Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2023 – 02:33 am GMT

PDB ID	:	1OJY
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	:	2003-07-16
Resolution	:	2.60 Å(reported)

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

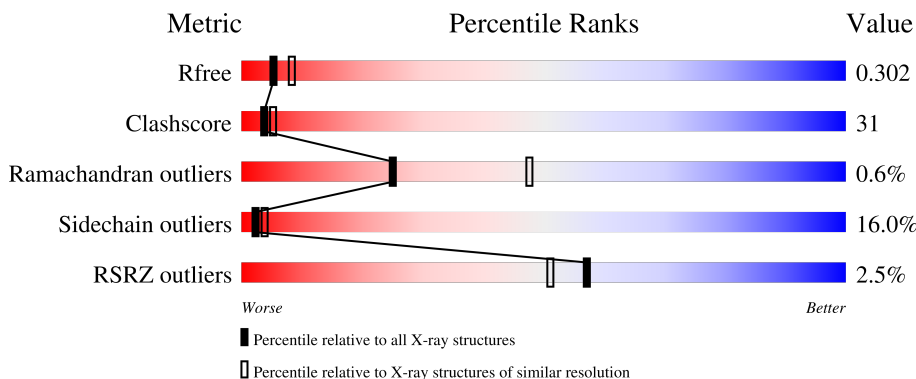|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 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	Percentile Ranks	Value
Rfree		0.302
Clashscore		31
Ramachandran outliers		0.6%
Sidechain outliers		16.0%
RSRZ outliers		2.5%

Worse — *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	3% — 52% 39% 8% ·
1	B	254	3% — 53% 37% 9%
1	C	254	3% — 48% 42% 9%
1	D	254	% — 50% 41% 8%

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	1254	-	-	X	-
2	ACT	B	1255	-	-	X	-
2	ACT	C	1256	-	-	X	-
2	ACT	D	1256	-	-	X	-
3	GOL	B	1256	-	X	-	-
3	GOL	C	1255	-	X	-	-
3	GOL	C	1258	-	X	-	X
3	GOL	D	1257	-	X	X	X
3	GOL	D	1258	-	X	X	X
3	GOL	D	1259	-	X	-	-
4	SO4	C	1254	-	-	X	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 8050 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	253	Total	C	N	O	S	0	0	0
			1961	1229	329	385	18			
1	C	253	Total	C	N	O	S	0	0	0
			1963	1231	329	385	18			
1	D	253	Total	C	N	O	S	0	0	0
			1961	1229	329	385	18			

There are 4 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
C	48	ILE	THR	SEE REMARK 999	UNP P08174
D	48	ILE	THR	SEE REMARK 999	UNP P08174

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

ACT

OXT

O^-

C

CH3

O

O

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

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

GOL

C3

OH O3

C1   C2

HO
O1

OH
O2

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
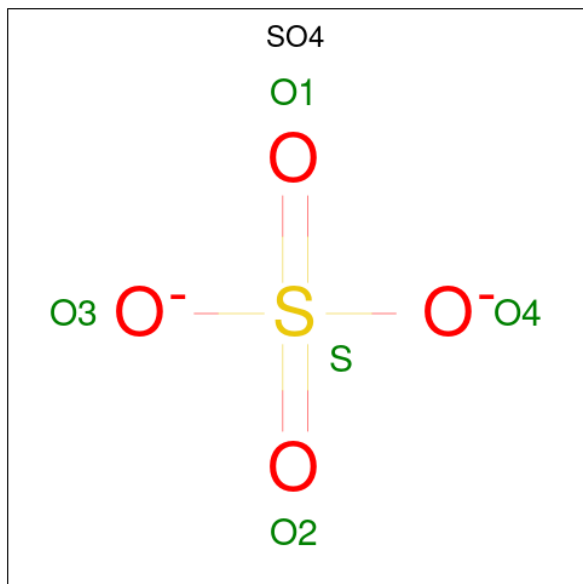
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total 5	O 4	S 1	0	0
4	C	1	Total 5	O 4	S 1	0	0
4	D	1	Total 5	O 4	S 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	25	Total 25	O 25	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	40	Total O 40 40		0	0
5	C	36	Total O 36 36		0	0
5	D	42	Total O 42 42		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.

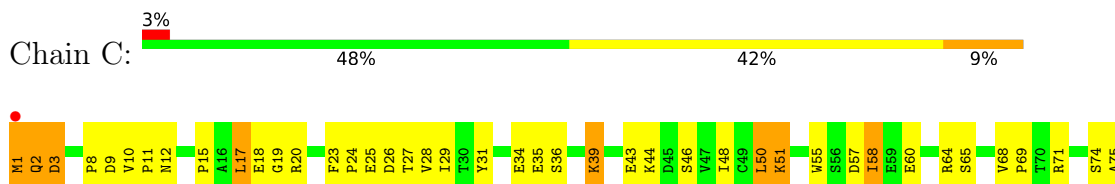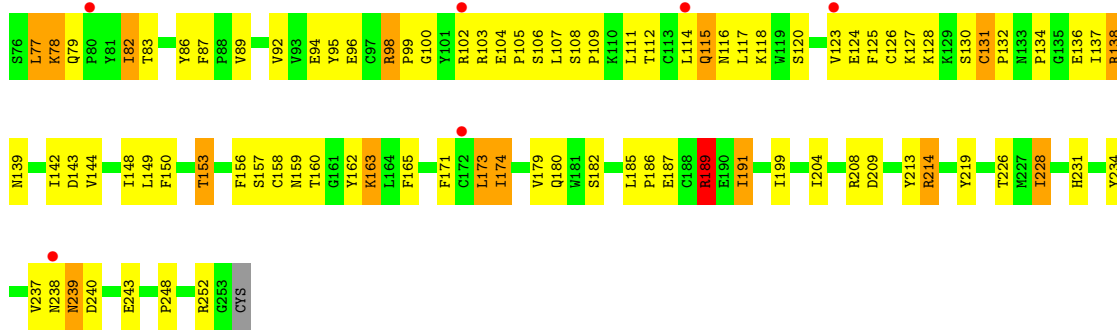- Molecule 1: COMPLEMENT DECAY-ACCELERATING FACTOR
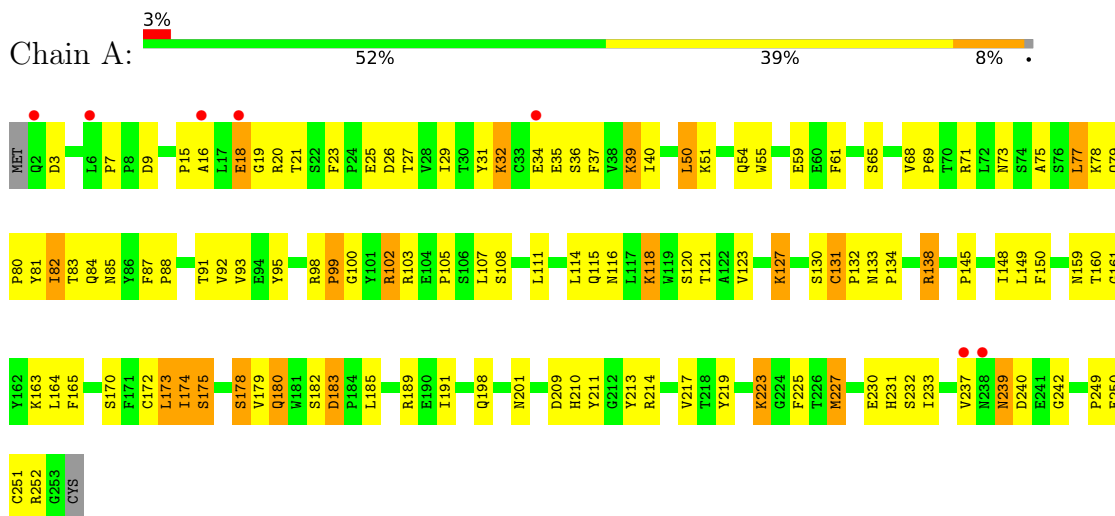
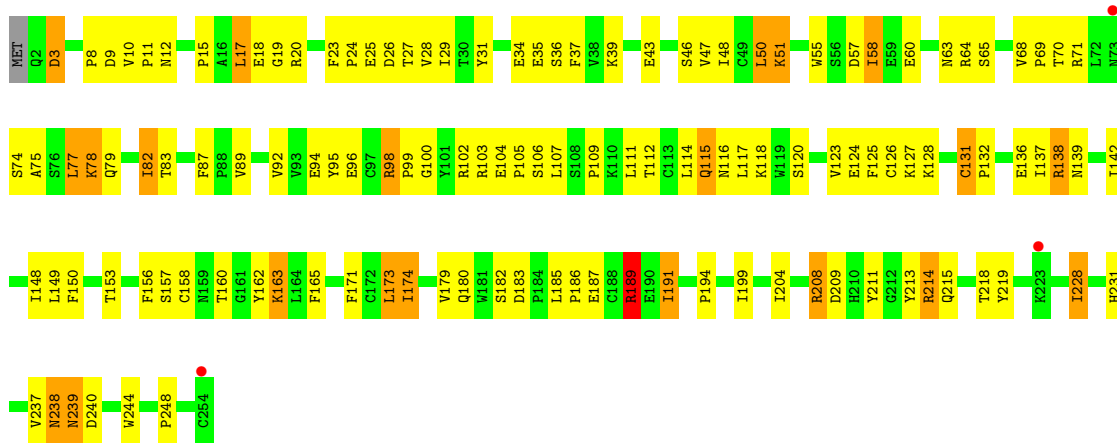Chain A:

