



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 12:26 AM EDT

PDB ID : 1OK9 / pdb_00001ok9
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, R.A.; Evans, D.J.; Morgan, B.P.; Smith, R.A.G.; Lea, S.M.
Deposited on : 2003-07-21
Resolution : 3.00 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

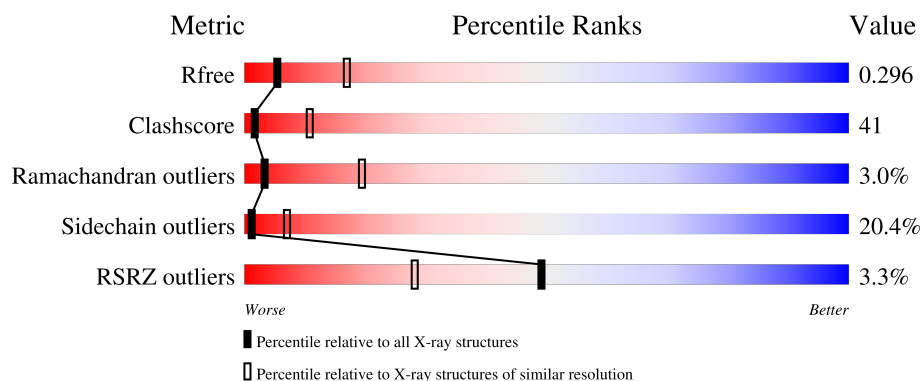
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	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
2	ACT	A	1255	-	-	X	-
2	ACT	A	1256	-	-	X	-
2	ACT	B	1255	-	-	X	-
2	ACT	B	1256	-	-	X	-
4	CL	A	1259[A]	-	-	X	-
4	CL	B	1259[A]	-	-	X	X
6	GOL	B	1261	-	X	-	-
6	GOL	B	1262	-	X	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 3991 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	254	Total	C	N	O	S	0	0	0
			1969	1234	330	386	19			
1	B	254	Total	C	N	O	S	0	0	0
			1969	1234	330	386	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	ILE	THR	conflict	UNP P08174
B	48	ILE	THR	conflict	UNP P08174

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

Continued on next page...

Continued from previous page...

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

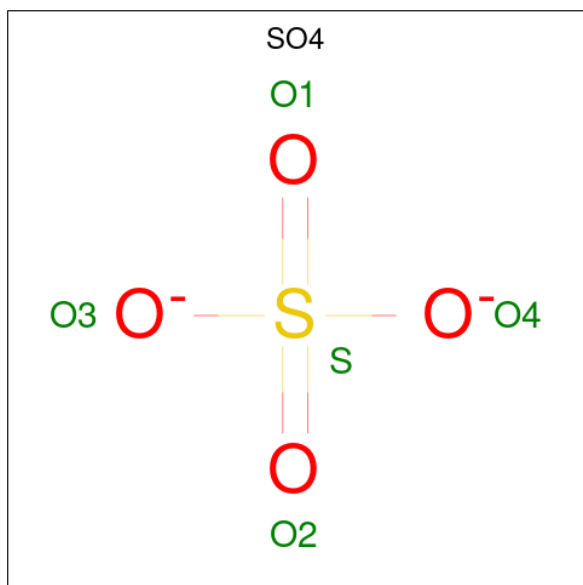
- Molecule 3 is PLATINUM (II) ION (CCD ID: PT) (formula: Pt).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Pt 1 1	0	1
3	B	1	Total Pt 1 1	0	1

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Cl 2 2	0	2
4	B	2	Total Cl 2 2	0	2

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

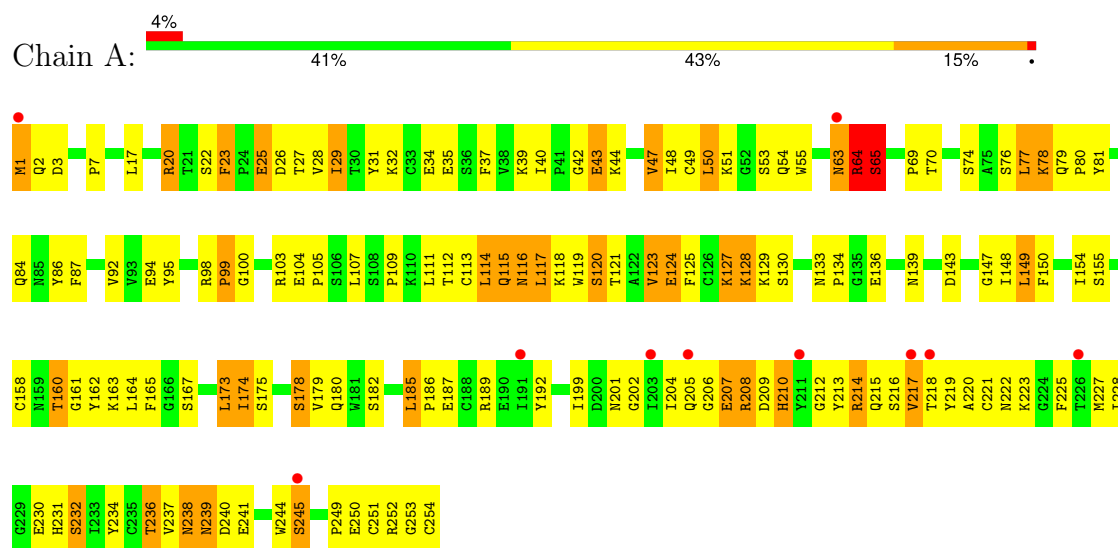
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total O 2 2	0	0
7	B	7	Total O 7 7	0	0

