



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 02:21 pm BST

PDB ID : 1OJW
Title : Decay accelerating factor (CD55): the structure of an intact human complement regulator.
Authors : Lukacik, P.; Roversi, P.; White, J.; Esser, D.; Smith, G.P.; Billington, J.; Williams, P.A.; Rudd, P.M.; Wormald, M.R.; Crispin, M.D.M.; Radcliffe, C.M.; Dwek, C.M.; Evans, D.J.; Morgan, B.P.; Smith, R.A.G.; Lea, S.M.
Deposited on : 2003-07-16
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) 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	:	2.11
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)	:	2.11

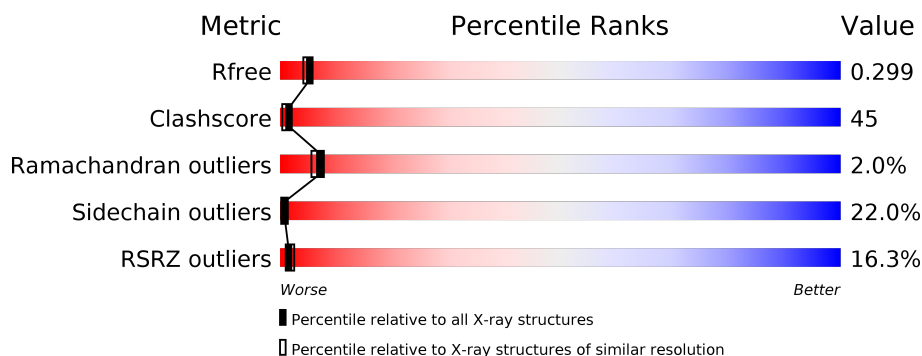
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	254	
1	B	254	

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	1256	-	X	X	X
3	GOL	A	1257	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3956 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.

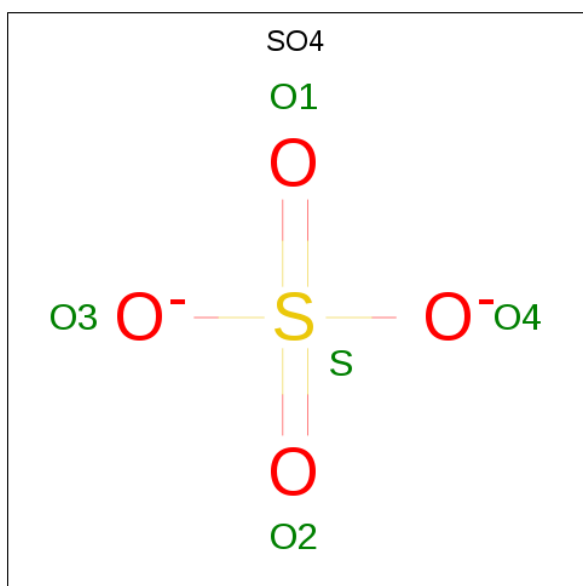
- Molecule 1 is a protein called COMPLEMENT DECAY-ACCELERATING FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			1955	1226	328	384	17			
1	B	251	Total	C	N	O	S	0	0	0
			1946	1221	326	382	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	ILE	THR	SEE REMARK 999	UNP P08174
B	48	ILE	THR	SEE REMARK 999	UNP P08174

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



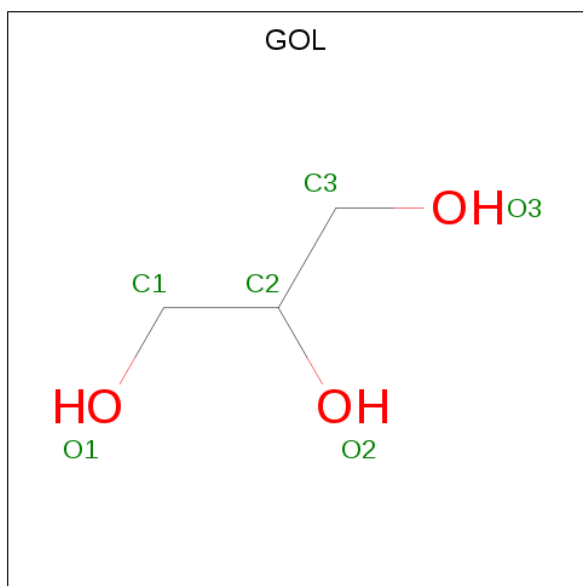
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

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

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



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

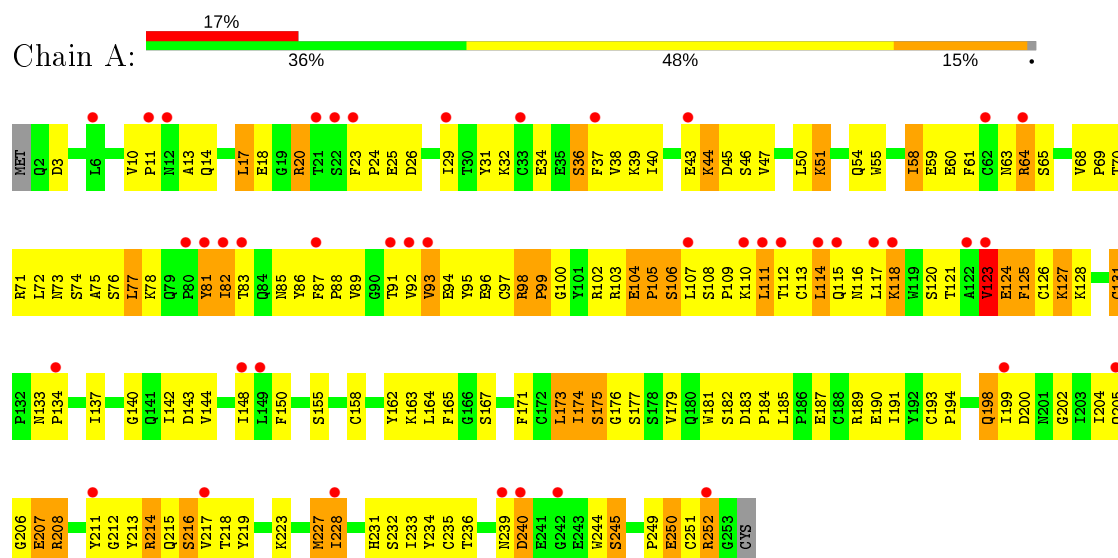
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	O	0	0
			9	9		
4	B	24	Total	O	0	0
			24	24		