- Molecule 1: COMPLEMENT DECAY-ACCELERATING FACTOR

Chain B:

- Molecule 1: COMPLEMENT DECAY-ACCELERATING FACTOR

Chain C:

• Molecule 1: COMPLEMENT DECAY-ACCELERATING FACTOR

Chain D:
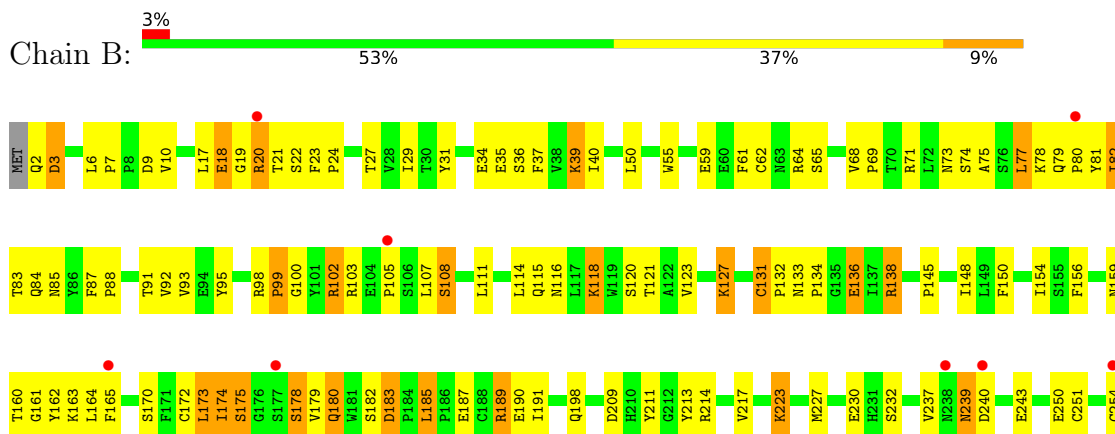
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	51.83Å 78.69Å 80.90Å 72.70° 79.38° 81.70°	Depositor
Resolution (Å)	16.00 – 2.60 15.99 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.3 (16.00-2.60) 94.4 (15.99-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.55 (at 2.58Å)	Xtriage
Refinement program	TNT 5F	Depositor
R, R_{free}	0.254 , (Not available) 0.251 , 0.302	Depositor DCC
R_{free} test set	1722 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	39.2	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.0	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8050	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 76.10 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1117e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: ACT, SO4, GOL

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	0.37	1/2008 (0.0%)	0.51	0/2731
1	B	0.34	0/2014	0.51	0/2739
1	C	0.32	0/2016	0.48	0/2741
1	D	0.31	0/2014	0.47	1/2739 (0.0%)
All	All	0.34	1/8052 (0.0%)	0.49	1/10950 (0.0%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	242	GLY	C-O	-5.08	1.15	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	238	ASN	N-CA-C	-5.31	96.66	111.00

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 (i)

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	109	0
1	B	1961	0	1855	111	0
1	C	1963	0	1862	143	0
1	D	1961	0	1855	138	0
2	A	4	0	3	4	0
2	B	4	0	3	5	0
2	C	4	0	3	3	0
2	D	4	0	3	2	0
3	B	6	0	4	0	0
3	C	12	0	8	4	0
3	D	18	0	12	10	0
4	C	10	0	0	2	0
4	D	5	0	0	0	0
5	A	25	0	0	6	0
5	B	40	0	0	9	1
5	C	36	0	0	10	0
5	D	42	0	0	4	1
All	All	8050	0	7458	478	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 31.