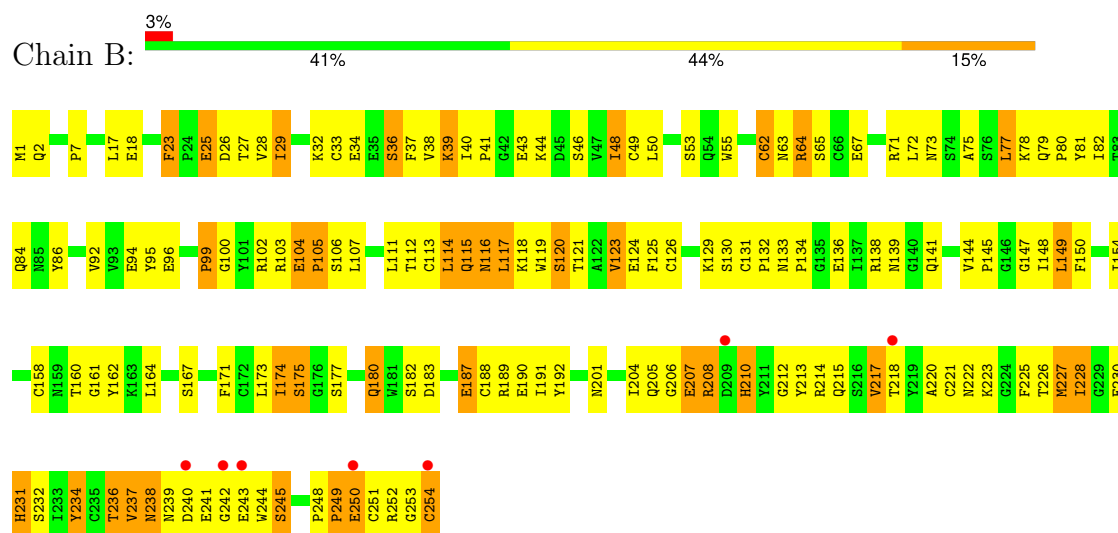
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 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	46.13Å 54.60Å 62.77Å 87.19° 85.61° 65.74°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.0 (20.00-3.00) 92.7 (20.00-3.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.11 (at 2.98Å)	Xtriage
Refinement program	TNT 5F	Depositor
R, R_{free}	0.240 , (Not available) 0.244 , 0.296	Depositor DCC
R_{free} test set	499 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	62.6	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,-h+k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	3991	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.72% 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: CL, PT, SO4, GOL, ACT

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	2/2022 (0.1%)	0.78	6/2749 (0.2%)
1	B	0.34	0/2022	0.72	1/2749 (0.0%)
All	All	0.37	2/4044 (0.0%)	0.75	7/5498 (0.1%)

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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	ASN	CA-CB	5.38	1.61	1.53
1	A	65	SER	CA-C	5.09	1.58	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	ASN	N-CA-C	-9.04	96.35	110.36
1	A	63	ASN	CA-C-N	8.20	136.47	121.70
1	A	63	ASN	C-N-CA	8.20	136.47	121.70
1	B	104	GLU	C-N-CD	-6.91	96.66	125.00
1	A	65	SER	N-CA-C	5.91	118.39	109.23
1	A	63	ASN	CA-C-O	-5.18	115.55	121.82
1	A	20	ARG	N-CA-C	5.02	117.92	110.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	62	CYS	Mainchain

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	1969	0	1867	144	0
1	B	1969	0	1867	180	0
2	A	8	0	6	6	0
2	B	8	0	6	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	2	0	0	3	0
4	B	2	0	0	3	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	B	12	0	8	0	0
7	A	2	0	0	0	0
7	B	7	0	0	0	0
All	All	3991	0	3754	317	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 41.