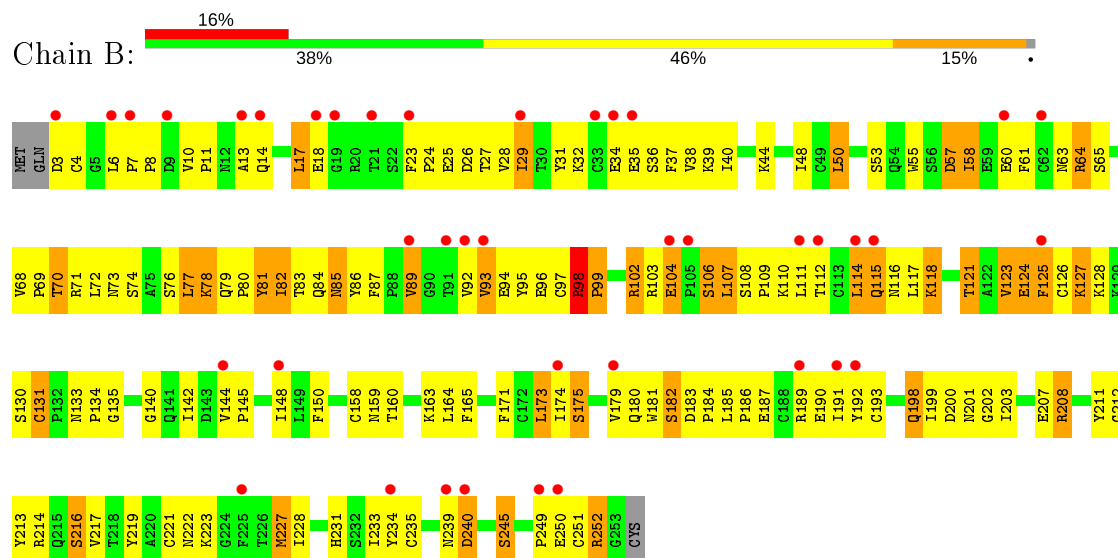
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: COMPLEMENT DECAY-ACCELERATING FACTOR



• Molecule 1: COMPLEMENT DECAY-ACCELERATING FACTOR



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.10Å 51.89Å 64.12Å 78.39° 83.66° 63.22°	Depositor
Resolution (Å)	28.00 – 2.30 24.33 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (28.00-2.30) 99.0 (24.33-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.80Å)	Xtriage
Refinement program	TNT 5F	Depositor
R, R_{free}	0.254 , (Not available) 0.268 , 0.299	Depositor DCC
R_{free} test set	739 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h-k,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	3956	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.52% 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	0.39	1/2008 (0.0%)	0.54	3/2731 (0.1%)
1	B	0.35	0/1999	0.54	2/2719 (0.1%)
All	All	0.37	1/4007 (0.0%)	0.54	5/5450 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	250	GLU	CD-OE2	-8.33	1.16	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	98	ARG	C-N-CD	-11.65	94.96	120.60
1	A	104	GLU	C-N-CD	-8.88	101.07	120.60
1	A	98	ARG	C-N-CD	-8.14	102.69	120.60
1	B	104	GLU	C-N-CD	-7.22	104.71	120.60
1	A	144	VAL	C-N-CD	-5.39	108.73	120.60

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	1955	0	1850	177	0
1	B	1946	0	1842	173	1
2	A	10	0	0	2	0
3	A	12	0	8	6	0
4	A	9	0	0	2	0
4	B	24	0	0	4	0
All	All	3956	0	3700	346	1

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 45.