All (478) 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:189:ARG:HH11	1:B:189:ARG:HB3	1.16	1.11
1:D:157:SER:HA	3:D:1257:GOL:H12	1.33	1.05
1:A:223:LYS:HE3	1:A:223:LYS:HA	1.33	1.05
1:B:223:LYS:HA	1:B:223:LYS:HE3	1.33	1.04
1:A:163:LYS:HD3	1:A:165:PHE:HE1	1.22	1.02
1:B:163:LYS:HD3	1:B:165:PHE:HE1	1.23	1.01
1:B:214:ARG:HH11	1:D:238:ASN:ND2	1.63	0.95
1:B:20:ARG:HG2	1:B:20:ARG:HH21	1.30	0.95
1:A:214:ARG:HH11	1:C:238:ASN:ND2	1.64	0.94
1:B:150:PHE:CE2	1:B:174:ILE:HG22	2.03	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:PHE:CE2	1:A:174:ILE:HG22	2.03	0.93
1:D:18:GLU:HG3	1:D:19:GLY:HA2	1.50	0.91
1:B:154:ILE:HD11	2:B:1255:ACT:H3	1.53	0.90
1:A:163:LYS:HD3	1:A:165:PHE:CE1	2.06	0.90
1:B:163:LYS:HD3	1:B:165:PHE:CE1	2.06	0.90
1:B:154:ILE:HD11	2:B:1255:ACT:CH3	2.04	0.88
1:B:7:PRO:HG3	1:B:29:ILE:HD13	1.52	0.88
1:D:69:PRO:HG2	1:D:77:LEU:HD21	1.56	0.88
1:C:69:PRO:HG2	1:C:77:LEU:HD21	1.56	0.88
1:A:16:ALA:HB2	1:A:32:LYS:HE2	1.55	0.87
1:A:214:ARG:NH2	1:C:160:THR:HG23	1.90	0.86
1:B:189:ARG:HB3	1:B:189:ARG:NH1	1.90	0.85
1:B:150:PHE:HE2	1:B:174:ILE:HG22	1.42	0.85
1:C:44:LYS:O	5:C:2009:HOH:O	1.94	0.84
1:A:191:ILE:HD12	1:A:237:VAL:CG1	2.09	0.83
1:A:150:PHE:HE2	1:A:174:ILE:HG22	1.42	0.83
1:B:150:PHE:HB2	1:B:179:VAL:HG11	1.59	0.83
1:B:191:ILE:HD12	1:B:237:VAL:CG1	2.09	0.83
1:A:150:PHE:HB2	1:A:179:VAL:HG11	1.59	0.82
1:B:29:ILE:HD12	1:B:55:TRP:CH2	2.14	0.81
1:A:131:CYS:HB2	1:A:148:ILE:O	1.81	0.81
1:C:78:LYS:HD2	1:C:96:GLU:HB3	1.64	0.80
1:D:78:LYS:HD2	1:D:96:GLU:HB3	1.64	0.80
1:B:7:PRO:CG	1:B:29:ILE:HD13	2.11	0.79
1:C:18:GLU:HG3	1:C:19:GLY:HA2	1.65	0.78
1:B:20:ARG:HG2	1:B:20:ARG:NH2	1.93	0.78
1:C:107:LEU:HD12	1:C:124:GLU:O	1.84	0.78
1:B:214:ARG:HH11	1:D:238:ASN:CG	1.88	0.77
1:D:107:LEU:HD12	1:D:124:GLU:O	1.84	0.77
1:B:7:PRO:HD3	1:B:23:PHE:CE2	2.19	0.77
1:B:189:ARG:HH11	1:B:189:ARG:CB	1.96	0.76
1:B:173:LEU:HD22	1:B:182:SER:HB3	1.67	0.76
1:A:173:LEU:HD22	1:A:182:SER:HB3	1.67	0.75
1:A:237:VAL:O	1:A:237:VAL:HG12	1.87	0.75
1:C:102:ARG:HG3	1:C:102:ARG:HH11	1.50	0.75
1:D:102:ARG:HG3	1:D:102:ARG:HH11	1.49	0.74
1:B:237:VAL:HG12	1:B:237:VAL:O	1.87	0.74
1:C:103:ARG:O	1:C:105:PRO:HD3	1.88	0.74
1:A:16:ALA:HB2	1:A:32:LYS:CE	2.16	0.74
1:B:131:CYS:HB2	1:B:148:ILE:O	1.87	0.74
1:B:80:PRO:HG2	1:B:84:GLN:OE1	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:GLU:HG3	1:D:19:GLY:CA	2.18	0.73
1:D:103:ARG:O	1:D:105:PRO:HD3	1.87	0.73
1:C:39:LYS:HG3	5:C:2008:HOH:O	1.89	0.73
1:A:80:PRO:HG2	1:A:84:GLN:OE1	1.89	0.72
1:B:36:SER:O	1:B:64:ARG:HA	1.89	0.72
1:C:69:PRO:HD3	1:C:87:PHE:CE1	2.24	0.71
1:A:69:PRO:HG2	1:A:77:LEU:HD21	1.71	0.71
1:B:145:PRO:O	1:D:228:ILE:HG23	1.90	0.71
1:A:77:LEU:HD13	1:A:95:TYR:CE2	2.26	0.71
1:A:165:PHE:CZ	1:A:189:ARG:HD2	2.26	0.71
1:B:77:LEU:HD13	1:B:95:TYR:CE2	2.26	0.71
1:D:69:PRO:HD3	1:D:87:PHE:CE1	2.24	0.71
1:B:161:GLY:C	1:B:191:ILE:HG13	2.10	0.71
1:B:6:LEU:O	5:B:2001:HOH:O	2.09	0.71
1:B:69:PRO:HG2	1:B:77:LEU:HD21	1.71	0.71
1:C:171:PHE:HB3	1:C:173:LEU:CD1	2.21	0.71
1:D:157:SER:CA	3:D:1257:GOL:H12	2.15	0.70
1:D:171:PHE:HB3	1:D:173:LEU:CD1	2.21	0.70
1:C:82:ILE:HG23	1:C:83:THR:HG23	1.73	0.70
1:B:20:ARG:HH21	1:B:20:ARG:CG	2.03	0.70
1:B:23:PHE:CD2	1:B:55:TRP:HZ2	2.10	0.70
1:B:187:GLU:OE1	1:B:189:ARG:NH2	2.24	0.70
1:D:12:ASN:C	1:D:34:GLU:HG3	2.12	0.70
1:A:214:ARG:HH22	1:C:160:THR:HG23	1.57	0.70
1:D:82:ILE:HG23	1:D:83:THR:HG23	1.73	0.69
1:D:163:LYS:HB2	1:D:191:ILE:HD11	1.74	0.69
1:A:191:ILE:HD12	1:A:237:VAL:HG11	1.74	0.69
1:A:214:ARG:NH1	1:C:238:ASN:ND2	2.40	0.69
1:C:12:ASN:C	1:C:34:GLU:HG3	2.11	0.69
1:C:29:ILE:HD13	1:C:55:TRP:CH2	2.27	0.69
1:D:18:GLU:CG	1:D:19:GLY:HA2	2.22	0.69
1:D:29:ILE:HD13	1:D:55:TRP:CH2	2.27	0.69
1:B:7:PRO:HG3	1:B:29:ILE:CD1	2.22	0.69
1:B:34:GLU:O	1:B:37:PHE:HB2	1.93	0.69
1:B:191:ILE:HD12	1:B:237:VAL:HG11	1.75	0.69
1:B:20:ARG:NH2	1:B:22:SER:O	2.26	0.69
1:C:237:VAL:HG12	1:C:237:VAL:O	1.91	0.69
1:C:171:PHE:HB3	1:C:173:LEU:HD11	1.75	0.69
1:A:34:GLU:O	1:A:37:PHE:HB2	1.93	0.68
1:D:171:PHE:HB3	1:D:173:LEU:HD11	1.75	0.68
1:A:115:GLN:OE1	1:A:115:GLN:N	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:SER:HA	3:D:1257:GOL:C1	2.17	0.68
