



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 03:04 AM GMT

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 validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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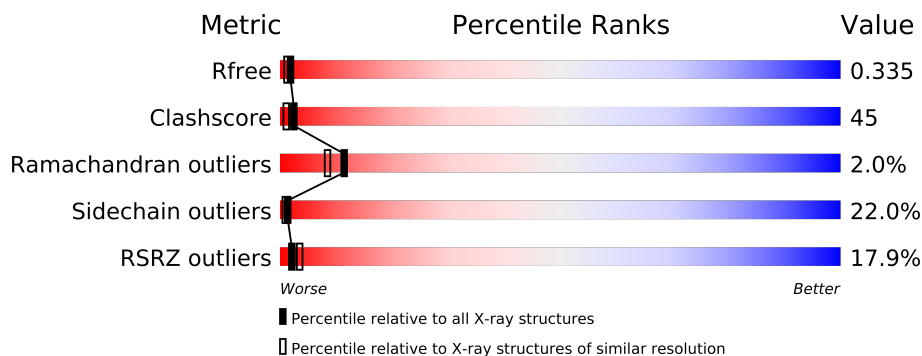
The following versions of software and data (see [references](#)) were used in the production of this report:

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

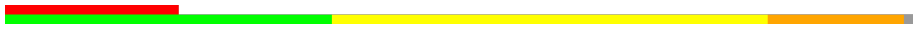

The reported resolution of this entry is 2.30 Å.

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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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  $\geq 3$ , 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	254	
1	B	254	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	GOL	A	1256	X	X
3	GOL	A	1257	X	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3956 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 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: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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

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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		

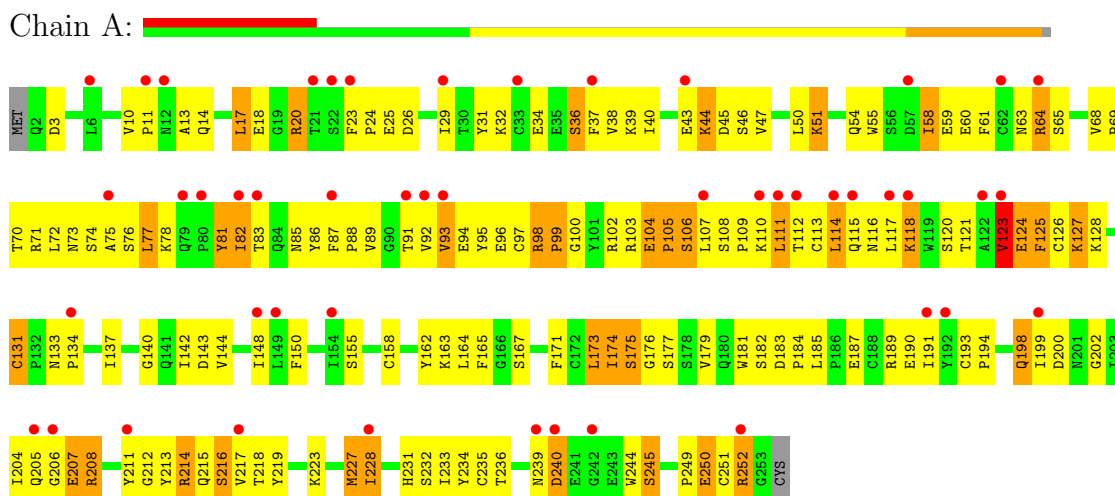
- Molecule 4 is water.