All (346) 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:252:ARG:HB2	1:A:252:ARG:NH1	1.29	1.38
1:B:252:ARG:HH21	1:B:252:ARG:HB3	0.94	1.10
1:A:250:GLU:OE2	1:A:252:ARG:NH2	1.85	1.08
1:B:252:ARG:HB3	1:B:252:ARG:NH2	1.72	1.03
1:A:252:ARG:HB2	1:A:252:ARG:CZ	1.86	1.02
1:A:252:ARG:CB	1:A:252:ARG:NH1	2.25	0.99
1:A:165:PHE:HD2	1:A:189:ARG:HG3	1.24	0.98
1:A:165:PHE:CD2	1:A:189:ARG:HG3	1.98	0.97
1:B:165:PHE:HD2	1:B:189:ARG:HG3	1.29	0.95
1:A:250:GLU:OE2	1:A:252:ARG:CZ	2.15	0.94
1:A:252:ARG:HB2	1:A:252:ARG:HH11	1.13	0.91
1:A:217:VAL:HG12	1:A:233:ILE:HG12	1.53	0.91
1:A:163:LYS:HG3	1:A:240:ASP:HB3	1.51	0.90
1:B:191:ILE:CD1	1:B:240:ASP:HA	2.03	0.88
1:B:163:LYS:HG3	1:B:240:ASP:HB3	1.54	0.87
1:B:252:ARG:HH21	1:B:252:ARG:CB	1.83	0.87
1:B:191:ILE:HD13	1:B:240:ASP:HA	1.56	0.87
1:A:191:ILE:HD13	1:A:240:ASP:HA	1.56	0.85
1:A:77:LEU:HB2	1:A:82:ILE:HD12	1.57	0.85
1:A:77:LEU:CB	1:A:82:ILE:HD12	2.06	0.84
1:B:78:LYS:HD3	1:B:96:GLU:HB3	1.57	0.83
1:B:28:VAL:CG2	1:B:48:ILE:HD12	2.08	0.83
1:B:165:PHE:CD2	1:B:189:ARG:HG3	2.13	0.83
1:A:110:LYS:O	1:A:111:LEU:HD23	1.77	0.82
1:B:227:MET:HE2	1:B:249:PRO:HB2	1.62	0.82
1:A:199:ILE:HD11	1:A:202:GLY:HA3	1.62	0.80
1:B:77:LEU:CB	1:B:82:ILE:HD12	2.11	0.80
1:A:252:ARG:CB	1:A:252:ARG:HH11	1.90	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:VAL:HG11	1:B:115:GLN:HA	1.64	0.78
1:A:250:GLU:OE2	1:A:252:ARG:NH1	2.17	0.76
1:A:55:TRP:H	3:A:1256:GOL:H12	1.50	0.76
1:B:148:ILE:HG22	1:B:181:TRP:CZ2	2.21	0.76
1:A:150:PHE:HB2	1:A:179:VAL:HG11	1.68	0.76
1:A:69:PRO:HG2	1:A:77:LEU:HD21	1.67	0.75
1:A:78:LYS:HD3	1:A:96:GLU:HB3	1.69	0.75
1:A:217:VAL:CG1	1:A:233:ILE:HG12	2.18	0.74
1:B:106:SER:C	1:B:107:LEU:HD23	2.07	0.74
1:A:73:ASN:O	1:A:98:ARG:HD2	1.88	0.73
1:B:217:VAL:CG1	1:B:233:ILE:HG12	2.18	0.73
1:A:106:SER:C	1:A:107:LEU:HD23	2.08	0.73
1:B:217:VAL:HG12	1:B:233:ILE:HG12	1.70	0.73
1:B:171:PHE:HB3	1:B:173:LEU:HD13	1.69	0.72
1:A:208:ARG:HG2	1:A:208:ARG:HH11	1.55	0.72
1:B:123:VAL:HG23	1:B:125:PHE:HD2	1.54	0.72
1:A:208:ARG:HB2	1:A:211:TYR:CZ	2.24	0.72
1:A:228:ILE:HG23	1:B:145:PRO:O	1.90	0.72
1:A:191:ILE:CD1	1:A:240:ASP:HA	2.20	0.71
1:A:89:VAL:HG13	1:A:113:CYS:O	1.90	0.71
1:A:207:GLU:HG2	1:A:208:ARG:H	1.56	0.71
1:B:131:CYS:HB2	1:B:148:ILE:O	1.90	0.71
1:B:28:VAL:HG22	1:B:48:ILE:HD12	1.71	0.70
1:B:10:VAL:HG23	1:B:31:TYR:CE1	2.27	0.70
1:A:171:PHE:HB3	1:A:173:LEU:HD13	1.73	0.70
1:B:77:LEU:HB2	1:B:82:ILE:HD12	1.73	0.69
1:A:231:HIS:ND1	4:A:2008:HOH:O	2.25	0.69
1:B:23:PHE:HB3	1:B:27:THR:HG21	1.74	0.69
1:A:45:ASP:HB3	1:A:61:PHE:CD2	2.28	0.68
1:A:217:VAL:HG12	1:A:233:ILE:CG1	2.24	0.68
1:A:25:GLU:O	1:A:26:ASP:HB2	1.90	0.68
1:A:85:ASN:ND2	4:A:2005:HOH:O	2.25	0.68
1:B:110:LYS:O	1:B:111:LEU:HD23	1.93	0.68
1:A:34:GLU:O	1:A:37:PHE:HB2	1.94	0.68
1:B:227:MET:CE	1:B:249:PRO:HB2	2.23	0.68
1:A:174:ILE:HD13	1:A:174:ILE:O	1.94	0.67
1:A:125:PHE:H	1:A:125:PHE:HD2	1.42	0.67
1:B:71:ARG:C	1:B:72:LEU:HD23	2.14	0.67
1:B:73:ASN:O	1:B:98:ARG:HD2	1.94	0.67
1:A:175:SER:OG	1:A:176:GLY:N	2.25	0.67
1:B:3:ASP:OD2	1:B:24:PRO:HA	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ASN:OD1	1:A:118:LYS:HG3	1.94	0.67
1:B:163:LYS:CG	1:B:240:ASP:HB3	2.23	0.67
1:B:103:ARG:NH2	1:B:107:LEU:O	2.28	0.66
1:A:109:PRO:HA	1:A:125:PHE:CD1	2.30	0.66
1:A:199:ILE:CD1	1:A:202:GLY:HA3	2.24	0.66
1:A:208:ARG:HG2	1:A:208:ARG:NH1	2.08	0.66
1:A:163:LYS:HG3	1:A:240:ASP:CB	2.24	0.66
1:A:36:SER:HB3	1:A:117:LEU:CD1	2.26	0.66
1:B:198:GLN:HA	1:B:198:GLN:NE2	2.09	0.66
1:A:252:ARG:CB	1:A:252:ARG:CZ	2.68	0.66
1:B:199:ILE:CD1	1:B:202:GLY:HA3	2.26	0.65
1:A:131:CYS:HB2	1:A:148:ILE:O	1.96	0.65
1:B:133:ASN:OD1	1:B:134:PRO:HD2	1.96	0.65
1:B:198:GLN:NE2	4:B:2021:HOH:O	2.23	0.65
1:B:234:TYR:H	1:B:245:SER:HB3	1.62	0.65
1:B:40:ILE:HD11	1:B:63:ASN:HB2	1.78	0.65
1:B:175:SER:HB3	1:B:180:GLN:HB2	1.78	0.65
1:B:68:VAL:HG12	1:B:69:PRO:HD2	1.80	0.64
1:B:69:PRO:HG2	1:B:77:LEU:HD21	1.79	0.64
1:B:77:LEU:HB3	1:B:82:ILE:HD12	1.78	0.64
1:A:38:VAL:HG11	1:A:86:TYR:HA	1.80	0.64
1:A:103:ARG:NH2	1:A:107:LEU:O	2.31	0.64
1:A:93:VAL:HG23	1:A:111:LEU:HB2	1.79	0.64
1:A:131:CYS:O	1:A:148:ILE:HD12	1.98	0.63
1:B:191:ILE:HD11	1:B:240:ASP:HA	1.79	0.63
1:B:48:ILE:CG2	1:B:50:LEU:HD21	2.28	0.63
1:A:111:LEU:HD22	1:A:120:SER:HG	1.62	0.63
1:A:71:ARG:O	1:A:72:LEU:HD23	1.99	0.63
1:A:55:TRP:HD1	3:A:1256:GOL:C2	2.12	0.63
1:B:48:ILE:HG23	1:B:50:LEU:HD21	1.80	0.63
1:B:48:ILE:HG23	1:B:50:LEU:CD2	2.29	0.62
1:A:240:ASP:OD1	1:A:240:ASP:N	2.33	0.62
1:A:10:VAL:HG23	1:A:31:TYR:CE1	2.35	0.62
1:B:148:ILE:HG22	1:B:181:TRP:HZ2	1.65	0.62
1:A:37:PHE:HA	1:A:63:ASN:O	2.00	0.61
1:A:25:GLU:OE2	1:A:51:LYS:NZ	2.34	0.61
1:B:94:GLU:HG3	1:B:110:LYS:HG2	1.82	0.61
1:B:163:LYS:HG3	1:B:240:ASP:CB	2.30	0.60
1:B:80:PRO:HG2	1:B:84:GLN:OE1	2.02	0.60
1:A:92:VAL:HA	1:A:111:LEU:O	2.01	0.60
1:A:17:LEU:O	1:A:20:ARG:HG3	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:GLU:HG3	1:B:208:ARG:H	1.66	0.60
1:A:111:LEU:HD22	1:A:120:SER:OG	2.01	0.60
1:A:94:GLU:HG3	1:A:110:LYS:HG2	1.84	0.59
1:A:133:ASN:OD1	1:A:134:PRO:HD2	2.03	0.59