1:A:183:ASP:O	2:A:1254:ACT:H1	1.94	0.68
1:B:223:LYS:HA	1:B:223:LYS:CE	2.20	0.68
1:D:187:GLU:OE1	1:D:189:ARG:NE	2.27	0.68
1:D:237:VAL:HG12	1:D:237:VAL:O	1.93	0.68
1:C:165:PHE:CD1	1:C:189:ARG:HG2	2.29	0.68
1:D:109:PRO:HA	1:D:125:PHE:CD1	2.29	0.68
1:B:115:GLN:N	1:B:115:GLN:OE1	2.27	0.67
1:B:198:GLN:NE2	5:B:2033:HOH:O	2.27	0.67
1:B:161:GLY:O	1:B:191:ILE:HG13	1.95	0.67
1:C:102:ARG:HG3	1:C:102:ARG:NH1	2.10	0.67
1:A:223:LYS:HA	1:A:223:LYS:CE	2.20	0.67
1:C:187:GLU:OE1	1:C:189:ARG:NE	2.27	0.67
1:D:165:PHE:CD1	1:D:189:ARG:HG2	2.29	0.67
1:D:102:ARG:HG3	1:D:102:ARG:NH1	2.09	0.67
1:C:109:PRO:HA	1:C:125:PHE:CD1	2.29	0.67
1:B:133:ASN:OD1	1:B:134:PRO:HD2	1.95	0.67
1:D:189:ARG:HH21	1:D:189:ARG:HG3	1.60	0.67
1:A:214:ARG:NH2	1:C:160:THR:CG2	2.59	0.66
1:C:189:ARG:HH21	1:C:189:ARG:HG3	1.60	0.66
1:D:163:LYS:HB2	1:D:191:ILE:CD1	2.25	0.66
1:C:189:ARG:HG3	1:C:189:ARG:NH2	2.09	0.66
1:C:10:VAL:HG21	1:C:58:ILE:HD13	1.78	0.66
1:C:108:SER:O	5:C:2014:HOH:O	2.13	0.66
1:D:10:VAL:HG21	1:D:58:ILE:HD13	1.78	0.65
1:D:36:SER:O	1:D:64:ARG:HA	1.96	0.65
1:C:18:GLU:HG3	1:C:19:GLY:CA	2.27	0.65
1:B:23:PHE:HB3	1:B:27:THR:HG21	1.79	0.65
1:C:27:THR:HG22	1:C:29:ILE:HD12	1.77	0.65
1:A:198:GLN:NE2	5:A:2017:HOH:O	2.30	0.65
1:D:189:ARG:HG3	1:D:189:ARG:NH2	2.10	0.65
1:D:149:LEU:HB2	5:D:2026:HOH:O	1.96	0.65
1:B:160:THR:O	1:D:214:ARG:NH1	2.29	0.65
1:A:133:ASN:OD1	1:A:134:PRO:HD2	1.98	0.64
1:B:138:ARG:HH22	3:D:1259:GOL:H12	1.61	0.64
1:C:173:LEU:HD22	1:C:182:SER:HB3	1.79	0.64
1:D:27:THR:HG22	1:D:29:ILE:HD12	1.77	0.64
1:D:173:LEU:HD22	1:D:182:SER:HB3	1.79	0.64
1:C:18:GLU:CG	1:C:19:GLY:HA2	2.27	0.63
1:C:12:ASN:O	1:C:34:GLU:HG3	1.99	0.63
1:A:214:ARG:HH11	1:C:238:ASN:CG	2.02	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:PRO:CG	1:A:29:ILE:HD13	2.27	0.63
1:D:12:ASN:O	1:D:34:GLU:HG3	1.99	0.63
1:D:77:LEU:O	1:D:82:ILE:HD12	1.99	0.63
1:C:158:CYS:H	3:C:1258:GOL:C2	2.12	0.62
1:A:95:TYR:HE1	1:A:111:LEU:HD12	1.65	0.62
1:A:23:PHE:HB3	1:A:27:THR:HG21	1.82	0.62
1:C:77:LEU:O	1:C:82:ILE:HD12	1.99	0.62
1:C:17:LEU:HB2	1:C:18:GLU:HA	1.82	0.62
1:C:157:SER:HA	3:C:1258:GOL:H12	1.81	0.62
1:A:7:PRO:HG3	1:A:29:ILE:CD1	2.29	0.62
1:C:107:LEU:HD12	1:C:124:GLU:C	2.20	0.62
1:A:159:ASN:ND2	5:A:2015:HOH:O	2.28	0.61
1:C:163:LYS:HB2	1:C:191:ILE:CD1	2.30	0.61
1:D:92:VAL:HG22	1:D:112:THR:OG1	2.00	0.61
1:A:16:ALA:HB2	1:A:32:LYS:NZ	2.15	0.61
1:B:95:TYR:HE1	1:B:111:LEU:HD12	1.65	0.61
1:A:29:ILE:HD12	1:A:55:TRP:CH2	2.35	0.61
1:B:81:TYR:CD2	1:B:93:VAL:HG12	2.36	0.61
1:C:163:LYS:HB2	1:C:191:ILE:HD11	1.82	0.61
1:C:92:VAL:HG22	1:C:112:THR:OG1	2.00	0.61
1:D:213:TYR:O	1:D:214:ARG:HB2	2.00	0.61
1:A:81:TYR:CD2	1:A:93:VAL:HG12	2.36	0.61
1:C:213:TYR:O	1:C:214:ARG:HB2	2.00	0.60
1:A:7:PRO:HG3	1:A:29:ILE:HD13	1.83	0.60
1:D:107:LEU:HD12	1:D:124:GLU:C	2.20	0.60
1:A:213:TYR:CE2	1:A:214:ARG:HD2	2.37	0.59
1:B:213:TYR:CE2	1:B:214:ARG:HD2	2.37	0.59
1:D:15:PRO:HD3	3:D:1258:GOL:C1	2.33	0.59
1:B:35:GLU:O	1:B:36:SER:HB2	2.04	0.58
1:D:185:LEU:HD13	2:D:1256:ACT:H3	1.85	0.58
1:A:214:ARG:HH21	1:C:160:THR:CG2	2.16	0.58
1:D:116:ASN:ND2	1:D:118:LYS:HD2	2.19	0.58
1:C:116:ASN:ND2	1:C:118:LYS:HD2	2.19	0.57
1:C:157:SER:HA	3:C:1258:GOL:C1	2.34	0.57
1:C:213:TYR:HE1	4:C:1254:SO4:O3	1.87	0.57
1:B:154:ILE:HD11	2:B:1255:ACT:H2	1.84	0.57
1:C:17:LEU:CB	1:C:18:GLU:HA	2.34	0.57
1:A:35:GLU:O	1:A:36:SER:HB2	2.03	0.57
1:A:161:GLY:O	1:A:191:ILE:HG13	2.05	0.57
1:B:18:GLU:N	1:B:19:GLY:HA2	2.19	0.57
1:A:111:LEU:HD22	1:A:120:SER:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:LEU:HD13	1:D:95:TYR:CE2	2.40	0.57
1:A:161:GLY:C	1:A:191:ILE:HG13	2.25	0.57
1:C:77:LEU:HD13	1:C:95:TYR:CE2	2.40	0.56
1:D:17:LEU:HB2	1:D:18:GLU:HA	1.87	0.56
1:A:95:TYR:CE1	1:A:111:LEU:HD12	2.40	0.56
1:A:183:ASP:OD1	1:A:183:ASP:N	2.37	0.56
1:D:69:PRO:CG	1:D:77:LEU:HD21	2.34	0.56
1:D:104:GLU:HG3	1:D:107:LEU:HG	1.87	0.56
1:D:18:GLU:CA	1:D:20:ARG:H	2.18	0.56
1:B:183:ASP:N	1:B:183:ASP:OD1	2.37	0.56
1:B:95:TYR:CE1	1:B:111:LEU:HD12	2.40	0.56
1:B:111:LEU:HD22	1:B:120:SER:O	2.05	0.56
1:D:18:GLU:HA	1:D:20:ARG:H	1.71	0.56
1:D:131:CYS:HB2	1:D:148:ILE:O	2.06	0.56
1:C:39:LYS:NZ	5:C:2008:HOH:O	2.28	0.56