All (317) 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:B:116:ASN:HB2	1:B:118:LYS:HE3	1.29	1.14
1:A:116:ASN:HB2	1:A:118:LYS:HE3	1.29	1.10
1:A:209:ASP:H	2:A:1256:ACT:H1	1.20	1.01
1:B:171:PHE:HD1	1:B:173:LEU:HD12	1.32	0.93
1:B:205:GLN:HE21	1:B:220:ALA:HB2	1.36	0.91
1:B:73:ASN:H	2:B:1256:ACT:H2	1.34	0.91
1:A:205:GLN:HE21	1:A:220:ALA:HB2	1.36	0.90
1:A:213:TYR:HB2	1:A:237:VAL:HG21	1.54	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLN:HG3	1:A:80:PRO:HA	1.55	0.88
1:A:227:MET:HE3	1:A:231:HIS:HA	1.58	0.85
1:B:99:PRO:HB2	1:B:174:ILE:HD12	1.61	0.82
1:A:252:ARG:HH21	1:A:254:CYS:HA	1.43	0.82
1:B:29:ILE:HD13	1:B:55:TRP:CH2	2.16	0.81
1:B:116:ASN:HB2	1:B:118:LYS:CE	2.11	0.81
1:B:252:ARG:HH11	1:B:254:CYS:H	1.28	0.80
1:A:29:ILE:HD13	1:A:55:TRP:CH2	2.16	0.80
1:B:173:LEU:HD13	1:B:182:SER:HB3	1.63	0.80
1:B:227:MET:HG3	1:B:249:PRO:HB2	1.62	0.80
1:B:252:ARG:NH1	1:B:254:CYS:H	1.80	0.79
1:A:209:ASP:H	2:A:1256:ACT:CH3	1.95	0.79
1:B:171:PHE:CD1	1:B:173:LEU:HD12	2.15	0.79
1:A:209:ASP:N	2:A:1256:ACT:H1	1.97	0.78
1:A:116:ASN:HB2	1:A:118:LYS:CE	2.11	0.78
1:A:227:MET:HB3	4:A:1259[A]:CL:CL	2.20	0.78
1:A:228:ILE:HG23	1:B:145:PRO:O	1.84	0.77
1:A:78:LYS:CE	1:A:94:GLU:HG2	2.15	0.77
1:A:25:GLU:OE1	1:A:51:LYS:HD3	1.85	0.77
1:B:237:VAL:HG22	1:B:242:GLY:HA2	1.67	0.76
1:B:213:TYR:CD2	1:B:214:ARG:HG3	2.21	0.76
1:A:81:TYR:HA	1:A:84:GLN:NE2	2.01	0.76
1:B:2:GLN:HG3	1:B:53:SER:HB2	1.67	0.76
1:A:133:ASN:HD22	1:A:134:PRO:HD2	1.51	0.75
1:B:81:TYR:HA	1:B:84:GLN:NE2	2.01	0.75
1:B:104:GLU:OE2	1:B:105:PRO:HD2	1.85	0.75
1:B:27:THR:O	1:B:48:ILE:HD13	1.87	0.75
1:B:237:VAL:HA	1:B:241:GLU:O	1.87	0.74
1:B:106:SER:C	1:B:107:LEU:HD23	2.10	0.74
1:A:107:LEU:HD13	1:A:123:VAL:CG2	2.18	0.74
1:A:130:SER:HB2	1:A:149:LEU:CD2	2.18	0.73
1:B:79:GLN:OE1	1:B:80:PRO:HA	1.89	0.73
1:A:185:LEU:HD12	1:A:186:PRO:HD2	1.71	0.72
1:B:227:MET:CG	1:B:249:PRO:HB2	2.19	0.72
1:A:28:VAL:CG2	1:A:48:ILE:HD12	2.19	0.72
1:A:227:MET:CE	1:A:231:HIS:HA	2.19	0.72
1:A:79:GLN:HG3	1:A:80:PRO:CA	2.19	0.71
1:B:27:THR:HG22	1:B:29:ILE:HD12	1.72	0.71
1:B:36:SER:O	1:B:64:ARG:HA	1.90	0.71
1:B:252:ARG:HG3	1:B:253:GLY:HA3	1.72	0.71
1:A:213:TYR:HB2	1:A:237:VAL:CG2	2.21	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ARG:HH21	1:A:254:CYS:CA	2.03	0.71
1:A:27:THR:HG22	1:A:29:ILE:HD12	1.72	0.71
1:A:100:GLY:C	1:A:129:LYS:HD2	2.16	0.70
1:B:39:LYS:HD3	1:B:39:LYS:N	2.07	0.70
1:B:171:PHE:HB3	1:B:173:LEU:CD1	2.21	0.70
1:A:205:GLN:HG3	1:A:218:THR:O	1.92	0.70
1:B:150:PHE:CE2	1:B:174:ILE:HG22	2.27	0.69
1:B:162:TYR:HD2	1:B:189:ARG:C	2.00	0.69
1:B:106:SER:O	1:B:107:LEU:HD23	1.92	0.69
1:B:161:GLY:C	1:B:191:ILE:HD12	2.17	0.69
1:A:127:LYS:HE2	1:A:128:LYS:H	1.58	0.69
1:B:205:GLN:HG3	1:B:218:THR:O	1.92	0.69
1:A:127:LYS:HE2	1:A:127:LYS:HA	1.75	0.68
1:B:162:TYR:CD2	1:B:190:GLU:HA	2.28	0.68
1:B:236:THR:N	1:B:243:GLU:O	2.24	0.68
1:A:20:ARG:HD2	1:A:22:SER:O	1.93	0.68
1:A:78:LYS:HE3	1:A:94:GLU:HG2	1.75	0.68
1:B:191:ILE:HD13	1:B:237:VAL:HG11	1.75	0.68
1:B:234:TYR:N	1:B:245:SER:OG	2.26	0.67
1:B:252:ARG:HD2	1:B:253:GLY:CA	2.24	0.67
1:B:133:ASN:OD1	1:B:134:PRO:HD2	1.95	0.66
1:B:252:ARG:HD2	1:B:253:GLY:HA2	1.77	0.66
1:B:29:ILE:HD13	1:B:55:TRP:HH2	1.59	0.66
1:B:205:GLN:NE2	1:B:220:ALA:HB2	2.11	0.65
1:A:165:PHE:HD2	1:A:189:ARG:CG	2.10	0.64
1:A:37:PHE:HD2	1:A:63:ASN:O	1.79	0.64
1:A:42:GLY:O	1:A:43:GLU:HG2	1.97	0.64
1:A:163:LYS:N	1:A:189:ARG:O	2.23	0.64
1:A:253:GLY:HA2	1:A:254:CYS:C	2.21	0.64
1:B:99:PRO:HB2	1:B:174:ILE:CD1	2.28	0.64
1:A:216:SER:HA	1:A:234:TYR:HA	1.80	0.64
1:B:73:ASN:H	2:B:1256:ACT:CH3	2.08	0.64
1:A:79:GLN:CG	1:A:80:PRO:HA	2.26	0.63
1:A:160:THR:HG21	1:B:214:ARG:NE	2.14	0.63
1:B:221:CYS:SG	1:B:227:MET:HE2	2.38	0.63
1:A:29:ILE:HD13	1:A:55:TRP:HH2	1.59	0.63
1:A:50:LEU:HD12	1:A:54:GLN:O	1.97	0.63
1:A:174:ILE:HD13	1:A:174:ILE:O	1.98	0.63
1:A:205:GLN:NE2	1:A:220:ALA:HB2	2.11	0.63
1:B:227:MET:HA	1:B:250:GLU:O	2.00	0.62
1:A:116:ASN:OD1	1:A:118:LYS:HD2	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:VAL:HG22	1:A:48:ILE:HD12	1.81	0.62
1:B:116:ASN:OD1	1:B:118:LYS:HD2	2.00	0.62
1:B:130:SER:HB2	1:B:149:LEU:CD2	2.29	0.61
1:A:34:GLU:O	1:A:37:PHE:HB2	1.99	0.61
1:B:77:LEU:O	1:B:82:ILE:HB	2.01	0.61
1:B:175:SER:HB3	1:B:180:GLN:HG2	1.83	0.60
1:A:127:LYS:HA	1:A:127:LYS:CE	2.27	0.60
1:B:213:TYR:CE2	1:B:214:ARG:HG3	2.35	0.60
1:B:39:LYS:HD3	1:B:39:LYS:H	1.67	0.59
1:B:252:ARG:HH11	1:B:254:CYS:N	1.99	0.59
1:B:29:ILE:O	1:B:46:SER:HB2	2.01	0.59
1:B:102:ARG:NH2	1:B:129:LYS:HG2	2.18	0.59
1:B:114:LEU:HD21	1:B:120:SER:HA	1.85	0.59
1:A:114:LEU:HD21	1:A:120:SER:HA	1.85	0.58
1:B:28:VAL:HG22	1:B:48:ILE:HG12	1.86	0.58
1:B:117:LEU:N	1:B:117:LEU:HD23	2.19	0.58