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

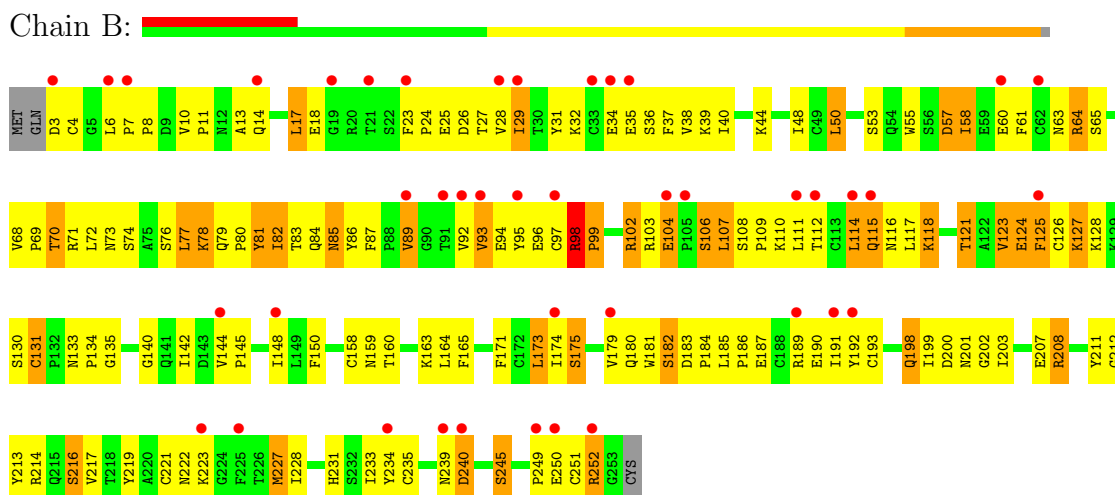
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.19 (at 2.80Å)	Xtriage
Refinement program	TNT 5F	Depositor
R, $R_{free}$	0.254 , (Not available) 0.294 , 0.335	Depositor DCC
$R_{free}$ test set	739 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.6	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 41.5	EDS
Estimated twinning fraction	0.000 for h-k,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 14559 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	3956	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities 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: 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 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	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

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 45.