1:D:15:PRO:HD3	3:D:1258:GOL:H11	1.88	0.56
1:C:104:GLU:HG3	1:C:107:LEU:HG	1.87	0.55
1:A:145:PRO:O	1:C:228:ILE:HG23	2.06	0.55
1:D:82:ILE:CG2	1:D:83:THR:HG23	2.37	0.55
1:A:239:ASN:HD22	1:B:105:PRO:HG3	1.71	0.55
1:C:82:ILE:CG2	1:C:83:THR:HG23	2.37	0.55
1:A:227:MET:HE3	5:A:2025:HOH:O	2.06	0.55
1:C:69:PRO:CG	1:C:77:LEU:HD21	2.34	0.55
1:C:131:CYS:HB2	1:C:148:ILE:O	2.06	0.55
1:C:204:ILE:HG12	1:C:219:TYR:CE2	2.42	0.55
1:C:27:THR:HG22	1:C:29:ILE:CD1	2.37	0.55
1:B:214:ARG:NH1	1:D:238:ASN:ND2	2.45	0.54
1:D:29:ILE:O	1:D:46:SER:HB2	2.08	0.54
1:D:204:ILE:HG12	1:D:219:TYR:CE2	2.42	0.54
1:A:120:SER:HB2	5:A:2010:HOH:O	2.07	0.54
1:A:231:HIS:HD2	1:C:143:ASP:OD2	1.91	0.54
1:C:29:ILE:O	1:C:46:SER:HB2	2.08	0.54
1:C:106:SER:O	1:C:107:LEU:HD23	2.08	0.54
1:C:144:VAL:O	5:C:2017:HOH:O	2.18	0.54
1:D:106:SER:O	1:D:107:LEU:HD23	2.08	0.54
1:D:27:THR:HG22	1:D:29:ILE:CD1	2.37	0.54
1:C:17:LEU:HB2	1:C:18:GLU:CA	2.37	0.54
1:B:73:ASN:O	1:B:98:ARG:HD2	2.07	0.54
1:C:17:LEU:HB2	1:C:18:GLU:CB	2.38	0.54
1:A:73:ASN:O	1:A:98:ARG:HD2	2.07	0.53
1:C:25:GLU:O	1:C:26:ASP:HB2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:TYR:CE2	1:A:217:VAL:HG12	2.44	0.53
1:C:17:LEU:CA	1:C:18:GLU:HB2	2.39	0.53
1:B:102:ARG:HE	1:B:127:LYS:HE3	1.73	0.53
1:D:25:GLU:O	1:D:26:ASP:HB2	2.07	0.53
1:B:211:TYR:CE2	1:B:217:VAL:HG12	2.44	0.53
1:B:239:ASN:O	1:B:240:ASP:HB2	2.08	0.53
1:C:185:LEU:HD13	2:C:1256:ACT:H3	1.91	0.53
1:A:75:ALA:HB1	1:A:95:TYR:HB3	1.92	0.52
1:A:102:ARG:HE	1:A:127:LYS:HE3	1.73	0.52
1:A:160:THR:O	1:C:214:ARG:NH1	2.43	0.52
1:C:29:ILE:HD13	1:C:55:TRP:HH2	1.72	0.52
1:A:239:ASN:O	1:A:240:ASP:HB2	2.08	0.52
1:D:17:LEU:CA	1:D:18:GLU:HB2	2.40	0.52
1:B:75:ALA:HB1	1:B:95:TYR:HB3	1.92	0.52
1:D:123:VAL:HG22	5:D:2018:HOH:O	2.09	0.52
1:D:29:ILE:HD13	1:D:55:TRP:HH2	1.72	0.52
1:B:123:VAL:HG22	5:B:2019:HOH:O	2.10	0.52
1:C:189:ARG:HH21	1:C:189:ARG:CG	2.23	0.52
1:D:189:ARG:HH21	1:D:189:ARG:CG	2.23	0.52
1:A:175:SER:N	1:A:178:SER:O	2.36	0.52
1:C:17:LEU:CB	1:C:18:GLU:CA	2.88	0.52
1:D:165:PHE:CD1	1:D:189:ARG:CG	2.93	0.52
1:A:223:LYS:HE3	1:A:223:LYS:CA	2.21	0.51
1:D:132:PRO:HG2	1:D:180:GLN:OE1	2.11	0.51
1:C:64:ARG:NH2	1:C:115:GLN:O	2.41	0.51
1:C:132:PRO:HG2	1:C:180:GLN:OE1	2.11	0.51
1:C:137:ILE:HD12	1:C:142:ILE:HG12	1.92	0.51
1:C:165:PHE:CD1	1:C:189:ARG:CG	2.93	0.51
1:C:239:ASN:O	1:C:240:ASP:HB2	2.10	0.51
1:B:175:SER:N	1:B:178:SER:O	2.36	0.51
1:D:17:LEU:CB	1:D:18:GLU:HA	2.40	0.51
1:D:64:ARG:NH2	1:D:115:GLN:O	2.41	0.51
1:D:17:LEU:HB2	1:D:18:GLU:CB	2.41	0.51
1:D:124:GLU:OE2	1:D:124:GLU:N	2.44	0.51
1:C:89:VAL:CG2	1:C:117:LEU:HD23	2.41	0.50
1:C:214:ARG:NH2	4:C:1254:SO4:O1	2.45	0.50
1:D:137:ILE:HD12	1:D:142:ILE:HG12	1.93	0.50
1:B:145:PRO:HD2	5:B:2028:HOH:O	2.10	0.50
1:C:124:GLU:OE2	1:C:124:GLU:N	2.44	0.50
1:C:204:ILE:HB	5:C:2027:HOH:O	2.11	0.50
1:D:37:PHE:HA	1:D:63:ASN:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:VAL:CG2	1:D:117:LEU:HD23	2.41	0.50
1:A:159:ASN:ND2	1:C:234:TYR:CE1	2.80	0.50
1:A:165:PHE:CE1	1:A:189:ARG:HD2	2.47	0.50
1:B:77:LEU:HD13	1:B:95:TYR:CZ	2.46	0.50
1:B:237:VAL:CG1	1:B:237:VAL:O	2.60	0.50
1:D:17:LEU:HB2	1:D:18:GLU:CA	2.41	0.50
1:D:47:VAL:HA	5:D:2005:HOH:O	2.11	0.50
1:B:223:LYS:HE3	1:B:223:LYS:CA	2.21	0.50
1:B:174:ILE:HD13	1:B:174:ILE:O	2.12	0.49
1:B:17:LEU:HD22	1:B:23:PHE:HZ	1.77	0.49
1:D:239:ASN:O	1:D:240:ASP:HB2	2.12	0.49
1:A:77:LEU:HD13	1:A:95:TYR:CZ	2.46	0.49
1:A:174:ILE:HD13	1:A:174:ILE:O	2.12	0.49
1:A:191:ILE:HG21	1:A:237:VAL:HG13	1.94	0.49
1:B:191:ILE:HG21	1:B:237:VAL:HG13	1.94	0.49
1:D:162:TYR:HD2	1:D:189:ARG:O	1.94	0.49
1:A:15:PRO:HD3	1:A:31:TYR:CE1	2.48	0.49
1:C:156:PHE:CD1	1:C:186:PRO:HG3	2.48	0.49
1:A:39:LYS:O	1:A:39:LYS:HG2	2.12	0.49
1:C:162:TYR:HD2	1:C:189:ARG:O	1.94	0.49
1:D:18:GLU:HA	1:D:20:ARG:N	2.28	0.49
1:B:20:ARG:NH2	5:B:2003:HOH:O	2.45	0.49
1:C:102:ARG:O	1:C:127:LYS:N	2.45	0.49
1:C:153:THR:O	5:C:2018:HOH:O	2.19	0.49
1:B:39:LYS:O	1:B:39:LYS:HG2	2.12	0.49
1:D:156:PHE:CD1	1:D:186:PRO:HG3	2.48	0.49
1:C:17:LEU:HB2	1:C:18:GLU:CD	2.33	0.48
1:A:77:LEU:HB3	1:A:82:ILE:HD12	1.96	0.48
1:B:74:SER:OG	5:B:2016:HOH:O	2.10	0.48
1:B:77:LEU:HB3	1:B:82:ILE:HD12	1.96	0.48
