:338:GLY:HA3	1.95	0.48
1:D:16:LYS:HE3	5:D:4106:HOH:O	2.12	0.48
1:A:187:ALA:HB2	1:A:338:GLY:HA3	1.96	0.48
1:D:225:GLU:HB2	1:D:227:MET:HG2	1.95	0.48
1:D:312:LEU:CD1	1:D:321:LEU:HD22	2.38	0.48
1:B:70:GLU:C	1:B:72:GLN:H	2.16	0.48
1:A:73:CYS:SG	1:A:124:LEU:CD1	3.02	0.47
1:C:181:LYS:HE2	1:D:151:SER:OG	2.14	0.47
1:A:54:ASN:HD21	1:A:60:ASP:N	2.12	0.47
1:A:129:LEU:HD22	1:A:130:GLU:N	2.30	0.47
1:D:101:LEU:HD13	1:D:178:ILE:HG22	1.97	0.47
1:C:119:GLN:O	1:C:122:LYS:CD	2.63	0.47
1:B:187:ALA:HB2	1:B:338:GLY:CA	2.45	0.47
1:B:23:ALA:O	1:B:25:GLU:HG3	2.14	0.47
1:A:106:TYR:O	1:A:172:MET:HG3	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:75:THR:OG1	1:C:76:SER:N	2.46	0.47
1:D:252:LEU:O	1:D:256:GLU:HG3	2.14	0.47
1:D:199:ARG:O	1:D:363:PRO:HD3	2.15	0.47
1:A:218:ARG:HH21	1:A:273:MET:CB	2.21	0.47
1:A:129:LEU:HD22	1:A:130:GLU:H	1.80	0.47
1:A:187:ALA:HB2	1:A:338:GLY:CA	2.44	0.47
1:C:230:LEU:HD21	1:C:232:LEU:HD21	1.97	0.47
1:D:142:ARG:HG3	1:D:166:VAL:CG2	2.45	0.47
1:B:78:ASN:O	1:B:81:SER:HB3	2.15	0.47
1:B:83:LEU:O	1:B:87:LEU:HD23	2.15	0.47
1:B:162:GLN:HB3	1:D:75:THR:CG2	2.46	0.46
1:B:66:GLY:O	1:B:68:SEP:N	2.49	0.46
1:D:69:ILE:O	1:D:72:GLN:HB2	2.16	0.46
1:A:341:VAL:HG12	5:A:1226:HOH:O	2.16	0.46
1:D:320:DSN:HA	5:D:4167:HOH:O	2.14	0.46
1:C:334:ILE:HD12	1:C:334:ILE:N	2.31	0.46
1:D:325:GLN:NE2	3:D:386:NAG:H82	2.28	0.46
1:B:244:LEU:HD12	1:B:244:LEU:N	2.31	0.46
1:A:36:SER:HB2	1:A:87:LEU:HD11	1.98	0.46
1:D:47:ASP:HB3	5:D:4132:HOH:O	2.14	0.45
1:A:95:ASP:HB3	5:A:1150:HOH:O	2.15	0.45
1:C:1:GLY:CA	1:C:61:LYS:HD3	2.44	0.45
1:B:294:THR:O	1:B:298:MET:HG3	2.17	0.45
1:C:278:ILE:CG2	1:C:356:GLU:HG2	2.42	0.45
1:C:69:ILE:HD12	5:C:3166:HOH:O	2.16	0.45
1:A:108:GLU:HB3	1:A:111:TYR:CD1	2.51	0.45
1:D:157:ILE:CD1	1:D:177:ALA:HB1	2.47	0.45
1:A:154:ASN:ND2	1:B:154:ASN:ND2	2.65	0.45
1:C:187:ALA:HB2	1:C:338:GLY:HA3	1.99	0.45
1:C:93:PRO:HG3	1:D:91:THR:O	2.17	0.45
1:B:60:ASP:O	1:B:61:LYS:CB	2.65	0.44
1:D:219:VAL:CG2	1:D:220:ALA:N	2.81	0.44
1:A:114:LEU:HA	1:A:115:PRO:HD2	1.88	0.44
1:B:162:GLN:HB3	1:D:75:THR:HG23	1.98	0.44
1:D:137:ALA:HB1	1:D:140:GLN:HB3	1.99	0.44
1:B:58:ARG:CB	1:B:61:LYS:NZ	2.73	0.44
1:A:341:VAL:HG22	1:A:342:VAL:O	2.16	0.44
1:B:112:PRO:HG3	5:B:2148:HOH:O	2.17	0.44
1:A:281:TYR:HB2	1:A:359:ARG:HA	1.99	0.44
1:A:276:ARG:HE	1:A:356:GLU:CD	2.21	0.44