1:A:78:LYS:HE2	1:A:94:GLU:HG2	1.85	0.57
1:A:165:PHE:HD2	1:A:189:ARG:HG3	1.68	0.57
1:B:26:ASP:C	1:B:48:ILE:HD11	2.28	0.57
1:A:117:LEU:HD23	1:A:117:LEU:N	2.19	0.57
1:A:40:ILE:CG2	1:A:43:GLU:HG3	2.34	0.57
1:A:40:ILE:HG22	1:A:43:GLU:HG3	1.86	0.57
1:B:252:ARG:CG	1:B:253:GLY:HA3	2.33	0.57
1:A:160:THR:HG21	1:B:214:ARG:HE	1.70	0.57
1:A:209:ASP:CB	2:A:1256:ACT:H1	2.36	0.56
1:A:104:GLU:N	1:A:125:PHE:O	2.37	0.56
1:A:199:ILE:HD11	1:A:202:GLY:HA3	1.86	0.56
1:A:204:ILE:HG23	1:A:217:VAL:HG23	1.88	0.55
1:B:75:ALA:HB2	1:B:126:CYS:SG	2.46	0.55
1:B:228:ILE:HB	1:B:250:GLU:CD	2.31	0.55
1:B:154:ILE:HD11	2:B:1255:ACT:H2	1.88	0.55
1:B:64:ARG:CB	1:B:117:LEU:HD11	2.37	0.55
1:A:154:ILE:HD11	2:A:1255:ACT:H2	1.88	0.55
1:A:127:LYS:HE2	1:A:128:LYS:N	2.22	0.55
1:B:150:PHE:HE2	1:B:174:ILE:HG22	1.70	0.54
1:B:204:ILE:HG23	1:B:217:VAL:HG23	1.88	0.54
1:B:48:ILE:CD1	1:B:49:CYS:H	2.20	0.54
1:B:230:GLU:O	1:B:249:PRO:HB3	2.07	0.54
1:B:231:HIS:CE1	4:B:1259[A]:CL:CL	2.97	0.54
1:B:171:PHE:HB3	1:B:173:LEU:HD11	1.88	0.54
1:B:208:ARG:CG	1:B:208:ARG:HH11	2.21	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ARG:HH11	1:B:208:ARG:HG3	1.73	0.53
1:B:2:GLN:HG3	1:B:53:SER:CB	2.38	0.53
1:A:1:MET:C	1:A:3:ASP:H	2.16	0.53
1:B:38:VAL:HG11	1:B:86:TYR:HA	1.89	0.53
1:A:208:ARG:HG3	1:A:208:ARG:HH11	1.73	0.53
1:B:71:ARG:C	1:B:72:LEU:HD23	2.33	0.53
1:A:192:TYR:CE1	1:A:210:HIS:HB2	2.44	0.53
1:B:37:PHE:HB3	1:B:62:CYS:HB3	1.90	0.52
1:B:77:LEU:HD13	1:B:95:TYR:CE2	2.44	0.52
1:A:107:LEU:HD13	1:A:123:VAL:HG21	1.89	0.52
1:B:192:TYR:CE1	1:B:210:HIS:HB2	2.44	0.52
1:A:208:ARG:HH11	1:A:208:ARG:CG	2.21	0.52
1:B:23:PHE:N	1:B:23:PHE:CD2	2.78	0.52
1:B:252:ARG:NH1	1:B:254:CYS:N	2.53	0.52
1:A:69:PRO:HG2	1:A:77:LEU:HD21	1.91	0.51
1:A:115:GLN:O	1:A:117:LEU:HD23	2.11	0.51
1:A:207:GLU:HG3	1:A:208:ARG:N	2.25	0.51
1:B:115:GLN:O	1:B:117:LEU:HD23	2.11	0.51
1:B:217:VAL:HG12	1:B:244:TRP:CZ3	2.46	0.51
1:A:160:THR:HG23	1:B:214:ARG:HH11	1.75	0.51
1:B:173:LEU:CD1	1:B:182:SER:HB3	2.36	0.51
1:B:252:ARG:HD2	1:B:253:GLY:HA3	1.91	0.51
1:B:64:ARG:HB2	1:B:117:LEU:HD11	1.92	0.51
1:A:217:VAL:HG12	1:A:244:TRP:CZ3	2.46	0.51
1:B:187:GLU:OE1	1:B:189:ARG:NE	2.44	0.51
1:B:231:HIS:CD2	4:B:1259[A]:CL:CL	3.00	0.51
1:A:212:GLY:O	1:A:215:GLN:HB2	2.11	0.50
1:B:212:GLY:O	1:B:215:GLN:HB2	2.11	0.50
1:A:78:LYS:HE3	1:A:94:GLU:CG	2.42	0.50
1:A:143:ASP:HB3	1:A:155:SER:OG	2.11	0.50
1:B:73:ASN:N	2:B:1256:ACT:H2	2.15	0.50
1:A:23:PHE:N	1:A:23:PHE:CD2	2.78	0.50
1:A:174:ILE:HA	1:A:179:VAL:HA	1.93	0.50
1:A:252:ARG:NE	1:A:253:GLY:HA3	2.27	0.50
1:B:27:THR:HG22	1:B:29:ILE:CD1	2.40	0.50
1:B:207:GLU:HG3	1:B:208:ARG:N	2.25	0.50
1:A:27:THR:HG22	1:A:29:ILE:CD1	2.40	0.50
1:B:227:MET:O	1:B:228:ILE:HD13	2.12	0.50
1:B:138:ARG:O	1:B:188:CYS:HB2	2.12	0.49
1:B:227:MET:SD	1:B:249:PRO:HB2	2.51	0.49
1:B:144:VAL:HG22	1:B:154:ILE:HG22	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:GLU:O	1:A:26:ASP:HB2	2.11	0.49
1:A:165:PHE:N	1:A:187:GLU:O	2.41	0.49
1:B:103:ARG:NH2	1:B:125:PHE:HB2	2.27	0.49
1:B:144:VAL:HG12	1:B:144:VAL:O	2.11	0.49
1:B:25:GLU:O	1:B:26:ASP:HB2	2.11	0.48
1:B:213:TYR:CG	1:B:214:ARG:HG3	2.47	0.48
1:B:39:LYS:O	1:B:41:PRO:HD3	2.14	0.48
1:B:162:TYR:CE2	1:B:190:GLU:HB2	2.48	0.48
1:B:53:SER:O	1:B:53:SER:OG	2.30	0.48
1:A:112:THR:O	1:A:119:TRP:HA	2.14	0.48
1:A:173:LEU:HD22	1:A:182:SER:HB3	1.94	0.48
1:A:139:ASN:HB3	1:A:162:TYR:CE1	2.49	0.48
1:B:213:TYR:CE2	1:B:214:ARG:CG	2.97	0.48
1:B:139:ASN:HB3	1:B:162:TYR:CE1	2.49	0.48
1:A:77:LEU:CD1	1:A:95:TYR:CZ	2.97	0.47
1:B:7:PRO:HG2	1:B:17:LEU:HD21	1.96	0.47
1:B:191:ILE:CD1	1:B:237:VAL:HG11	2.44	0.47
1:B:214:ARG:HA	1:B:234:TYR:CD2	2.48	0.47
1:A:7:PRO:HG2	1:A:17:LEU:HD21	1.96	0.47
1:A:127:LYS:HE2	1:A:127:LYS:CA	2.43	0.47
1:B:39:LYS:H	1:B:39:LYS:CD	2.26	0.47
1:B:48:ILE:HD12	1:B:49:CYS:N	2.30	0.47
1:B:112:THR:O	1:B:119:TRP:HA	2.14	0.47
1:B:234:TYR:H	1:B:245:SER:HG	1.55	0.47
1:A:31:TYR:HE2	1:A:47:VAL:HG22	1.80	0.47
1:B:144:VAL:HG22	1:B:154:ILE:CG2	2.44	0.47
1:A:222:ASN:O	1:A:225:PHE:HB2	2.14	0.47
1:A:238:ASN:O	1:A:241:GLU:N	2.48	0.47
1:B:182:SER:OG	1:B:183:ASP:OD1	2.31	0.47
1:B:227:MET:HE1	1:B:231:HIS:HE1	1.78	0.47
1:B:227:MET:CE	1:B:231:HIS:CE1	2.98	0.47
1:A:107:LEU:HD13	1:A:123:VAL:HG23	1.96	0.46
1:B:48:ILE:CD1	1:B:49:CYS:N	2.79	0.46
1:B:103:ARG:NH1	1:B:107:LEU:O	2.45	0.46
1:A:64:ARG:HA	1:A:64:ARG:HD3	1.51	0.46
1:B:99:PRO:HA	1:B:100:GLY:HA2	1.53	0.46
1:A:53:SER:O	1:A:53:SER:OG	2.30	0.46
1:A:37:PHE:HD2	1:A:63:ASN:C	2.23	0.46
1:A:35:GLU:C	1:A:37:PHE:H	2.22	0.46
1:A:150:PHE:CE2	1:A:174:ILE:HG22	2.51	0.46
1:B:27:THR:C	1:B:48:ILE:HD13	2.40	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:TYR:CD1	1:B:245:SER:HB3	2.50	0.46