1:C:138:ARG:O	1:C:139:ASN:HB2	2.14	0.48
1:A:210:HIS:CD2	5:A:2021:HOH:O	2.66	0.48
1:B:170:SER:CB	2:B:1255:ACT:H1	2.43	0.48
1:D:15:PRO:CD	3:D:1258:GOL:H12	2.42	0.48
1:A:170:SER:OG	2:A:1254:ACT:H1	2.14	0.48
1:D:138:ARG:O	1:D:139:ASN:HB2	2.14	0.48
1:D:199:ILE:HG21	1:D:248:PRO:HB2	1.96	0.48
1:C:78:LYS:HG3	1:C:94:GLU:O	2.14	0.48
1:D:78:LYS:HG3	1:D:94:GLU:O	2.14	0.48
1:D:104:GLU:O	1:D:107:LEU:N	2.40	0.48
1:C:68:VAL:HA	1:C:87:PHE:HE1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:VAL:HA	1:D:87:PHE:HE1	1.79	0.48
1:D:102:ARG:O	1:D:127:LYS:N	2.45	0.48
1:B:132:PRO:HG2	1:B:180:GLN:OE1	2.14	0.47
1:C:18:GLU:CA	1:C:20:ARG:H	2.27	0.47
1:C:226:THR:O	1:C:252:ARG:N	2.46	0.47
1:C:128:LYS:HD3	1:C:150:PHE:O	2.14	0.47
1:D:183:ASP:O	2:D:1256:ACT:OXT	2.32	0.47
1:B:69:PRO:HD3	1:B:87:PHE:CE1	2.49	0.47
1:A:69:PRO:HD3	1:A:87:PHE:CE1	2.50	0.47
1:D:17:LEU:CB	1:D:18:GLU:CA	2.92	0.47
1:D:75:ALA:HB2	1:D:126:CYS:SG	2.55	0.47
1:D:156:PHE:CE1	1:D:186:PRO:HD3	2.50	0.47
1:A:132:PRO:HG2	1:A:180:GLN:OE1	2.14	0.47
1:C:75:ALA:HB2	1:C:126:CYS:SG	2.55	0.47
1:A:51:LYS:HD2	5:A:2003:HOH:O	2.15	0.47
1:C:99:PRO:HA	1:C:100:GLY:HA2	1.54	0.47
1:B:3:ASP:OD2	1:B:24:PRO:HA	2.15	0.46
1:A:217:VAL:HG22	1:A:233:ILE:CG1	2.44	0.46
1:C:156:PHE:CE1	1:C:186:PRO:HD3	2.50	0.46
1:D:109:PRO:HA	1:D:125:PHE:CG	2.50	0.46
1:D:214:ARG:HD2	1:D:214:ARG:HA	1.44	0.46
1:B:156:PHE:HZ	2:B:1255:ACT:H2	1.81	0.46
1:C:106:SER:C	1:C:107:LEU:HD23	2.35	0.46
1:C:174:ILE:O	1:C:174:ILE:HD13	2.15	0.46
1:C:209:ASP:N	1:C:209:ASP:OD2	2.48	0.46
1:D:99:PRO:HA	1:D:100:GLY:HA2	1.54	0.46
1:D:106:SER:C	1:D:107:LEU:HD23	2.35	0.46
1:D:138:ARG:HA	1:D:138:ARG:HD3	1.40	0.46
1:D:174:ILE:HD13	1:D:174:ILE:O	2.16	0.46
1:C:109:PRO:HA	1:C:125:PHE:CG	2.50	0.46
1:D:64:ARG:HB3	1:D:117:LEU:HD11	1.98	0.46
1:D:209:ASP:OD2	1:D:209:ASP:N	2.48	0.46
1:A:237:VAL:CG1	1:A:237:VAL:O	2.59	0.45
1:A:138:ARG:HA	1:A:138:ARG:HD3	1.42	0.45
1:B:162:TYR:CD2	1:B:190:GLU:HA	2.51	0.45
1:D:15:PRO:HD3	3:D:1258:GOL:H12	1.96	0.45
1:A:191:ILE:CD1	1:A:240:ASP:HA	2.47	0.45
1:D:162:TYR:CD2	1:D:189:ARG:O	2.70	0.45
1:A:7:PRO:HG3	1:A:29:ILE:HD12	1.98	0.45
1:B:108:SER:O	5:B:2019:HOH:O	2.21	0.45
1:C:64:ARG:HB3	1:C:117:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:PRO:CD	3:D:1258:GOL:C1	2.94	0.45
1:C:1:MET:HG2	1:C:3:ASP:HB2	1.98	0.45
1:D:111:LEU:HD22	1:D:120:SER:O	2.17	0.45
1:A:77:LEU:HG	1:A:81:TYR:HB2	1.99	0.45
1:C:162:TYR:CD2	1:C:189:ARG:O	2.70	0.45
1:B:99:PRO:HA	1:B:100:GLY:HA2	1.54	0.45
1:C:111:LEU:HD22	1:C:120:SER:O	2.17	0.45
1:A:7:PRO:HG2	1:A:29:ILE:HD13	1.99	0.45
1:B:7:PRO:HD3	1:B:23:PHE:HE2	1.75	0.45
1:B:40:ILE:HG13	1:B:61:PHE:O	2.16	0.45
1:B:10:VAL:CG2	1:B:31:TYR:CE1	3.00	0.45
1:B:102:ARG:HH11	1:B:127:LYS:HE3	1.82	0.45
1:B:107:LEU:HB3	1:B:123:VAL:HG21	1.99	0.45
1:C:104:GLU:O	1:C:107:LEU:N	2.40	0.45
1:D:237:VAL:O	1:D:237:VAL:CG1	2.65	0.44
1:A:165:PHE:CE2	1:A:189:ARG:NH2	2.85	0.44
1:A:252:ARG:HH12	1:D:208:ARG:HE	1.65	0.44
1:B:191:ILE:CD1	1:B:240:ASP:HA	2.48	0.44
1:B:68:VAL:HG13	1:B:69:PRO:HD2	2.00	0.44
1:C:130:SER:HA	1:C:149:LEU:HD23	1.98	0.44
1:A:99:PRO:HA	1:A:100:GLY:HA2	1.54	0.44
1:A:107:LEU:HB3	1:A:123:VAL:HG21	1.99	0.44
1:C:123:VAL:O	1:C:125:PHE:HD2	2.00	0.44
1:A:40:ILE:HG13	1:A:61:PHE:O	2.16	0.44
1:B:77:LEU:HG	1:B:81:TYR:HB2	1.99	0.44
1:B:138:ARG:HA	1:B:138:ARG:HD3	1.42	0.44
1:A:102:ARG:HH11	1:A:127:LYS:HE3	1.82	0.44
1:C:17:LEU:N	1:C:18:GLU:HB2	2.33	0.44
1:D:123:VAL:O	1:D:125:PHE:HD2	2.00	0.44
1:B:24:PRO:HB2	5:B:2005:HOH:O	2.17	0.44
1:B:250:GLU:HG2	1:B:251:CYS:N	2.32	0.43
1:C:15:PRO:HA	1:C:31:TYR:HA	2.00	0.43
1:C:134:PRO:O	2:C:1256:ACT:H3	2.17	0.43
1:C:204:ILE:CB	5:C:2027:HOH:O	2.66	0.43
1:D:109:PRO:CA	1:D:125:PHE:CD1	3.00	0.43
1:B:92:VAL:HA	1:B:111:LEU:O	2.18	0.43
1:C:18:GLU:HA	1:C:20:ARG:H	1.83	0.43
1:A:183:ASP:O	2:A:1254:ACT:OXT	2.36	0.43
1:C:199:ILE:HG21	1:C:248:PRO:HB2	2.01	0.43
1:D:17:LEU:N	1:D:18:GLU:HB2	2.33	0.43
1:D:194:PRO:O	1:D:244:TRP:NE1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:VAL:HG13	1:A:69:PRO:HD2	2.00	0.43
1:A:92:VAL:HA	1:A:111:LEU:O	2.19	0.43
1:B:116:ASN:ND2	1:B:118:LYS:HB2	2.34	0.43
1:C:3:ASP:OD2	1:C:24:PRO:HA	2.19	0.43