1:A:199:ARG:CD	1:A:199:ARG:N	2.80	0.44
1:C:68:SEP:C	1:C:71:ALA:H	2.31	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:96:VAL:HG23	1:C:97:TYR:CD2	2.53	0.44
1:C:162:GLN:CA	1:C:162:GLN:HE21	2.31	0.44
1:A:142:ARG:HH11	1:A:163:PRO:HD3	1.82	0.44
1:B:220:ALA:HB1	1:B:272:VAL:HG12	2.00	0.44
1:B:58:ARG:HB3	1:B:61:LYS:HZ3	1.80	0.44
1:A:286:LYS:HG3	1:A:333:GLU:HG2	1.99	0.44
1:C:373:THR:O	1:C:374:ASN:HB2	2.17	0.44
1:B:252:LEU:HD22	1:B:363:PRO:HB3	1.99	0.44
1:D:162:GLN:CD	1:D:162:GLN:N	2.69	0.43
1:D:288:GLU:HA	1:D:330:ALA:O	2.18	0.43
1:A:8:MET:SD	1:A:261:PHE:HD1	2.41	0.43
1:B:73:CYS:C	1:B:75:THR:H	2.22	0.43
1:C:89:GLN:NE2	1:C:370:HIS:NE2	2.65	0.43
1:B:9:GLU:OE2	1:B:58:ARG:NH2	2.51	0.43
1:A:137:ALA:O	1:A:140:GLN:HB3	2.18	0.43
1:C:381:ARG:HD3	1:C:383:VAL:CG1	2.48	0.43
1:D:46:LYS:HD2	1:D:313:SER:OG	2.19	0.43
1:B:15:PHE:O	1:B:19:LYS:HG3	2.17	0.43
1:B:222:MET:HE3	1:B:222:MET:H	1.83	0.43
1:C:189:LYS:HZ3	1:D:140:GLN:HG3	1.83	0.43
1:B:75:THR:O	1:B:76:SER:HB2	2.18	0.43
1:A:296:VAL:O	1:A:300:MET:HG3	2.18	0.43
1:A:61:LYS:HG2	1:A:61:LYS:O	2.18	0.43
1:C:228:LYS:HE3	1:C:358:PHE:HD2	1.83	0.43
1:D:78:ASN:CG	1:D:78:ASN:O	2.56	0.43
1:A:42:TYR:OH	1:A:50:ARG:NH1	2.51	0.43
1:D:73:CYS:SG	1:D:124:LEU:CD1	3.06	0.43
1:C:162:GLN:H	1:C:162:GLN:CD	2.21	0.43
1:A:189:LYS:CE	1:A:341:VAL:HG21	2.49	0.43
1:C:214:ILE:HD11	1:C:277:LYS:CG	2.49	0.43
1:B:298:MET:HA	1:B:302:ILE:O	2.19	0.43
1:C:143:GLU:HG3	1:D:190:ASP:OD2	2.19	0.43
1:B:57:VAL:HG12	1:B:57:VAL:O	2.19	0.42
1:C:183:LEU:HD12	1:C:338:GLY:CA	2.49	0.42
1:A:69:ILE:HG23	1:A:70:GLU:N	2.34	0.42
1:B:96:VAL:HG23	1:B:97:TYR:CD2	2.54	0.42
1:C:93:PRO:HD3	1:D:93:PRO:HD3	2.00	0.42
1:D:244:LEU:HD22	1:D:259:ILE:HD12	2.02	0.42
1:B:335:ASN:HD22	1:B:335:ASN:C	2.21	0.42
1:A:36:SER:HB2	1:A:87:LEU:CD1	2.50	0.42
1:C:40:MET:SD	1:C:128:GLY:HA3	2.60	0.42
1:B:43:LEU:HD21	1:B:80:HIS:CE1	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:136:THR:HG23	5:A:1214:HOH:O	2.20	0.42
1:D:178:ILE:HD12	1:D:178:ILE:C	2.39	0.42
1:B:79:VAL:HG21	1:B:124:LEU:HD11	2.01	0.42
1:D:9:GLU:OE2	1:D:58:ARG:HD2	2.19	0.42
1:C:77:VAL:HG23	1:C:79:VAL:HG23	2.01	0.42
1:D:202:GLU:OE2	1:D:249:VAL:HG23	2.19	0.42
1:B:69:ILE:HG23	1:B:70:GLU:N	2.34	0.42
1:C:162:GLN:OE1	2:C:386:NAG:H81	2.20	0.42
1:B:105:LEU:HD22	1:B:172:MET:HG2	2.02	0.42