All (346) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:252:ARG:HH21	1:B:252:ARG:CB	1.83	0.87
1:B:163:LYS:HG3	1:B:240:ASP:HB3	1.54	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:123:VAL:HG23	1:B:125:PHE:HD2	1.54	0.72
1:A:208:ARG:HG2	1:A:208:ARG:HH11	1.55	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:207:GLU:HG2	1:A:208:ARG:H	1.56	0.71
1:A:89:VAL:HG13	1:A:113:CYS:O	1.90	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:B:227:MET:CE	1:B:249:PRO:HB2	2.23	0.68
1:A:34:GLU:O	1:A:37:PHE:HB2	1.94	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:B:3:ASP:OD2	1:B:24:PRO:HA	1.95	0.67
1:A:175:SER:OG	1:A:176:GLY:N	2.25	0.67
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:198:GLN:HA	1:B:198:GLN:NE2	2.09	0.66
1:A:36:SER:HB3	1:A:117:LEU:CD1	2.26	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:93:VAL:HG23	1:A:111:LEU:HB2	1.79	0.64
1:A:103:ARG:NH2	1:A:107:LEU:O	2.31	0.64
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:131:CYS:O	1:A:148:ILE:HD12	1.98	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:B:148:ILE:HG22	1:B:181:TRP:HZ2	1.65	0.62
1:A:10:VAL:HG23	1:A:31:TYR:CE1	2.35	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
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:B:76:SER:O	1:B:96:GLU:HG2	2.03	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:133:ASN:OD1	1:A:134:PRO:HD2	2.03	0.59
1:B:93:VAL:HG23	1:B:111:LEU:HB2	1.85	0.59
1:A:14:GLN:OE1	1:A:14:GLN:HA	2.02	0.59
1:A:36:SER:HB3	1:A:117:LEU:HD13	1.83	0.59
1:A:68:VAL:HG12	1:A:69:PRO:HD2	1.84	0.58
1:A:17:LEU:O	1:A:18:GLU:HB2	2.03	0.58
1:B:163:LYS:HE3	1:B:165:PHE:CE1	2.38	0.58
1:A:171:PHE:HB3	1:A:173:LEU:CD1	2.33	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:B:228:ILE:N	1:B:250:GLU:O	2.36	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: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:40:ILE:HD11	1:A:63:ASN:HB2	1.87	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:240:ASP:N	1:B:240:ASP:OD1	2.38	0.56
1:B:199:ILE:HD12	1:B:202:GLY:HA3	1.87	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:N	1:B:72:LEU:HD23	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
1:B:81:TYR:CD2	1:B:93:VAL:HA	2.42	0.55
1:B:34:GLU:O	1:B:37:PHE:HB2	2.06	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:219:TYR:CD1	1:B:249:PRO:HD2	2.43	0.54
1:A:40:ILE:HD12	1:A:61:PHE:O	2.08	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:HG3	1:B:102:ARG:O	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:B:74:SER:C	1:B:98:ARG:HG3	2.30	0.52
1:A:140:GLY:HA2	1:A:158:CYS:HA	1.92	0.52
1:A:55:TRP:HB2	3:A:1256:GOL:H12	1.91	0.51
1:B:165:PHE:CE2	1:B:189:ARG:HB2	2.46	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:A:234:TYR:O	1:A:245:SER:HB3	2.11	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:B:107:LEU:CD1	1:B:123:VAL:HB	2.42	0.50
1:A:36:SER:HB3	1:A:117:LEU:HD11	1.92	0.50
1:B:216:SER:HB2	1:B:234:TYR:CD1	2.46	0.50
1:B:201:ASN:O	1:B:222:ASN:ND2	2.44	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:228:ILE:HG13	1:B:252:ARG:HB2	1.94	0.50
1:B:114:LEU:HB2	1:B:118:LYS:O	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:191:ILE:HD13	1:B:240:ASP:CA	2.37	0.49
1:A:77:LEU:HD13	1:A:95:TYR:CE2	2.46	0.49
1:B:200:ASP:O	1:B:201:ASN:HB2	2.12	0.49
1:B:183:ASP:HB3	1:B:184:PRO:HD2	1.95	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:200:ASP:O	1:B:251:CYS:HB2	2.13	0.49
1:B:36:SER:HB3	1:B:117:LEU:CD1	2.43	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:B:82:ILE:HG23	1:B:83:THR:HG23	1.95	0.47
1:A:107:LEU:HD23	1:A:107:LEU:N	2.25	0.47
1:A:40:ILE:CG2	1:A:43:GLU:HG3	2.44	0.47
1:A:13:ALA:HB1	1:A:31:TYR:HB3	1.97	0.47
1:B:140:GLY:HA2	1:B:158:CYS:HA	1.96	0.47
1:B:203:ILE:HA	4:B:2021:HOH:O	2.14	0.47
1:A:11:PRO:HB2	1:A:60:GLU:OE2	2.15	0.47
1:A:163:LYS:HE3	1:A:165:PHE:CE1	2.49	0.47
1:B:97:CYS:SG	1:B:103:ARG:HG2	2.55	0.47
1:A:198:GLN:CA	1:A:198:GLN:NE2	2.77	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
1:B:165:PHE:HE2	1:B:189:ARG:HB2	1.78	0.46
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:123:VAL:HG23	1:B:125:PHE:CD2	2.43	0.46
1:B:79:GLN:OE1	1:B:82:ILE:HG22	2.15	0.46
1:A:228:ILE:HA	1:B:145:PRO:O	2.14	0.46
1:A:217:VAL:HG13	1:A:217:VAL:O	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:45:ASP:HB3	1:A:61:PHE:CE2	2.50	0.46
1:B:130:SER:C	1:B:179:VAL:HG21	2.36	0.46
1:A:208:ARG:CB	1:A:211:TYR:CZ	2.98	0.46
1:A:185:LEU:HD12	1:A:185:LEU:HA	1.78	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:194:PRO:O	1:A:244:TRP:NE1	2.41	0.46
1:B:219:TYR:CD1	1:B:249:PRO:CD	2.98	0.46
1:A:204:ILE:HG13	1:A:219:TYR:CE2	2.51	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:99:PRO:HA	1:A:100:GLY:HA2	1.53	0.45
1:A:112:THR:CG2	1:A:113:CYS:N	2.79	0.45
1:B:69:PRO:HD3	1:B:87:PHE:CE1	2.52	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:A:198:GLN:CA	1:A:198:GLN:HE21	2.29	0.45
1:A:76:SER:O	1:A:96:GLU:HG2	2.16	0.45
1:B:252:ARG:NH2	1:B:252:ARG:CB	2.59	0.45
1:B:159:ASN:ND2	4:B:2020:HOH:O	2.47	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:61:PHE:N	1:A:61:PHE:CD1	2.85	0.44
1:A:127:LYS:HD2	1:A:127:LYS:HA	1.40	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:250:GLU:CD	1:A:252:ARG:HH22	2.15	0.44
1:A:104:GLU:OE2	1:A:105:PRO:HD2	2.18	0.44
1:A:71:ARG:C	1:A:72:LEU:HD23	2.38	0.44
1:A:214:ARG:HA	1:A:214:ARG:HD3	1.58	0.44
1:B:135:GLY:O	1:B:142:ILE:HD12	2.17	0.44
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:B:96:GLU:O	1:B:96:GLU:HG3	2.17	0.44
1:B:199:ILE:HD12	1:B:202:GLY:CA	2.47	0.44
1:A:44:LYS:HB2	1:A:44:LYS:HE2	1.38	0.44
1:B:10:VAL:HA	1:B:11:PRO:HD3	1.90	0.44
1:A:148:ILE:CG2	1:A:181:TRP:HZ2	2.31	0.44
1:B:77:LEU:HD13	1:B:95:TYR:CZ	2.53	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:124:GLU:OE2	1:B:127:LYS:HE2	2.17	0.44
1:A:97:CYS:SG	1:A:103:ARG:HG2	2.57	0.43
1:A:207:GLU:CG	1:A:208:ARG:N	2.81	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:B:77:LEU:CD1	1:B:95:TYR:CE2	3.01	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: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:B:208:ARG:NH1	1:B:208:ARG:HG3	2.34	0.43
1:A:183:ASP:HB3	1:A:184:PRO:HD2	2.00	0.43
1:A:217:VAL:CG1	1:A:217:VAL:O	2.67	0.43
1:A:123:VAL:HG23	1:A:125:PHE:HD2	1.83	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:B:199:ILE:HD11	1:B:202:GLY:HA3	2.01	0.42
1:A:213:TYR:HE1	2:A:1254:SO4:O3	2.02	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:20:ARG:H	1:A:20:ARG:HG3	1.67	0.42
1:A:208:ARG:CG	1:A:208:ARG:HH11	2.24	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:98:ARG:HA	1:B:99:PRO:HD3	1.75	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: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
1:A:123:VAL:HG23	1:A:125:PHE:CD2	2.55	0.41
1:B:74:SER:OG	1:B:126:CYS:HB2	2.20	0.41
1:A:38:VAL:HG12	1:A:86:TYR:CD2	2.55	0.41
1:B:221:CYS:SG	1:B:227:MET:HE3	2.60	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:133:ASN:HA	1:B:134:PRO:HD3	1.94	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:68:VAL:HA	1:B:87:PHE:CE1	2.56	0.41
1:B:231:HIS:CD2	1:B:231:HIS:H	2.37	0.41
1:A:55:TRP:CD1	3:A:1256:GOL:C2	2.99	0.41
1:B:58:ILE:O	1:B:58:ILE:HG23	2.20	0.41
1:A:55:TRP:H	3:A:1256:GOL:C1	2.28	0.41
1:A:198:GLN:OE1	1:A:204:ILE:HD12	2.21	0.41
1:A:162:TYR:CD2	1:A:190:GLU:HA	2.55	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:B:227:MET:HG3	1:B:228:ILE:N	2.35	0.41
1:A:114:LEU:CD1	1:A:114:LEU:N	2.83	0.41
1:A:58:ILE:O	1:A:58:ILE:HG23	2.21	0.40
1:B:23:PHE:CD2	1:B:55:TRP:HZ2	2.39	0.40
1:A:39:LYS:HA	1:A:61:PHE:O	2.21	0.40
1:A:174:ILE:HA	1:A:179:VAL:HA	2.02	0.40
1:B:4:CYS:SG	1:B:53:SER:HA	2.61	0.40
1:B:185:LEU:HA	1:B:185:LEU:HD12	1.89	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:B:106:SER:O	1:B:107:LEU:HD23	2.22	0.40
1:A:227:MET:HE3	1:B:144:VAL:HG11	2.03	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	Distance(Å)	Clash(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%)	11	8
1	B	249/254 (98%)	222 (89%)	22 (9%)	5 (2%)	11	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	499/508 (98%)	439 (88%)	50 (10%)	10 (2%)	11	8