1:A:116:ASN:ND2	1:A:118:LYS:HB2	2.34	0.43
1:D:3:ASP:OD2	1:D:24:PRO:HA	2.19	0.43
1:A:252:ARG:HH12	1:D:208:ARG:HH21	1.66	0.43
1:C:134:PRO:HA	2:C:1256:ACT:H2	1.99	0.43
1:C:214:ARG:HD2	1:C:214:ARG:HA	1.43	0.43
1:A:219:TYR:CD1	1:A:249:PRO:HD2	2.54	0.43
1:B:7:PRO:HG2	1:B:29:ILE:HD13	1.98	0.43
1:A:250:GLU:HG2	1:A:251:CYS:N	2.34	0.43
1:A:18:GLU:N	1:A:19:GLY:HA2	2.33	0.43
1:D:15:PRO:HA	1:D:31:TYR:HA	2.00	0.43
1:C:109:PRO:HB3	1:C:125:PHE:CD1	2.54	0.42
1:C:159:ASN:ND2	3:C:1255:GOL:H12	2.34	0.42
1:C:173:LEU:O	1:C:179:VAL:HA	2.19	0.42
1:D:70:THR:HA	5:D:2011:HOH:O	2.17	0.42
1:D:109:PRO:HB3	1:D:125:PHE:CD1	2.54	0.42
1:A:103:ARG:O	1:A:105:PRO:HD3	2.19	0.42
1:C:103:ARG:NH2	1:C:125:PHE:HB2	2.34	0.42
1:C:138:ARG:HA	1:C:138:ARG:HD3	1.40	0.42
1:C:237:VAL:O	1:C:237:VAL:CG1	2.62	0.42
1:B:20:ARG:HH22	1:B:22:SER:HB3	1.84	0.42
1:B:103:ARG:O	1:B:105:PRO:HD3	2.19	0.42
1:D:158:CYS:H	3:D:1257:GOL:C2	2.33	0.42
1:A:130:SER:HA	1:A:149:LEU:HA	2.01	0.42
1:C:23:PHE:CD2	1:C:23:PHE:N	2.88	0.42
1:C:68:VAL:HG13	1:C:69:PRO:HD2	2.02	0.42
1:D:173:LEU:O	1:D:179:VAL:HA	2.19	0.42
1:A:88:PRO:HD2	1:A:91:THR:OG1	2.19	0.42
1:D:68:VAL:HG13	1:D:69:PRO:HD2	2.02	0.42
1:D:103:ARG:NH2	1:D:125:PHE:HB2	2.34	0.42
1:D:111:LEU:HD23	1:D:111:LEU:HA	1.86	0.42
1:A:165:PHE:CD2	1:A:189:ARG:CZ	3.03	0.42
1:B:10:VAL:HG23	1:B:31:TYR:CE1	2.54	0.42
1:D:23:PHE:CD2	1:D:23:PHE:N	2.88	0.42
1:D:25:GLU:OE2	1:D:51:LYS:HD2	2.19	0.42
1:D:75:ALA:HB1	1:D:96:GLU:O	2.20	0.42
1:A:170:SER:HG	2:A:1254:ACT:H1	1.85	0.42
1:C:25:GLU:OE2	1:C:51:LYS:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:ALA:HB1	1:C:96:GLU:O	2.20	0.42
1:C:35:GLU:O	1:C:36:SER:HB2	2.20	0.42
1:B:164:LEU:HD23	1:B:165:PHE:N	2.35	0.42
1:D:35:GLU:O	1:D:36:SER:HB2	2.20	0.42
1:A:25:GLU:O	1:A:26:ASP:HB2	2.20	0.42
1:A:87:PHE:HD2	1:A:91:THR:HG21	1.85	0.42
1:B:136:GLU:OE2	1:D:218:THR:OG1	2.38	0.42
1:A:133:ASN:HA	1:A:134:PRO:HD3	1.92	0.41
1:A:82:ILE:HG23	1:A:83:THR:HG23	2.02	0.41
1:A:164:LEU:HD23	1:A:165:PHE:N	2.35	0.41
1:B:88:PRO:HD2	1:B:91:THR:OG1	2.19	0.41
1:C:28:VAL:HG22	1:C:48:ILE:HB	2.02	0.41
1:C:48:ILE:HG23	1:C:50:LEU:HD13	2.02	0.41
1:D:128:LYS:HD3	1:D:150:PHE:O	2.20	0.41
1:B:185:LEU:HD12	1:B:185:LEU:HA	1.86	0.41
1:B:82:ILE:HG23	1:B:83:THR:HG23	2.02	0.41
1:B:214:ARG:NH1	1:D:238:ASN:CG	2.65	0.41
1:D:17:LEU:HB2	1:D:18:GLU:HB2	2.01	0.41
1:D:160:THR:CG2	1:D:213:TYR:CE2	3.02	0.41
1:A:23:PHE:CD2	1:A:55:TRP:HZ2	2.38	0.41
1:A:239:ASN:ND2	1:B:105:PRO:HG3	2.34	0.41
1:D:48:ILE:HG23	1:D:50:LEU:HD13	2.02	0.41
1:D:131:CYS:O	1:D:148:ILE:HD12	2.21	0.41
1:A:50:LEU:HB2	1:A:54:GLN:O	2.21	0.41
1:D:11:PRO:HD2	1:D:60:GLU:HG3	2.02	0.41
1:B:87:PHE:HD2	1:B:91:THR:HG21	1.85	0.41
1:C:173:LEU:HD22	1:C:182:SER:CB	2.46	0.41
1:D:8:PRO:HD2	1:D:31:TYR:OH	2.21	0.41
1:D:28:VAL:HG22	1:D:48:ILE:HB	2.02	0.41
1:D:156:PHE:CD1	1:D:186:PRO:HD3	2.56	0.41
1:C:8:PRO:HD2	1:C:31:TYR:OH	2.21	0.41
1:C:11:PRO:HD2	1:C:60:GLU:HG3	2.02	0.41
1:C:109:PRO:CA	1:C:125:PHE:CD1	3.00	0.41
1:C:111:LEU:HD23	1:C:111:LEU:HA	1.86	0.41
1:C:131:CYS:O	1:C:148:ILE:HD12	2.21	0.41
1:D:123:VAL:O	1:D:125:PHE:CD2	2.74	0.41
1:D:171:PHE:HB3	1:D:173:LEU:HD13	2.00	0.41
1:D:173:LEU:HD22	1:D:182:SER:CB	2.46	0.41
1:D:211:TYR:HA	1:D:215:GLN:OE1	2.21	0.41
1:B:163:LYS:HG3	1:B:240:ASP:CG	2.41	0.41
1:C:74:SER:O	1:C:98:ARG:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:N	1:C:2:GLN:HB3	2.37	0.40
1:C:89:VAL:HG22	1:C:117:LEU:HD23	2.02	0.40
1:C:123:VAL:O	1:C:125:PHE:CD2	2.74	0.40
1:C:156:PHE:CD1	1:C:186:PRO:HD3	2.56	0.40
1:C:204:ILE:N	5:C:2027:HOH:O	2.04	0.40
1:D:89:VAL:HG22	1:D:117:LEU:HD23	2.02	0.40
1:A:252:ARG:HH22	1:D:208:ARG:HE	1.69	0.40
1:B:159:ASN:ND2	5:B:2030:HOH:O	2.48	0.40
1:D:74:SER:O	1:D:98:ARG:HB2	2.21	0.40
1:B:150:PHE:HA	1:B:172:CYS:SG	2.62	0.40
1:C:86:TYR:HB2	5:C:2007:HOH:O	2.21	0.40
1:C:171:PHE:HB3	1:C:173:LEU:HD13	2.00	0.40
1:A:150:PHE:HA	1:A:172:CYS:SG	2.62	0.40
1:A:201:ASN:ND2	1:A:225:PHE:CE2	2.90	0.40
1:B:23:PHE:CD2	1:B:55:TRP:CZ2	3.01	0.40
1:C:17:LEU:HB2	1:C:18:GLU:HB2	2.03	0.40
1:C:89:VAL:CG2	1:C:117:LEU:CD2	3.00	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)
5:B:2004:HOH:O	5:D:2017:HOH:O[1_854]	0.18	2.02