1:C:115:PRO:O	1:C:119:GLN:HG3	2.20	0.41
1:C:242:LEU:HD13	1:C:268:THR:HG21	2.02	0.41
1:D:156:ILE:HD12	1:D:179:VAL:HG11	2.02	0.41
1:C:84:ARG:HD2	1:C:124:LEU:HB3	2.01	0.41
1:B:108:GLU:HG2	1:B:134:PHE:HB2	2.02	0.41
1:C:75:THR:O	1:C:76:SER:HB2	2.20	0.41
1:A:159:ASN:HD21	1:C:76:SER:HB3	1.85	0.41
1:B:252:LEU:HD22	1:B:363:PRO:CB	2.51	0.41
1:C:294:THR:O	1:C:298:MET:HG3	2.21	0.41
1:C:36:SER:HA	1:C:83:LEU:HD21	2.01	0.41
1:B:70:GLU:C	1:B:72:GLN:N	2.73	0.41
1:A:199:ARG:CD	1:A:199:ARG:H	2.32	0.41
1:C:108:GLU:OE1	1:C:134:PHE:N	2.51	0.41
1:A:341:VAL:CG2	1:A:342:VAL:N	2.83	0.41
1:B:242:LEU:HD11	1:B:369:LYS:HE2	2.03	0.41
1:C:110:ARG:NH1	1:C:135:GLN:NE2	2.68	0.41
1:D:321:LEU:HD23	1:D:321:LEU:C	2.40	0.41
1:A:75:THR:OG1	1:A:76:SER:N	2.53	0.41
1:D:41:VAL:HG22	1:D:105:LEU:HD11	2.02	0.41
1:A:181:LYS:HE3	5:A:2157:HOH:O	2.19	0.41
1:C:93:PRO:CG	1:D:91:THR:O	2.69	0.41
1:A:342:VAL:HG12	1:A:346:GLU:HB2	2.02	0.41
1:C:69:ILE:HA	1:C:72:GLN:NE2	2.35	0.41
1:A:206:LYS:HZ1	1:A:384:SER:CB	2.33	0.41
1:C:311:ASN:ND2	1:C:313:SER:H	2.18	0.41
1:B:32:ILE:HG13	1:B:87:LEU:HD21	2.02	0.41
1:D:60:ASP:HB2	1:D:61:LYS:H	1.54	0.41
1:A:204:GLU:HG2	1:A:205:SER:N	2.35	0.41
1:A:76:SER:C	1:A:78:ASN:H	2.25	0.41
1:D:19:LYS:HB3	1:D:19:LYS:HE2	1.94	0.41
1:C:73:CYS:SG	1:C:124:LEU:HD11	2.60	0.41
1:C:245:LEU:HA	1:C:246:PRO:HD3	1.91	0.41
1:B:181:LYS:HA	1:B:181:LYS:HD2	1.78	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:281:TYR:HB2	1:D:359:ARG:HA	2.02	0.40
1:C:200:VAL:HG12	1:C:201:THR:HG23	2.03	0.40
1:B:233:PRO:HG3	5:B:2094:HOH:O	2.21	0.40
1:B:160:VAL:HG22	1:B:327:VAL:HG21	2.03	0.40
1:C:50:ARG:HH22	1:C:70:GLU:CD	2.22	0.40
1:A:157:ILE:HD13	1:A:177:ALA:HB1	2.03	0.40
1:C:54:ASN:HD22	1:C:59:PHE:HB2	1.87	0.40
1:C:199:ARG:CD	1:C:199:ARG:N	2.78	0.40
1:B:8:MET:SD	1:B:264:LEU:HD23	2.62	0.40
1:D:79:VAL:HB	1:D:124:LEU:CD1	2.51	0.40
1:B:258:ILE:HD13	1:B:258:ILE:H	1.86	0.40
1:D:37:ALA:HB1	1:D:174:LEU:HD11	2.02	0.40
1:D:122:LYS:HE2	1:D:126:ARG:NH1	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	374/385 (97%)	361 (96%)	9 (2%)	4 (1%)	21	7
1	B	378/385 (98%)	363 (96%)	11 (3%)	4 (1%)	21	7
1	C	366/385 (95%)	347 (95%)	16 (4%)	3 (1%)	27	12
1	D	378/385 (98%)	368 (97%)	8 (2%)	2 (0%)	38	23
All	All	1496/1540 (97%)	1439 (96%)	44 (3%)	13 (1%)	25	10