1:B:77:LEU:HB3	1:B:82:ILE:HB	1.97	0.46
1:A:3:ASP:O	1:A:53:SER:HB2	2.16	0.46
1:A:78:LYS:HE3	1:A:94:GLU:CD	2.41	0.46
1:A:213:TYR:HA	1:A:237:VAL:HG23	1.98	0.46
1:B:39:LYS:N	1:B:39:LYS:CD	2.78	0.46
1:B:107:LEU:HD13	1:B:123:VAL:HG21	1.98	0.46
1:B:213:TYR:CE2	1:B:214:ARG:CD	2.99	0.46
1:B:234:TYR:HD1	1:B:245:SER:HB3	1.81	0.46
1:A:124:GLU:H	1:A:124:GLU:HG2	1.50	0.45
1:A:208:ARG:CG	1:A:208:ARG:NH1	2.79	0.45
1:B:131:CYS:HB3	1:B:132:PRO:HD2	1.99	0.45
1:B:162:TYR:CD2	1:B:190:GLU:CA	2.97	0.45
1:B:162:TYR:HE2	1:B:190:GLU:HB2	1.82	0.45
1:A:81:TYR:HA	1:A:84:GLN:HE21	1.80	0.45
1:A:214:ARG:HD3	1:A:214:ARG:HA	1.41	0.45
1:A:165:PHE:CD2	1:A:189:ARG:CD	2.99	0.45
1:A:230:GLU:HA	1:A:230:GLU:OE1	2.16	0.45
1:B:252:ARG:CD	1:B:253:GLY:HA3	2.46	0.45
1:B:48:ILE:HD13	1:B:49:CYS:H	1.80	0.45
1:A:236:THR:CG2	1:A:245:SER:HA	2.47	0.45
1:B:208:ARG:CG	1:B:208:ARG:NH1	2.79	0.45
1:B:71:ARG:O	1:B:72:LEU:HD23	2.16	0.45
1:B:227:MET:HE3	1:B:227:MET:HB2	1.72	0.45
1:A:219:TYR:CD1	1:A:249:PRO:CD	3.00	0.45
1:B:191:ILE:HD13	1:B:237:VAL:CG1	2.46	0.45
1:A:221:CYS:SG	1:A:227:MET:HA	2.56	0.44
1:B:226:THR:O	1:B:251:CYS:HA	2.17	0.44
1:B:78:LYS:HG2	1:B:96:GLU:HB3	1.99	0.44
1:B:107:LEU:HD13	1:B:123:VAL:CG2	2.47	0.44
1:B:131:CYS:HB3	1:B:132:PRO:CD	2.48	0.44
1:A:100:GLY:CA	1:A:129:LYS:HD2	2.47	0.44
1:B:227:MET:SD	1:B:231:HIS:CE1	3.04	0.44
1:B:236:THR:OG1	1:B:243:GLU:HB3	2.18	0.43
1:A:133:ASN:HD22	1:A:134:PRO:CD	2.27	0.43
1:A:175:SER:N	1:A:178:SER:O	2.48	0.43
1:B:111:LEU:HD23	1:B:111:LEU:HA	1.89	0.43
1:A:65:SER:HB2	1:A:87:PHE:C	2.44	0.43
1:A:77:LEU:HD13	1:A:95:TYR:CZ	2.53	0.43
1:A:103:ARG:NH1	1:A:107:LEU:O	2.51	0.43
1:A:160:THR:CG2	1:B:214:ARG:NH1	2.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ARG:HA	1:B:234:TYR:HD2	1.84	0.43
1:B:78:LYS:HE2	1:B:94:GLU:HG2	2.00	0.43
1:A:63:ASN:ND2	1:A:86:TYR:OH	2.46	0.43
1:B:154:ILE:HD11	2:B:1255:ACT:CH3	2.48	0.43
1:A:35:GLU:C	1:A:37:PHE:N	2.76	0.42
1:A:74:SER:O	1:A:98:ARG:HB2	2.19	0.42
1:A:252:ARG:CB	1:A:253:GLY:HA3	2.48	0.42
1:B:81:TYR:HA	1:B:84:GLN:HE21	1.80	0.42
1:B:226:THR:O	1:B:250:GLU:O	2.37	0.42
1:B:112:THR:H	1:B:120:SER:HG	1.67	0.42
1:B:248:PRO:O	1:B:249:PRO:O	2.37	0.42
1:B:77:LEU:HD12	1:B:77:LEU:HA	1.78	0.42
1:B:112:THR:HG22	1:B:113:CYS:N	2.33	0.42
1:A:178:SER:HB2	1:A:179:VAL:H	1.72	0.42
1:B:236:THR:O	1:B:237:VAL:HG23	2.19	0.42
1:A:112:THR:HG22	1:A:113:CYS:N	2.33	0.42
1:B:187:GLU:CD	1:B:189:ARG:HE	2.28	0.42
1:A:111:LEU:HD23	1:A:111:LEU:HA	1.89	0.42
1:A:133:ASN:ND2	1:A:134:PRO:HD2	2.28	0.42
1:A:103:ARG:NH1	1:A:109:PRO:HD3	2.35	0.42
1:A:161:GLY:HA2	1:A:237:VAL:HG11	2.02	0.42
1:A:175:SER:O	1:A:175:SER:OG	2.29	0.42
1:B:162:TYR:HD2	1:B:189:ARG:O	2.03	0.42
1:B:28:VAL:CG2	1:B:48:ILE:HG12	2.49	0.41
1:B:148:ILE:HG13	1:B:148:ILE:O	2.20	0.41
1:B:227:MET:CG	1:B:249:PRO:CB	2.94	0.41
1:A:148:ILE:O	1:A:148:ILE:HG13	2.20	0.41
1:B:225:PHE:HB3	1:B:251:CYS:HB3	2.03	0.41
1:B:238:ASN:C	1:B:239:ASN:CG	2.88	0.41
1:A:25:GLU:HA	1:A:49:CYS:SG	2.61	0.41
1:A:154:ILE:HD11	2:A:1255:ACT:CH3	2.48	0.41
1:B:17:LEU:O	1:B:18:GLU:HB2	2.20	0.41
1:B:234:TYR:CE1	1:B:236:THR:HG22	2.55	0.41
1:A:77:LEU:HD13	1:A:95:TYR:CE2	2.56	0.41
1:B:175:SER:HB3	1:B:180:GLN:CG	2.49	0.41
1:A:158:CYS:SG	1:A:164:LEU:HA	2.60	0.41
1:A:227:MET:CB	4:A:1259[A]:CL:CL	3.01	0.41
1:A:99:PRO:HA	1:A:100:GLY:HA2	1.53	0.41
1:A:252:ARG:NH2	1:A:254:CYS:CA	2.79	0.41
1:B:34:GLU:O	1:B:37:PHE:HB2	2.21	0.41
1:B:77:LEU:HD13	1:B:95:TYR:CZ	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ARG:NH2	1:A:107:LEU:O	2.54	0.41
1:A:199:ILE:CD1	1:A:251:CYS:SG	3.08	0.41
4:A:1258[A]:CL:CL	1:B:133:ASN:OD1	2.76	0.41
1:B:40:ILE:HB	1:B:43:GLU:HG3	2.02	0.41
1:B:227:MET:SD	1:B:249:PRO:CB	3.09	0.41
1:B:236:THR:CG2	1:B:245:SER:HA	2.51	0.41
1:B:252:ARG:HA	1:B:253:GLY:HA2	1.78	0.41
1:A:78:LYS:HB2	1:A:94:GLU:O	2.21	0.41
1:A:179:VAL:C	1:A:180:GLN:HG2	2.46	0.41
1:A:185:LEU:HD12	1:A:185:LEU:HA	1.77	0.41
1:B:158:CYS:SG	1:B:164:LEU:HA	2.61	0.41
1:B:201:ASN:C	1:B:222:ASN:ND2	2.79	0.40
1:B:239:ASN:HA	1:B:240:ASP:HA	1.75	0.40
1:A:201:ASN:C	1:A:222:ASN:ND2	2.79	0.40
1:A:160:THR:CG2	1:B:214:ARG:HH11	2.33	0.40
1:B:33:CYS:HB3	1:B:37:PHE:HB3	2.03	0.40
1:A:232:SER:O	1:B:141:GLN:NE2	2.54	0.40
1:A:252:ARG:HB3	1:A:253:GLY:HA3	2.04	0.40
1:B:25:GLU:HA	1:B:49:CYS:SG	2.62	0.40
1:B:227:MET:HG2	4:B:1258[A]:CL:CL	2.58	0.40
1:A:165:PHE:O	1:A:187:GLU:N	2.49	0.40
1:A:239:ASN:HA	1:A:240:ASP:HA	1.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	252/254 (99%)	218 (86%)	27 (11%)	7 (3%)	4	21
1	B	252/254 (99%)	222 (88%)	22 (9%)	8 (3%)	3	18
All	All	504/508 (99%)	440 (87%)	49 (10%)	15 (3%)	3	19