1:B:76:SER:O	1:B:96:GLU:HG2	2.03	0.59
1:A:14:GLN:OE1	1:A:14:GLN:HA	2.02	0.59
1:B:93:VAL:HG23	1:B:111:LEU:HB2	1.85	0.59
1:A:36:SER:HB3	1:A:117:LEU:HD13	1.83	0.59
1:A:17:LEU:O	1:A:18:GLU:HB2	2.03	0.58
1:A:68:VAL:HG12	1:A:69:PRO:HD2	1.84	0.58
1:A:171:PHE:HB3	1:A:173:LEU:CD1	2.33	0.58
1:B:163:LYS:HE3	1:B:165:PHE:CE1	2.38	0.58
1:A:148:ILE:HG22	1:A:181:TRP:CZ2	2.39	0.58
1:A:59:GLU:OE1	1:A:59:GLU:N	2.36	0.58
1:A:150:PHE:CE2	1:A:174:ILE:HG22	2.39	0.58
1:A:198:GLN:NE2	1:A:198:GLN:HA	2.18	0.58
1:A:165:PHE:CE2	1:A:189:ARG:HB2	2.38	0.58
1:A:217:VAL:O	1:A:232:SER:HB2	2.04	0.58
1:B:25:GLU:O	1:B:26:ASP:HB2	2.03	0.58
1:B:208:ARG:HB2	1:B:211:TYR:CZ	2.38	0.58
1:A:81:TYR:CD2	1:A:93:VAL:HA	2.39	0.57
1:A:206:GLY:O	1:A:207:GLU:O	2.23	0.57
1:A:86:TYR:O	1:A:88:PRO:HD3	2.04	0.57
1:B:228:ILE:N	1:B:250:GLU:O	2.36	0.57
1:A:40:ILE:HD11	1:A:63:ASN:HB2	1.87	0.57
1:A:77:LEU:HB3	1:A:82:ILE:HD12	1.85	0.57
1:B:77:LEU:HD13	1:B:95:TYR:CE2	2.39	0.57
1:A:207:GLU:CG	1:A:208:ARG:H	2.15	0.57
1:A:36:SER:O	1:A:64:ARG:HA	2.05	0.57
1:A:3:ASP:OD2	1:A:24:PRO:HA	2.05	0.56
1:B:199:ILE:HD12	1:B:202:GLY:HA3	1.87	0.56
1:B:240:ASP:N	1:B:240:ASP:OD1	2.38	0.56
1:B:148:ILE:HG22	1:B:181:TRP:CH2	2.39	0.56
1:B:190:GLU:HG2	1:B:192:TYR:CE1	2.40	0.56
1:A:125:PHE:CD2	1:A:125:PHE:N	2.72	0.56
1:B:107:LEU:N	1:B:107:LEU:HD23	2.20	0.55
1:B:70:THR:N	4:B:2014:HOH:O	2.27	0.55
1:A:55:TRP:HD1	3:A:1256:GOL:O2	1.88	0.55
1:B:72:LEU:HD23	1:B:72:LEU:N	2.21	0.55
1:B:81:TYR:HB3	1:B:93:VAL:HG12	1.87	0.55
1:B:92:VAL:HA	1:B:111:LEU:O	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:GLU:O	1:B:37:PHE:HB2	2.06	0.55
1:B:81:TYR:CD2	1:B:93:VAL:HA	2.42	0.55
1:A:165:PHE:HE2	1:A:189:ARG:HB2	1.70	0.54
1:A:20:ARG:HD3	1:A:23:PHE:CE1	2.41	0.54
1:A:74:SER:OG	1:A:126:CYS:HB2	2.08	0.54
1:A:107:LEU:HD13	1:A:123:VAL:HB	1.90	0.54
1:A:204:ILE:O	1:A:204:ILE:HG22	2.08	0.54
1:A:88:PRO:HG2	1:A:91:THR:OG1	2.08	0.54
1:B:116:ASN:OD1	1:B:118:LYS:HB2	2.07	0.54
1:B:148:ILE:CG2	1:B:181:TRP:HZ2	2.20	0.54
1:A:40:ILE:HD12	1:A:61:PHE:O	2.08	0.54
1:B:219:TYR:CD1	1:B:249:PRO:HD2	2.43	0.54
1:A:38:VAL:HG11	1:A:86:TYR:CA	2.37	0.53
1:A:106:SER:O	1:A:107:LEU:HD23	2.08	0.53
1:A:215:GLN:NE2	2:A:1255:SO4:O3	2.39	0.53
1:B:102:ARG:O	1:B:102:ARG:HG3	2.08	0.53
1:B:207:GLU:HG3	1:B:208:ARG:N	2.23	0.53
1:A:163:LYS:CG	1:A:240:ASP:HB3	2.33	0.53
1:A:38:VAL:HG11	1:A:86:TYR:HB2	1.91	0.53
1:B:38:VAL:HG11	1:B:86:TYR:HA	1.90	0.53
1:B:227:MET:HG2	1:B:231:HIS:CE1	2.44	0.52
1:B:40:ILE:HD12	1:B:61:PHE:O	2.09	0.52
1:B:13:ALA:HB1	1:B:31:TYR:HB3	1.91	0.52
1:B:8:PRO:HD3	1:B:55:TRP:CD1	2.44	0.52
1:A:23:PHE:CD2	1:A:55:TRP:HZ2	2.26	0.52
1:A:212:GLY:O	1:A:235:CYS:HB3	2.10	0.52
1:A:140:GLY:HA2	1:A:158:CYS:HA	1.92	0.52
1:B:74:SER:C	1:B:98:ARG:HG3	2.30	0.52
1:A:55:TRP:HB2	3:A:1256:GOL:H12	1.91	0.51
1:A:234:TYR:O	1:A:245:SER:HB3	2.11	0.51
1:B:89:VAL:CG1	1:B:115:GLN:HA	2.37	0.51
1:B:160:THR:HG22	1:B:213:TYR:CE2	2.45	0.51
1:B:165:PHE:CE2	1:B:189:ARG:HB2	2.46	0.51
1:B:14:GLN:HA	1:B:14:GLN:OE1	2.11	0.51
1:A:104:GLU:N	1:A:125:PHE:O	2.41	0.51
1:A:208:ARG:HB2	1:A:211:TYR:OH	2.10	0.51
1:B:28:VAL:HG23	1:B:48:ILE:HD12	1.90	0.51
1:B:109:PRO:HA	1:B:125:PHE:CD1	2.47	0.50
1:B:217:VAL:HG12	1:B:233:ILE:CG1	2.40	0.50
1:A:36:SER:HB3	1:A:117:LEU:HD11	1.92	0.50
1:B:107:LEU:CD1	1:B:123:VAL:HB	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:ASN:O	1:B:222:ASN:ND2	2.44	0.50
1:B:216:SER:HB2	1:B:234:TYR:CD1	2.46	0.50
1:B:116:ASN:OD1	1:B:116:ASN:O	2.30	0.50
1:B:17:LEU:O	1:B:18:GLU:HB2	2.11	0.50
1:B:114:LEU:HB2	1:B:118:LYS:O	2.11	0.50
1:B:228:ILE:HG13	1:B:252:ARG:HB2	1.94	0.50
1:A:68:VAL:HA	1:A:87:PHE:HE1	1.77	0.50
1:B:131:CYS:HA	1:B:179:VAL:HG23	1.94	0.50
1:B:165:PHE:CD2	1:B:189:ARG:NH2	2.80	0.49
1:B:68:VAL:HA	1:B:87:PHE:HE1	1.77	0.49
1:A:77:LEU:HD13	1:A:95:TYR:CE2	2.46	0.49
1:B:191:ILE:HD13	1:B:240:ASP:CA	2.37	0.49
1:B:183:ASP:HB3	1:B:184:PRO:HD2	1.95	0.49
1:B:200:ASP:O	1:B:201:ASN:HB2	2.12	0.49
1:B:231:HIS:CD2	1:B:231:HIS:N	2.80	0.49
1:B:180:GLN:OE1	1:B:180:GLN:HA	2.12	0.49
1:B:208:ARG:HB2	1:B:211:TYR:CE1	2.48	0.49
1:B:36:SER:HB3	1:B:117:LEU:CD1	2.43	0.49
1:B:200:ASP:O	1:B:251:CYS:HB2	2.13	0.49
1:A:38:VAL:HG11	1:A:86:TYR:CB	2.43	0.49
1:B:104:GLU:N	1:B:125:PHE:O	2.43	0.48
1:B:198:GLN:CA	1:B:198:GLN:NE2	2.73	0.48
1:B:208:ARG:HH11	1:B:208:ARG:HG3	1.79	0.48
1:B:163:LYS:CE	1:B:165:PHE:CE1	2.97	0.48
1:B:77:LEU:CD1	1:B:95:TYR:CZ	2.96	0.48
1:B:127:LYS:HD2	1:B:127:LYS:HA	1.41	0.47
1:A:219:TYR:CD1	1:A:249:PRO:HD2	2.49	0.47
1:B:7:PRO:HG3	1:B:29:ILE:HD12	1.96	0.47
1:A:107:LEU:HD23	1:A:107:LEU:N	2.25	0.47
1:A:13:ALA:HB1	1:A:31:TYR:HB3	1.97	0.47
1:A:40:ILE:CG2	1:A:43:GLU:HG3	2.44	0.47
1:B:140:GLY:HA2	1:B:158:CYS:HA	1.96	0.47
1:B:82:ILE:HG23	1:B:83:THR:HG23	1.95	0.47
1:A:11:PRO:HB2	1:A:60:GLU:OE2	2.15	0.47
1:B:203:ILE:HA	4:B:2021:HOH:O	2.14	0.47
1:A:163:LYS:HE3	1:A:165:PHE:CE1	2.49	0.47
1:A:198:GLN:CA	1:A:198:GLN:NE2	2.77	0.47
1:B:97:CYS:SG	1:B:103:ARG:HG2	2.55	0.47
1:A:214:ARG:NH1	1:B:160:THR:O	2.23	0.47