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ASP
1	A	67	ASP
1	B	61	LYS
1	C	60	ASP
1	C	67	ASP

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Mol	Chain	Res	Type
1	C	76	SER
1	D	60	ASP
1	D	76	SER
1	B	60	ASP
1	A	76	SER
1	B	67	ASP
1	B	76	SER
1	A	77	VAL

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	324/326 (99%)	316 (98%)	8 (2%)	60	50
1	B	326/326 (100%)	317 (97%)	9 (3%)	56	45
1	C	322/326 (99%)	309 (96%)	13 (4%)	42	29
1	D	326/326 (100%)	318 (98%)	8 (2%)	60	50
All	All	1298/1304 (100%)	1260 (97%)	38 (3%)	55	44

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ASP
1	A	75	THR
1	A	135	GLN
1	A	162	GLN
1	A	199	ARG
1	A	201	THR
1	A	254	GLN
1	A	325	GLN
1	B	16	LYS
1	B	58	ARG
1	B	110	ARG
1	B	116	GLU
1	B	118	LEU
1	B	222	MET

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Mol	Chain	Res	Type
1	B	253	GLU
1	B	258	ILE
1	B	335	ASN
1	C	8	MET
1	C	25	GLU
1	C	108	GLU
1	C	122	LYS
1	C	139	ASP
1	C	162	GLN
1	C	199	ARG
1	C	214	ILE
1	C	227	MET
1	C	253	GLU
1	C	271	ASN
1	C	274	GLU
1	C	311	ASN
1	D	58	ARG
1	D	60	ASP
1	D	119	GLN
1	D	140	GLN
1	D	162	GLN
1	D	203	GLN
1	D	216	LEU
1	D	335	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	89	GLN
1	A	119	GLN
1	A	135	GLN
1	A	154	ASN
1	A	159	ASN
1	A	162	GLN
1	A	213	GLN
1	A	254	GLN
1	A	325	GLN
1	B	89	GLN
1	B	152	GLN
1	B	154	ASN
1	B	169	GLN

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Mol	Chain	Res	Type
1	B	203	GLN
1	B	254	GLN
1	B	271	ASN
1	B	335	ASN
1	C	54	ASN
1	C	72	GLN
1	C	88	ASN
1	C	89	GLN
1	C	135	GLN
1	C	140	GLN
1	C	154	ASN
1	C	162	GLN
1	C	169	GLN
1	C	194	GLN
1	C	203	GLN
1	C	213	GLN
1	C	254	GLN
1	C	271	ASN
1	C	311	ASN
1	D	119	GLN
1	D	135	GLN
1	D	140	GLN
1	D	152	GLN
1	D	162	GLN
1	D	194	GLN
1	D	203	GLN
1	D	271	ASN
1	D	335	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