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	237	VAL
1	A	64	ARG
1	A	239	ASN
1	B	249	PRO
1	B	238	ASN
1	A	2	GLN
1	A	99	PRO
1	A	105	PRO
1	B	99	PRO
1	B	105	PRO
1	B	228	ILE
1	A	147	GLY
1	A	206	GLY
1	B	147	GLY
1	B	206	GLY

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	225/225 (100%)	179 (80%)	46 (20%)	1	7
1	B	225/225 (100%)	179 (80%)	46 (20%)	1	7
All	All	450/450 (100%)	358 (80%)	92 (20%)	1	7

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	23	PHE
1	A	25	GLU
1	A	29	ILE
1	A	32	LYS
1	A	39	LYS
1	A	43	GLU
1	A	44	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	47	VAL
1	A	50	LEU
1	A	64	ARG
1	A	65	SER
1	A	70	THR
1	A	76	SER
1	A	77	LEU
1	A	78	LYS
1	A	92	VAL
1	A	114	LEU
1	A	115	GLN
1	A	116	ASN
1	A	117	LEU
1	A	120	SER
1	A	121	THR
1	A	123	VAL
1	A	124	GLU
1	A	127	LYS
1	A	128	LYS
1	A	136	GLU
1	A	149	LEU
1	A	160	THR
1	A	167	SER
1	A	173	LEU
1	A	174	ILE
1	A	178	SER
1	A	185	LEU
1	A	207	GLU
1	A	208	ARG
1	A	210	HIS
1	A	214	ARG
1	A	217	VAL
1	A	223	LYS
1	A	232	SER
1	A	236	THR
1	A	238	ASN
1	A	245	SER
1	A	250	GLU
1	B	1	MET
1	B	23	PHE
1	B	25	GLU
1	B	29	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	32	LYS
1	B	36	SER
1	B	39	LYS
1	B	44	LYS
1	B	48	ILE
1	B	50	LEU
1	B	63	ASN
1	B	64	ARG
1	B	65	SER
1	B	67	GLU
1	B	77	LEU
1	B	92	VAL
1	B	114	LEU
1	B	115	GLN
1	B	116	ASN
1	B	117	LEU
1	B	120	SER
1	B	121	THR
1	B	123	VAL
1	B	124	GLU
1	B	136	GLU
1	B	149	LEU
1	B	160	THR
1	B	167	SER
1	B	174	ILE
1	B	175	SER
1	B	177	SER
1	B	180	GLN
1	B	187	GLU
1	B	207	GLU
1	B	208	ARG
1	B	210	HIS
1	B	217	VAL
1	B	223	LYS
1	B	227	MET
1	B	231	HIS
1	B	232	SER
1	B	234	TYR
1	B	236	THR
1	B	245	SER
1	B	250	GLU
1	B	254	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	73	ASN
1	A	84	GLN
1	A	133	ASN
1	A	159	ASN
1	A	180	GLN
1	A	198	GLN
1	A	205	GLN
1	A	222	ASN
1	A	239	ASN
1	B	84	GLN
1	B	141	GLN
1	B	159	ASN
1	B	205	GLN
1	B	222	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](#)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 for Mogul analysis.