1:A:124:GLU:OE2	1:A:127:LYS:HE2	2.14	0.47
1:B:217:VAL:HG13	1:B:217:VAL:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ILE:HG22	1:A:181:TRP:CH2	2.49	0.46
1:B:112:THR:HG22	1:B:114:LEU:CD1	2.45	0.46
1:B:165:PHE:HE2	1:B:189:ARG:HB2	1.78	0.46
1:B:123:VAL:HG23	1:B:125:PHE:CD2	2.43	0.46
1:A:228:ILE:HA	1:B:145:PRO:O	2.14	0.46
1:B:79:GLN:OE1	1:B:82:ILE:HG22	2.15	0.46
1:A:217:VAL:HG13	1:A:217:VAL:O	2.15	0.46
1:A:45:ASP:HB3	1:A:61:PHE:CE2	2.50	0.46
1:A:185:LEU:HD12	1:A:185:LEU:HA	1.78	0.46
1:A:208:ARG:CB	1:A:211:TYR:CZ	2.98	0.46
1:B:130:SER:C	1:B:179:VAL:HG21	2.36	0.46
1:A:194:PRO:O	1:A:244:TRP:NE1	2.41	0.46
1:A:75:ALA:HB1	1:A:95:TYR:HB3	1.97	0.46
1:B:198:GLN:HE21	1:B:198:GLN:CA	2.29	0.46
1:A:204:ILE:HG13	1:A:219:TYR:CE2	2.51	0.46
1:B:219:TYR:CD1	1:B:249:PRO:CD	2.98	0.46
1:A:69:PRO:HD3	1:A:87:PHE:CE1	2.51	0.45
1:B:10:VAL:CG2	1:B:31:TYR:CE1	2.98	0.45
1:B:36:SER:HB3	1:B:117:LEU:HD12	1.98	0.45
1:A:112:THR:CG2	1:A:113:CYS:N	2.79	0.45
1:A:99:PRO:HA	1:A:100:GLY:HA2	1.53	0.45
1:A:198:GLN:CA	1:A:198:GLN:HE21	2.29	0.45
1:A:47:VAL:HG23	1:A:55:TRP:CE3	2.50	0.45
1:B:107:LEU:HD13	1:B:123:VAL:HB	1.98	0.45
1:B:69:PRO:HD3	1:B:87:PHE:CE1	2.52	0.45
1:A:76:SER:O	1:A:96:GLU:HG2	2.16	0.45
1:B:159:ASN:ND2	4:B:2020:HOH:O	2.47	0.45
1:B:252:ARG:NH2	1:B:252:ARG:CB	2.59	0.45
1:A:143:ASP:HB3	1:A:155:SER:OG	2.16	0.45
1:B:171:PHE:O	1:B:182:SER:N	2.47	0.45
1:B:6:LEU:HA	1:B:23:PHE:HE2	1.81	0.45
1:A:218:THR:HA	1:A:232:SER:HB3	1.99	0.45
1:A:127:LYS:HD2	1:A:127:LYS:HA	1.40	0.44
1:A:61:PHE:N	1:A:61:PHE:CD1	2.85	0.44
1:A:98:ARG:HA	1:A:99:PRO:HD3	1.76	0.44
1:B:213:TYR:O	1:B:214:ARG:HB2	2.16	0.44
1:A:104:GLU:OE2	1:A:105:PRO:HD2	2.18	0.44
1:A:250:GLU:CD	1:A:252:ARG:HH22	2.15	0.44
1:A:214:ARG:HA	1:A:214:ARG:HD3	1.58	0.44
1:A:71:ARG:C	1:A:72:LEU:HD23	2.38	0.44
1:B:135:GLY:O	1:B:142:ILE:HD12	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ARG:HH21	1:A:125:PHE:HB2	1.82	0.44
1:B:35:GLU:O	1:B:36:SER:HB2	2.18	0.44
1:A:44:LYS:HB2	1:A:44:LYS:HE2	1.38	0.44
1:B:199:ILE:HD12	1:B:202:GLY:CA	2.47	0.44
1:B:96:GLU:O	1:B:96:GLU:HG3	2.17	0.44
1:A:148:ILE:CG2	1:A:181:TRP:HZ2	2.31	0.44
1:B:10:VAL:HA	1:B:11:PRO:HD3	1.90	0.44
1:B:124:GLU:OE2	1:B:127:LYS:HE2	2.17	0.44
1:B:77:LEU:HD13	1:B:95:TYR:CZ	2.53	0.44
1:A:207:GLU:CG	1:A:208:ARG:N	2.81	0.43
1:A:97:CYS:SG	1:A:103:ARG:HG2	2.57	0.43
1:B:74:SER:O	1:B:98:ARG:HG3	2.18	0.43
1:B:85:ASN:N	1:B:85:ASN:ND2	2.66	0.43
1:A:208:ARG:NH2	1:A:215:GLN:HE22	2.16	0.43
1:B:216:SER:CB	1:B:234:TYR:CD1	3.01	0.43
1:B:57:ASP:O	1:B:58:ILE:HB	2.17	0.43
1:B:77:LEU:CD1	1:B:95:TYR:CE2	3.01	0.43
1:A:93:VAL:CG2	1:A:111:LEU:HB2	2.45	0.43
1:A:38:VAL:CG1	1:A:86:TYR:HB2	2.48	0.43
1:A:216:SER:HA	1:A:234:TYR:HA	1.99	0.43
1:B:128:LYS:HE2	1:B:150:PHE:O	2.18	0.43
1:A:165:PHE:CD2	1:A:189:ARG:CG	2.88	0.43
1:A:183:ASP:HB3	1:A:184:PRO:HD2	2.00	0.43
1:B:208:ARG:NH1	1:B:208:ARG:HG3	2.34	0.43
1:A:123:VAL:HG23	1:A:125:PHE:HD2	1.83	0.43
1:A:217:VAL:CG1	1:A:217:VAL:O	2.67	0.43
1:A:40:ILE:HB	1:A:43:GLU:HG3	2.01	0.42
1:B:160:THR:CG2	1:B:213:TYR:CE2	3.02	0.42
1:A:213:TYR:HE1	2:A:1254:SO4:O3	2.02	0.42
1:B:199:ILE:HD11	1:B:202:GLY:HA3	2.01	0.42
1:A:128:LYS:HE2	1:A:150:PHE:O	2.20	0.42
1:A:82:ILE:HG23	1:A:83:THR:HG23	2.01	0.42
1:A:208:ARG:CG	1:A:208:ARG:HH11	2.24	0.42
1:A:20:ARG:H	1:A:20:ARG:HG3	1.67	0.42
1:A:64:ARG:H	1:A:64:ARG:HG3	1.72	0.42
1:A:217:VAL:CG1	1:A:233:ILE:CG1	2.92	0.42
1:B:208:ARG:CB	1:B:211:TYR:CE1	3.02	0.42
1:B:212:GLY:O	1:B:235:CYS:HB3	2.20	0.42
1:B:98:ARG:HA	1:B:99:PRO:HD3	1.75	0.42
1:A:137:ILE:HG12	1:A:185:LEU:HG	2.01	0.42
1:A:200:ASP:O	1:A:251:CYS:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:VAL:HG23	1:A:125:PHE:CD2	2.55	0.41
1:A:38:VAL:HG12	1:A:86:TYR:CD2	2.55	0.41
1:B:74:SER:OG	1:B:126:CYS:HB2	2.20	0.41
1:B:64:ARG:NH2	1:B:115:GLN:O	2.53	0.41
1:B:199:ILE:H	1:B:199:ILE:HG13	1.71	0.41
1:B:207:GLU:CG	1:B:208:ARG:N	2.82	0.41
1:B:201:ASN:C	1:B:222:ASN:ND2	2.74	0.41
1:B:221:CYS:SG	1:B:227:MET:HE3	2.60	0.41
1:B:133:ASN:HA	1:B:134:PRO:HD3	1.94	0.41
1:B:68:VAL:HA	1:B:87:PHE:CE1	2.56	0.41
1:A:55:TRP:CD1	3:A:1256:GOL:C2	2.99	0.41
1:B:231:HIS:H	1:B:231:HIS:CD2	2.37	0.41
1:B:58:ILE:O	1:B:58:ILE:HG23	2.20	0.41
1:A:162:TYR:CD2	1:A:190:GLU:HA	2.55	0.41
1:A:198:GLN:OE1	1:A:204:ILE:HD12	2.21	0.41
1:A:55:TRP:H	3:A:1256:GOL:C1	2.28	0.41
1:A:173:LEU:HD22	1:A:182:SER:CB	2.51	0.41
1:B:71:ARG:O	1:B:72:LEU:HD23	2.21	0.41
1:A:114:LEU:CD1	1:A:114:LEU:N	2.83	0.41
1:B:227:MET:HG3	1:B:228:ILE:N	2.35	0.41
1:A:58:ILE:O	1:A:58:ILE:HG23	2.21	0.40
1:A:39:LYS:HA	1:A:61:PHE:O	2.21	0.40
1:B:23:PHE:CD2	1:B:55:TRP:HZ2	2.39	0.40
1:A:174:ILE:HA	1:A:179:VAL:HA	2.02	0.40
1:B:185:LEU:HA	1:B:185:LEU:HD12	1.89	0.40
1:B:4:CYS:SG	1:B:53:SER:HA	2.61	0.40
1:A:173:LEU:HD22	1:A:182:SER:HB3	2.02	0.40
1:B:24:PRO:HG2	1:B:27:THR:OG1	2.21	0.40
1:B:85:ASN:N	1:B:85:ASN:HD22	2.20	0.40
1:A:227:MET:HE3	1:B:144:VAL:HG11	2.03	0.40
1:B:106:SER:O	1:B:107:LEU:HD23	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:THR:OG1	1:B:200:ASP:OD2[1_665]	2.09	0.11