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	1
1	B	222/225 (99%)	176 (79%)	46 (21%)	2	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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	0.62	0	6,6,6	0.70	0
2	SO4	A	1255	-	4,4,4	0.70	0	6,6,6	0.73	0
3	GOL	A	1256	-	5,5,5	4.55	5 (100%)	5,5,5	5.65	3 (60%)
3	GOL	A	1257	-	5,5,5	4.51	5 (100%)	5,5,5	5.71	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
2	SO4	A	1254	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1255	-	-	0/0/0/0	0/0/0/0
3	GOL	A	1256	-	-	0/4/4/4	0/0/0/0
3	GOL	A	1257	-	-	0/4/4/4	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1256	GOL	C3-C2	-7.50	1.21	1.52
3	A	1257	GOL	C3-C2	-7.44	1.21	1.52
3	A	1256	GOL	O1-C1	4.47	1.61	1.42
3	A	1257	GOL	O1-C1	4.41	1.61	1.42
3	A	1256	GOL	O3-C3	3.38	1.57	1.42
3	A	1257	GOL	O3-C3	3.30	1.56	1.42
3	A	1257	GOL	C1-C2	-2.97	1.40	1.52
3	A	1256	GOL	C1-C2	-2.90	1.40	1.52
3	A	1256	GOL	O2-C2	-2.75	1.35	1.43
3	A	1257	GOL	O2-C2	-2.72	1.35	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1257	GOL	O3-C3-C2	10.42	160.53	109.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1256	GOL	O3-C3-C2	10.34	160.14	109.71
3	A	1257	GOL	O2-C2-C3	6.57	138.13	108.22
3	A	1256	GOL	O2-C2-C3	6.41	137.43	108.22
3	A	1256	GOL	O1-C1-C2	3.33	125.96	109.71
3	A	1257	GOL	O1-C1-C2	3.28	125.69	109.71