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
5	SO4	A	1260	-	4,4,4	0.46	0	6,6,6	0.75	0
2	ACT	A	1256	-	3,3,3	1.29	1 (33%)	3,3,3	0.75	0
6	GOL	B	1261	-	5,5,5	4.76	5 (100%)	5,5,5	6.08	3 (60%)
2	ACT	B	1255	-	3,3,3	1.29	1 (33%)	3,3,3	0.77	0
6	GOL	B	1262	-	5,5,5	4.78	5 (100%)	5,5,5	6.08	3 (60%)
2	ACT	A	1255	-	3,3,3	1.28	1 (33%)	3,3,3	0.77	0
2	ACT	B	1256	-	3,3,3	1.34	1 (33%)	3,3,3	0.75	0
5	SO4	B	1260	-	4,4,4	0.46	0	6,6,6	0.75	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
6	GOL	B	1262	-	-	3/4/4/4	-
6	GOL	B	1261	-	-	3/4/4/4	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1262	GOL	C3-C2	-7.99	1.21	1.51
6	B	1261	GOL	C3-C2	-7.97	1.21	1.51
6	B	1262	GOL	O1-C1	4.57	1.61	1.42
6	B	1261	GOL	O1-C1	4.56	1.61	1.42
6	B	1262	GOL	O3-C3	3.44	1.56	1.42
6	B	1261	GOL	O3-C3	3.42	1.56	1.42
6	B	1262	GOL	C1-C2	-3.05	1.40	1.51
6	B	1261	GOL	C1-C2	-3.04	1.40	1.51
6	B	1262	GOL	O2-C2	-2.89	1.35	1.43
6	B	1261	GOL	O2-C2	-2.82	1.35	1.43
2	B	1256	ACT	O-C	2.24	1.32	1.22
2	A	1256	ACT	O-C	2.17	1.31	1.22
2	B	1255	ACT	O-C	2.14	1.31	1.22
2	A	1255	ACT	O-C	2.13	1.31	1.22