19 non-standard protein/DNA/RNA residues 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$
1	DSN	A	164	1	5,5,6	7.74	2 (40%)	3,5,7	2.24	1 (33%)
1	DSN	A	236	1	5,5,6	7.43	2 (40%)	3,5,7	0.71	0
1	DSN	A	320	1	5,5,6	8.03	2 (40%)	3,5,7	1.45	1 (33%)
1	SEP	A	344	1	9,9,10	6.15	2 (22%)	10,12,14	2.07	2 (20%)
1	SEP	A	68	1	9,9,10	5.96	2 (22%)	10,12,14	1.78	1 (10%)
1	DSN	B	164	1	5,5,6	8.16	2 (40%)	3,5,7	0.69	0
1	DSN	B	236	1	5,5,6	8.03	2 (40%)	3,5,7	0.81	0
1	DSN	B	320	1	5,5,6	7.28	2 (40%)	3,5,7	0.50	0
1	SEP	B	344	1	9,9,10	6.11	2 (22%)	10,12,14	1.92	1 (10%)
1	SEP	B	68	1	5,5,10	8.03	2 (40%)	3,5,14	4.48	2 (66%)
1	DSN	C	164	1	5,5,6	7.96	2 (40%)	3,5,7	1.24	1 (33%)
1	DSN	C	236	1	5,5,6	7.64	2 (40%)	3,5,7	1.40	1 (33%)
1	DSN	C	320	1	5,5,6	7.91	2 (40%)	3,5,7	0.34	0
1	SEP	C	68	1	5,5,10	7.95	2 (40%)	3,5,14	2.70	1 (33%)
1	DSN	D	164	1	5,5,6	7.84	2 (40%)	3,5,7	1.51	1 (33%)
1	DSN	D	236	1	5,5,6	8.07	2 (40%)	3,5,7	0.34	0
1	DSN	D	320	1	5,5,6	7.36	2 (40%)	3,5,7	0.43	0
1	SEP	D	344	1	9,9,10	6.11	2 (22%)	10,12,14	2.36	3 (30%)
1	SEP	D	68	1	9,9,10	6.05	2 (22%)	10,12,14	2.55	2 (20%)

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
1	DSN	A	164	1	-	0/2/4/6	0/0/0/0
1	DSN	A	236	1	-	0/2/4/6	0/0/0/0
1	DSN	A	320	1	-	0/2/4/6	0/0/0/0
1	SEP	A	344	1	-	0/6/8/10	0/0/0/0
1	SEP	A	68	1	-	0/6/8/10	0/0/0/0
1	DSN	B	164	1	-	0/2/4/6	0/0/0/0
1	DSN	B	236	1	-	0/2/4/6	0/0/0/0
1	DSN	B	320	1	-	0/2/4/6	0/0/0/0
1	SEP	B	344	1	-	0/6/8/10	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	B	68	1	-	0/2/4/10	0/0/0/0
1	DSN	C	164	1	-	0/2/4/6	0/0/0/0
1	DSN	C	236	1	-	0/2/4/6	0/0/0/0
1	DSN	C	320	1	-	0/2/4/6	0/0/0/0
1	SEP	C	68	1	-	0/2/4/10	0/0/0/0
1	DSN	D	164	1	1/1/1/2	0/2/4/6	0/0/0/0
1	DSN	D	236	1	-	0/2/4/6	0/0/0/0
1	DSN	D	320	1	-	0/2/4/6	0/0/0/0
1	SEP	D	344	1	-	0/6/8/10	0/0/0/0
1	SEP	D	68	1	-	0/6/8/10	0/0/0/0