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	250/254 (98%)	217 (87%)	28 (11%)	5 (2%)	7	6
1	B	249/254 (98%)	222 (89%)	22 (9%)	5 (2%)	7	6
All	All	499/508 (98%)	439 (88%)	50 (10%)	10 (2%)	7	6

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	GLU
1	B	99	PRO
1	B	98	ARG
1	A	99	PRO
1	A	205	GLN
1	A	105	PRO
1	B	58	ILE
1	B	123	VAL
1	B	186	PRO
1	A	123	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	223/225 (99%)	171 (77%)	52 (23%)	1	0
1	B	222/225 (99%)	176 (79%)	46 (21%)	1	1
All	All	445/450 (99%)	347 (78%)	98 (22%)	1	1

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	20	ARG
1	A	29	ILE
1	A	32	LYS
1	A	36	SER
1	A	44	LYS
1	A	46	SER
1	A	50	LEU
1	A	51	LYS
1	A	54	GLN
1	A	58	ILE
1	A	64	ARG
1	A	65	SER
1	A	70	THR
1	A	77	LEU
1	A	81	TYR
1	A	82	ILE
1	A	93	VAL
1	A	102	ARG
1	A	106	SER
1	A	108	SER
1	A	111	LEU
1	A	114	LEU
1	A	115	GLN
1	A	118	LYS
1	A	121	THR
1	A	123	VAL
1	A	124	GLU
1	A	125	PHE
1	A	127	LYS
1	A	131	CYS
1	A	142	ILE
1	A	164	LEU
1	A	167	SER
1	A	173	LEU
1	A	174	ILE
1	A	175	SER
1	A	177	SER
1	A	187	GLU
1	A	193	CYS
1	A	198	GLN
1	A	208	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	214	ARG
1	A	216	SER
1	A	223	LYS
1	A	227	MET
1	A	228	ILE
1	A	236	THR
1	A	239	ASN
1	A	240	ASP
1	A	245	SER
1	A	252	ARG
1	B	17	LEU
1	B	29	ILE
1	B	32	LYS
1	B	39	LYS
1	B	44	LYS
1	B	50	LEU
1	B	57	ASP
1	B	60	GLU
1	B	64	ARG
1	B	65	SER
1	B	70	THR
1	B	77	LEU
1	B	78	LYS
1	B	81	TYR
1	B	82	ILE
1	B	85	ASN
1	B	89	VAL
1	B	93	VAL
1	B	102	ARG
1	B	106	SER
1	B	107	LEU
1	B	108	SER
1	B	114	LEU
1	B	115	GLN
1	B	118	LYS
1	B	121	THR
1	B	124	GLU
1	B	125	PHE
1	B	127	LYS
1	B	131	CYS
1	B	164	LEU
1	B	173	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	174	ILE
1	B	175	SER
1	B	182	SER
1	B	187	GLU
1	B	193	CYS
1	B	198	GLN
1	B	208	ARG
1	B	216	SER
1	B	223	LYS
1	B	227	MET
1	B	239	ASN
1	B	240	ASP
1	B	245	SER
1	B	252	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	85	ASN
1	A	198	GLN
1	A	205	GLN
1	A	222	ASN
1	A	231	HIS
1	B	85	ASN
1	B	115	GLN
1	B	159	ASN
1	B	198	GLN
1	B	222	ASN
1	B	231	HIS