There are no chirality outliers.

There are no torsion outliers.

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	252/254 (99%)	1.19	48 (19%)	2 3	25, 61, 87, 99	0
1	B	251/254 (98%)	1.15	42 (16%)	2 4	27, 59, 85, 102	0
All	All	503/508 (99%)	1.17	90 (17%)	2 3	25, 60, 86, 102	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	LEU	6.1
1	B	240	ASP	5.9
1	A	240	ASP	5.7
1	B	3	ASP	4.9
1	B	7	PRO	4.6
1	B	239	ASN	4.5
1	B	179	VAL	4.1
1	A	112	THR	3.8
1	A	114	LEU	3.7
1	B	62	CYS	3.6
1	A	122	ALA	3.6
1	A	82	ILE	3.5
1	A	117	LEU	3.5
1	A	22	SER	3.5
1	B	105	PRO	3.4
1	B	249	PRO	3.4
1	A	239	ASN	3.3
1	A	148	ILE	3.3
1	B	33	CYS	3.3
1	B	23	PHE	3.3
1	B	250	GLU	3.2
1	B	34	GLU	3.2
1	A	21	THR	3.1
1	B	148	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	23	PHE	3.0
1	A	115	GLN	3.0
1	A	87	PHE	3.0
1	A	107	LEU	3.0
1	A	205	GLN	2.9
1	B	29	ILE	2.9
1	A	110	LYS	2.8
1	A	64	ARG	2.8
1	A	123	VAL	2.8
1	B	234	TYR	2.7
1	B	111	LEU	2.7
1	B	192	TYR	2.7
1	A	149	LEU	2.7
1	B	19	GLY	2.7
1	A	11	PRO	2.6
1	B	60	GLU	2.6
1	B	93	VAL	2.6
1	A	252	ARG	2.6
1	B	115	GLN	2.5
1	A	83	THR	2.5
1	B	91	THR	2.5
1	A	12	ASN	2.5
1	B	189	ARG	2.5
1	A	33	CYS	2.5
1	A	80	PRO	2.4
1	A	134	PRO	2.4
1	B	114	LEU	2.4
1	A	211	TYR	2.4
1	B	225	PHE	2.4
1	B	92	VAL	2.4
1	B	89	VAL	2.4
1	A	29	ILE	2.4
1	A	43	GLU	2.4
1	B	35	GLU	2.4
1	A	111	LEU	2.3
1	A	118	LYS	2.3
1	A	6	LEU	2.3
1	A	228	ILE	2.3
1	B	144	VAL	2.3
1	A	242	GLY	2.3
1	B	191	ILE	2.2
1	A	92	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	97	CYS	2.2
1	A	199	ILE	2.2
1	B	174	ILE	2.2
1	B	252	ARG	2.2
1	B	28	VAL	2.2
1	B	104	GLU	2.2
1	B	112	THR	2.2
1	B	125	PHE	2.1
1	A	217	VAL	2.1
1	A	37	PHE	2.1
1	A	75	ALA	2.1
1	A	79	GLN	2.1
1	A	91	THR	2.1
1	A	62	CYS	2.1
1	A	206	GLY	2.1
1	B	95	TYR	2.1
1	B	21	THR	2.1
1	A	154	ILE	2.1
1	A	191	ILE	2.1
1	A	93	VAL	2.0
1	A	192	TYR	2.0
1	B	223	LYS	2.0
1	A	57	ASP	2.0
1	B	14	GLN	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	1256	6/6	0.51	8.17	96,96,96,96	0
3	GOL	A	1257	6/6	0.36	6.35	85,85,85,85	0
2	SO4	A	1254	5/5	0.13	-2.37	50,50,50,50	0
2	SO4	A	1255	5/5	0.16	-3.12	75,75,75,76	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.