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	344	SEP	O-C	18.01	1.23	1.11
1	B	164	DSN	O-C	18.00	1.23	1.11
1	D	344	SEP	O-C	17.90	1.23	1.11
1	B	344	SEP	O-C	17.87	1.23	1.11
1	D	68	SEP	O-C	17.84	1.23	1.11
1	B	68	SEP	O-C	17.78	1.23	1.11
1	D	236	DSN	O-C	17.77	1.23	1.11
1	A	320	DSN	O-C	17.76	1.23	1.11
1	B	236	DSN	O-C	17.74	1.23	1.11
1	C	68	SEP	O-C	17.61	1.23	1.11
1	C	164	DSN	O-C	17.56	1.23	1.11
1	A	68	SEP	O-C	17.55	1.23	1.11
1	D	164	DSN	O-C	17.34	1.23	1.11
1	C	320	DSN	O-C	17.27	1.23	1.11
1	A	164	DSN	O-C	17.10	1.23	1.11
1	C	236	DSN	O-C	16.85	1.23	1.11
1	A	236	DSN	O-C	16.46	1.22	1.11
1	D	320	DSN	O-C	16.24	1.22	1.11
1	B	320	DSN	O-C	16.02	1.22	1.11
1	C	320	DSN	CA-C	3.73	1.55	1.48
1	A	344	SEP	CA-C	3.59	1.55	1.48
1	B	344	SEP	CA-C	3.32	1.54	1.48
1	D	344	SEP	CA-C	3.23	1.54	1.48
1	D	236	DSN	CA-C	3.07	1.54	1.48
1	B	164	DSN	CA-C	2.94	1.53	1.48
1	B	320	DSN	CA-C	2.84	1.53	1.48
1	C	164	DSN	CA-C	2.81	1.53	1.48
1	C	236	DSN	CA-C	2.80	1.53	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	SEP	CA-C	2.70	1.53	1.48
1	B	236	DSN	CA-C	2.65	1.53	1.48
1	D	320	DSN	CA-C	2.61	1.53	1.48
1	A	320	DSN	CA-C	2.61	1.53	1.48
1	A	164	DSN	CA-C	2.59	1.53	1.48
1	D	164	DSN	CA-C	2.58	1.53	1.48
1	C	68	SEP	CA-C	2.41	1.52	1.48
1	B	68	SEP	CA-C	2.40	1.52	1.48
1	D	68	SEP	CA-C	2.33	1.52	1.48
1	A	236	DSN	CA-C	2.21	1.52	1.48

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	68	SEP	P-OG-CB	-6.63	99.00	118.19
1	B	68	SEP	C-CA-N	-6.30	107.54	113.83
1	D	344	SEP	P-OG-CB	-6.09	100.59	118.19
1	A	344	SEP	P-OG-CB	-5.49	102.32	118.19
1	B	344	SEP	P-OG-CB	-5.00	103.73	118.19
1	A	68	SEP	P-OG-CB	-4.81	104.28	118.19
1	C	68	SEP	OG-CB-CA	-4.55	111.62	113.63
1	B	68	SEP	OG-CB-CA	-4.53	111.62	113.63
1	A	164	DSN	C-CA-N	-3.87	109.97	113.83
1	D	68	SEP	C-CA-N	-3.36	110.47	113.83
1	D	344	SEP	OG-CB-CA	2.68	112.48	108.69
1	D	164	DSN	C-CA-N	2.49	116.31	113.83
1	A	320	DSN	C-CA-N	2.45	116.27	113.83
1	D	344	SEP	C-CA-N	2.32	116.15	113.83
1	A	344	SEP	C-CA-N	-2.28	111.55	113.83
1	C	236	DSN	C-CA-N	-2.21	111.62	113.83
1	C	164	DSN	C-CA-N	2.10	115.92	113.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	164	DSN	CA

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

6 carbohydrates 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	NAG	A	386	1,2	12,14,15	0.62	0	15,19,21	0.92	1 (6%)
2	NAG	A	387	2	12,14,15	0.53	0	15,19,21	0.70	0
2	NAG	B	386	1,2	12,14,15	0.73	0	15,19,21	0.81	0
2	NAG	B	387	2	12,14,15	0.50	0	15,19,21	0.91	1 (6%)
2	NAG	C	386	1,2	12,14,15	0.58	0	15,19,21	0.93	1 (6%)
2	NAG	C	387	2	12,14,15	0.62	0	15,19,21	0.94	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
2	NAG	A	386	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	387	2	-	0/6/23/26	0/1/1/1
2	NAG	B	386	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	387	2	-	0/6/23/26	0/1/1/1
2	NAG	C	386	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	387	2	-	0/6/23/26	1/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	387	NAG	C2-N2-C7	-2.88	118.25	123.09
2	A	386	NAG	C2-N2-C7	-2.76	118.45	123.09
2	C	386	NAG	C3-C2-N2	-2.64	107.73	111.76