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	1254	-	4,4,4	0.40	0	6,6,6	0.76	0
3	GOL	A	1256	-	5,5,5	4.54	5 (100%)	5,5,5	5.68	3 (60%)
2	SO4	A	1255	-	4,4,4	0.45	0	6,6,6	0.80	0
3	GOL	A	1257	-	5,5,5	4.50	5 (100%)	5,5,5	5.74	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	1256	-	-	3/4/4/4	-
3	GOL	A	1257	-	-	1/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1256	GOL	C3-C2	-7.38	1.21	1.51
3	A	1257	GOL	C3-C2	-7.32	1.21	1.51
3	A	1256	GOL	O1-C1	4.59	1.61	1.42
3	A	1257	GOL	O1-C1	4.54	1.61	1.42
3	A	1256	GOL	O3-C3	3.47	1.57	1.42
3	A	1257	GOL	O3-C3	3.38	1.56	1.42
3	A	1257	GOL	C1-C2	-2.83	1.40	1.51
3	A	1256	GOL	O2-C2	-2.82	1.35	1.43
3	A	1257	GOL	O2-C2	-2.79	1.35	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1256	GOL	C1-C2	-2.75	1.40	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1257	GOL	O3-C3-C2	10.50	160.53	110.20
3	A	1256	GOL	O3-C3-C2	10.41	160.14	110.20
3	A	1257	GOL	O2-C2-C3	6.59	138.13	109.12
3	A	1256	GOL	O2-C2-C3	6.43	137.43	109.12
3	A	1256	GOL	O1-C1-C2	3.29	125.96	110.20
3	A	1257	GOL	O1-C1-C2	3.23	125.69	110.20