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1262	GOL	O3-C3-C2	11.12	160.45	110.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1261	GOL	O3-C3-C2	11.12	160.45	110.38
6	B	1261	GOL	O2-C2-C3	6.97	138.03	109.18
6	B	1262	GOL	O2-C2-C3	6.94	137.91	109.18
6	B	1262	GOL	O1-C1-C2	3.44	125.85	110.38
6	B	1261	GOL	O1-C1-C2	3.44	125.85	110.38

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1261	GOL	C1-C2-C3-O3
6	B	1262	GOL	O1-C1-C2-C3
6	B	1262	GOL	C1-C2-C3-O3
6	B	1261	GOL	O1-C1-C2-O2
6	B	1262	GOL	O2-C2-C3-O3
6	B	1261	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1256	ACT	4	0
2	B	1255	ACT	2	0
2	A	1255	ACT	2	0
2	B	1256	ACT	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	254/254 (100%)	0.33	10 (3%) 43 24	31, 52, 78, 90	0
1	B	254/254 (100%)	0.19	7 (2%) 55 32	29, 48, 74, 84	0
All	All	508/508 (100%)	0.26	17 (3%) 49 28	29, 50, 75, 90	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	3.7
1	A	205	GLN	3.4
1	B	242	GLY	3.0
1	A	218	THR	2.9
1	A	217	VAL	2.5
1	B	218	THR	2.5
1	B	254	CYS	2.4
1	A	63	ASN	2.4
1	B	250	GLU	2.3
1	A	245	SER	2.2
1	B	243	GLU	2.2
1	A	191	ILE	2.2
1	B	209	ASP	2.2
1	A	226	THR	2.1
1	A	211	TYR	2.1
1	B	240	ASP	2.1
1	A	203	ILE	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
6	GOL	B	1261	6/6	0.37	0.27	75,75,75,75	0
2	ACT	A	1256	4/4	0.54	0.15	92,92,92,92	0
4	CL	B	1259[A]	1/1	0.68	0.45	47,47,47,47	1
5	SO4	B	1260	5/5	0.77	0.14	111,111,111,111	0
5	SO4	A	1260	5/5	0.80	0.12	107,107,107,107	0
6	GOL	B	1262	6/6	0.80	0.19	86,86,86,86	0
2	ACT	B	1256	4/4	0.87	0.10	33,34,34,34	0
4	CL	B	1258[A]	1/1	0.90	0.24	47,47,47,47	1
2	ACT	A	1255	4/4	0.91	0.10	51,51,51,51	0
2	ACT	B	1255	4/4	0.96	0.10	46,46,46,46	0
4	CL	A	1258[A]	1/1	0.96	0.16	73,73,73,73	1
3	PT	B	1257[A]	1/1	0.98	0.08	47,47,47,47	1
3	PT	A	1257[A]	1/1	0.98	0.07	73,73,73,73	1
4	CL	A	1259[A]	1/1	0.98	0.10	73,73,73,73	1

6.5 Other polymers [i](#)

There are no such residues in this entry.