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	387	NAG	C1-C2-C3-C4-C5-O5

5.6 Ligand geometry ⓘ

8 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	$\# Z > 2$
4	SO4	A	401	-	4,4,4	0.37	0	6,6,6	0.11	0
4	SO4	A	402	-	4,4,4	0.31	0	6,6,6	0.07	0
4	SO4	B	1401	-	4,4,4	0.28	0	6,6,6	0.09	0
4	SO4	B	1402	-	4,4,4	0.19	0	6,6,6	0.07	0
4	SO4	C	2401	-	4,4,4	0.37	0	6,6,6	0.08	0
4	SO4	D	3401	-	4,4,4	0.28	0	6,6,6	0.07	0
4	SO4	D	3402	-	4,4,4	0.31	0	6,6,6	0.07	0
3	NAG	D	386	1	12,14,15	0.74	0	15,19,21	0.81	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	SO4	A	401	-	-	0/0/0/0	0/0/0/0
4	SO4	A	402	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1401	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1402	-	-	0/0/0/0	0/0/0/0
4	SO4	C	2401	-	-	0/0/0/0	0/0/0/0
4	SO4	D	3401	-	-	0/0/0/0	0/0/0/0
4	SO4	D	3402	-	-	0/0/0/0	0/0/0/0
3	NAG	D	386	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	386	NAG	O7-C7-N2-C2
3	D	386	NAG	C8-C7-N2-C2