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1256	GOL	C1-C2-C3-O3
3	A	1257	GOL	O1-C1-C2-C3
3	A	1256	GOL	O2-C2-C3-O3
3	A	1256	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1254	SO4	1	0
3	A	1256	GOL	6	0
2	A	1255	SO4	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	252/254 (99%)	1.12	42 (16%) 1 2	25, 61, 87, 99	0
1	B	251/254 (98%)	1.10	40 (15%) 1 2	27, 59, 85, 102	0
All	All	503/508 (99%)	1.11	82 (16%) 1 2	25, 60, 86, 102	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	240	ASP	5.9
1	A	240	ASP	5.8
1	B	6	LEU	5.8
1	B	3	ASP	5.1
1	B	7	PRO	4.8
1	B	239	ASN	4.4
1	B	179	VAL	4.0
1	A	82	ILE	3.5
1	A	22	SER	3.5
1	B	105	PRO	3.4
1	B	23	PHE	3.4
1	A	239	ASN	3.4
1	A	112	THR	3.3
1	A	114	LEU	3.3
1	B	249	PRO	3.3
1	B	62	CYS	3.2
1	A	122	ALA	3.2
1	A	148	ILE	3.1
1	B	34	GLU	3.1
1	B	33	CYS	3.1
1	A	115	GLN	3.1
1	B	148	ILE	3.1
1	A	123	VAL	3.0
1	B	60	GLU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	19	GLY	3.0
1	B	29	ILE	3.0
1	A	21	THR	3.0
1	A	117	LEU	3.0
1	B	250	GLU	3.0
1	A	23	PHE	3.0
1	A	87	PHE	2.9
1	B	114	LEU	2.9
1	B	92	VAL	2.8
1	A	110	LYS	2.7
1	A	149	LEU	2.7
1	A	107	LEU	2.6
1	A	64	ARG	2.6
1	A	252	ARG	2.6
1	B	93	VAL	2.6
1	A	80	PRO	2.5
1	B	225	PHE	2.5
1	B	111	LEU	2.5
1	A	211	TYR	2.5
1	A	33	CYS	2.5
1	A	83	THR	2.5
1	B	192	TYR	2.4
1	B	91	THR	2.4
1	A	205	GLN	2.4
1	B	234	TYR	2.4
1	B	104	GLU	2.4
1	A	134	PRO	2.4
1	A	62	CYS	2.4
1	A	111	LEU	2.4
1	B	191	ILE	2.3
1	A	118	LYS	2.3
1	B	125	PHE	2.3
1	B	9	ASP	2.3
1	B	18	GLU	2.3
1	A	6	LEU	2.3
1	A	43	GLU	2.2
1	B	35	GLU	2.2
1	A	11	PRO	2.2
1	B	115	GLN	2.2
1	A	92	VAL	2.2
1	A	228	ILE	2.2
1	A	12	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	93	VAL	2.2
1	B	189	ARG	2.2
1	A	29	ILE	2.2
1	B	144	VAL	2.1
1	A	199	ILE	2.1
1	A	91	THR	2.1
1	B	89	VAL	2.1
1	A	37	PHE	2.1
1	B	14	GLN	2.1
1	A	217	VAL	2.0
1	B	174	ILE	2.0
1	B	21	THR	2.0
1	A	81	TYR	2.0
1	A	242	GLY	2.0
1	B	112	THR	2.0
1	B	13	ALA	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 carbohydrates 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(\AA^2)	Q<0.9
3	GOL	A	1257	6/6	0.73	0.39	85,85,85,85	0
3	GOL	A	1256	6/6	0.75	0.44	96,96,96,96	0
2	SO4	A	1255	5/5	0.90	0.17	75,75,75,76	0
2	SO4	A	1254	5/5	0.98	0.14	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.