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	383/385 (99%)	0.43	27 (7%) 16 16	13, 28, 50, 62	0
1	B	385/385 (100%)	0.38	25 (6%) 18 18	14, 26, 50, 75	0
1	C	374/385 (97%)	0.40	20 (5%) 25 26	12, 25, 49, 67	0
1	D	385/385 (100%)	0.24	14 (3%) 41 42	14, 26, 43, 59	0
All	All	1527/1540 (99%)	0.36	86 (5%) 24 24	12, 26, 49, 75	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	75	THR	8.5
1	A	77	VAL	8.2
1	B	77	VAL	8.1
1	B	69	ILE	7.1
1	C	354	VAL	6.5
1	C	69	ILE	6.5
1	B	67	ASP	6.1
1	A	74	GLY	5.5
1	C	75	THR	5.5
1	B	76	SER	5.4
1	C	61	LYS	5.3
1	B	73	CYS	5.0
1	C	74	GLY	4.8
1	A	60	ASP	4.7
1	A	319	GLU	4.7
1	C	76	SER	4.5
1	C	67	ASP	4.4
1	C	60	ASP	4.4
1	B	60	ASP	4.3
1	C	77	VAL	4.2
1	A	75	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	271	ASN	4.0
1	D	202	GLU	4.0
1	A	76	SER	4.0
1	B	250	SER	3.9
1	C	355	SER	3.8
1	C	78	ASN	3.8
1	D	249	VAL	3.8
1	C	68	SEP	3.7
1	A	73	CYS	3.6
1	A	250	SER	3.4
1	D	66	GLY	3.4
1	C	73	CYS	3.4
1	D	75	THR	3.4
1	B	74	GLY	3.4
1	D	203	GLN	3.3
1	C	126	ARG	3.3
1	A	47	ASP	3.3
1	C	66	GLY	3.3
1	D	126	ARG	3.3
1	A	249	VAL	3.2
1	B	78	ASN	3.1
1	A	71	ALA	3.0
1	D	73	CYS	2.9
1	C	222	MET	2.9
1	B	61	LYS	2.9
1	D	61	LYS	2.9
1	A	308	SER	2.8
1	D	69	ILE	2.8
1	B	122	LYS	2.7
1	A	111	TYR	2.7
1	B	72	GLN	2.7
1	A	110	ARG	2.6
1	B	319	GLU	2.6
1	B	320	DSN	2.6
1	B	70	GLU	2.6
1	C	257	SER	2.6
1	A	320	DSN	2.5
1	B	110	ARG	2.5
1	B	119	GLN	2.5
1	C	319	GLU	2.5
1	D	74	GLY	2.4
1	D	60	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	202	GLU	2.4
1	A	126	ARG	2.3
1	C	202	GLU	2.3
1	A	123	GLU	2.2
1	A	204	GLU	2.2
1	A	200	VAL	2.2
1	A	317	SER	2.2
1	A	113	ILE	2.2
1	B	126	ARG	2.2
1	A	169	GLN	2.1
1	B	254	GLN	2.1
1	D	21	HIS	2.1
1	A	66	GLY	2.1
1	B	58	ARG	2.1
1	A	67	ASP	2.1
1	D	76	SER	2.1
1	B	66	GLY	2.1
1	A	316	SER	2.0
1	A	34	ILE	2.0
1	C	72	GLN	2.0
1	A	224	SER	2.0
1	B	47	ASP	2.0
1	D	122	LYS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	SEP	D	344	10/11	0.22	2.70	25,36,52,53	0
1	SEP	C	68	6/11	0.50	2.39	63,65,65,65	0
1	DSN	A	164	6/7	0.22	1.78	38,39,42,45	0
1	DSN	D	320	6/7	0.22	1.46	34,37,39,42	0
1	DSN	D	164	6/7	0.21	1.34	37,38,41,45	0
1	DSN	B	320	6/7	0.25	1.26	32,37,40,44	0
1	DSN	C	164	6/7	0.17	0.93	29,31,33,36	0
1	SEP	D	68	10/11	0.26	0.92	53,57,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	DSN	B	236	6/7	0.15	0.86	23,29,31,35	0
1	DSN	C	320	6/7	0.20	0.80	31,36,38,41	0
1	DSN	A	320	6/7	0.25	0.24	45,49,51,53	0
1	SEP	A	68	10/11	0.17	0.10	50,55,60,61	0
1	SEP	B	68	6/11	0.34	0.03	67,68,68,69	0
1	SEP	B	344	10/11	0.12	-0.05	23,30,46,48	0
1	SEP	A	344	10/11	0.12	-0.08	40,44,51,51	0
1	DSN	B	164	6/7	0.10	-0.19	27,30,32,37	0
1	DSN	D	236	6/7	0.11	-0.42	18,22,25,27	0
1	DSN	A	236	6/7	0.07	-0.50	19,20,22,27	0
1	DSN	C	236	6/7	0.07	-1.00	20,24,26,28	0

6.3 Carbohydrates i

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	A	387	14/15	0.46	18.65	58,61,64,64	0
2	NAG	C	387	14/15	0.29	10.24	40,44,49,49	0
2	NAG	A	386	14/15	0.17	1.41	38,42,47,53	0
2	NAG	B	387	14/15	0.23	0.90	41,46,47,51	0
2	NAG	B	386	14/15	0.10	-0.09	21,26,30,35	0
2	NAG	C	386	14/15	0.08	-0.78	19,21,24,31	0

6.4 Ligands i

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	SO4	B	1402	5/5	0.22	6.96	89,89,90,90	0
4	SO4	D	3401	5/5	0.19	3.26	78,78,79,79	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	SO4	B	1401	5/5	0.25	2.95	99,99,99,99	0
4	SO4	C	2401	5/5	0.19	2.07	52,52,53,53	0
4	SO4	D	3402	5/5	0.23	1.60	74,74,74,74	0
3	NAG	D	386	14/15	0.18	1.53	32,37,41,41	0
4	SO4	A	402	5/5	0.17	1.14	56,56,58,58	0
4	SO4	A	401	5/5	0.15	0.05	52,52,53,54	0

6.5 Other polymers ⓘ

There are no such residues in this entry.