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%)	227 (91%)	22 (9%)	1 (0%)	34	57
1	B	251/254 (99%)	230 (92%)	20 (8%)	1 (0%)	34	57
1	C	251/254 (99%)	228 (91%)	21 (8%)	2 (1%)	19	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	251/254 (99%)	227 (90%)	22 (9%)	2 (1%)	19	39
All	All	1003/1016 (99%)	912 (91%)	85 (8%)	6 (1%)	25	47

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	17	LEU
1	D	17	LEU
1	D	189	ARG
1	C	189	ARG
1	A	99	PRO
1	B	99	PRO

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%)	186 (83%)	37 (17%)	2	3
1	B	224/225 (100%)	183 (82%)	41 (18%)	1	2
1	C	224/225 (100%)	190 (85%)	34 (15%)	3	4
1	D	224/225 (100%)	193 (86%)	31 (14%)	3	6
All	All	895/900 (99%)	752 (84%)	143 (16%)	2	4

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	9	ASP
1	A	18	GLU
1	A	20	ARG
1	A	21	THR
1	A	32	LYS
1	A	39	LYS
1	A	50	LEU

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Mol	Chain	Res	Type
1	A	59	GLU
1	A	65	SER
1	A	71	ARG
1	A	77	LEU
1	A	78	LYS
1	A	79	GLN
1	A	82	ILE
1	A	85	ASN
1	A	102	ARG
1	A	108	SER
1	A	114	LEU
1	A	118	LYS
1	A	121	THR
1	A	127	LYS
1	A	131	CYS
1	A	138	ARG
1	A	173	LEU
1	A	174	ILE
1	A	175	SER
1	A	178	SER
1	A	180	GLN
1	A	183	ASP
1	A	185	LEU
1	A	209	ASP
1	A	223	LYS
1	A	227	MET
1	A	230	GLU
1	A	232	SER
1	A	239	ASN
1	B	2	GLN
1	B	3	ASP
1	B	9	ASP
1	B	18	GLU
1	B	20	ARG
1	B	21	THR
1	B	39	LYS
1	B	50	LEU
1	B	59	GLU
1	B	65	SER
1	B	71	ARG
1	B	77	LEU
1	B	78	LYS

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Mol	Chain	Res	Type
1	B	79	GLN
1	B	82	ILE
1	B	85	ASN
1	B	102	ARG
1	B	108	SER
1	B	114	LEU
1	B	118	LYS
1	B	121	THR
1	B	127	LYS
1	B	131	CYS
1	B	136	GLU
1	B	138	ARG
1	B	173	LEU
1	B	174	ILE
1	B	175	SER
1	B	178	SER
1	B	180	GLN
1	B	183	ASP
1	B	185	LEU
1	B	189	ARG
1	B	209	ASP
1	B	223	LYS
1	B	227	MET
1	B	230	GLU
1	B	232	SER
1	B	239	ASN
1	B	243	GLU
1	B	254	CYS
1	C	1	MET
1	C	2	GLN
1	C	3	ASP
1	C	9	ASP
1	C	39	LYS
1	C	43	GLU
1	C	50	LEU
1	C	51	LYS
1	C	57	ASP
1	C	58	ILE
1	C	65	SER
1	C	71	ARG
1	C	77	LEU
1	C	78	LYS

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Mol	Chain	Res	Type
1	C	79	GLN
1	C	82	ILE
1	C	98	ARG
1	C	114	LEU
1	C	115	GLN
1	C	131	CYS
1	C	136	GLU
1	C	138	ARG
1	C	153	THR
1	C	163	LYS
1	C	173	LEU
1	C	174	ILE
1	C	189	ARG
1	C	191	ILE
1	C	208	ARG
1	C	214	ARG
1	C	228	ILE
1	C	231	HIS
1	C	239	ASN
1	C	243	GLU
1	D	3	ASP
1	D	9	ASP
1	D	39	LYS
1	D	43	GLU
1	D	50	LEU
1	D	51	LYS
1	D	57	ASP
1	D	58	ILE
1	D	65	SER
1	D	71	ARG
1	D	77	LEU
1	D	78	LYS
1	D	79	GLN
1	D	82	ILE
1	D	98	ARG
1	D	114	LEU
1	D	115	GLN
1	D	131	CYS
1	D	136	GLU
1	D	138	ARG
1	D	153	THR
1	D	163	LYS

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Mol	Chain	Res	Type
1	D	173	LEU
1	D	174	ILE
1	D	189	ARG
1	D	191	ILE
1	D	208	ARG
1	D	214	ARG
1	D	228	ILE
1	D	231	HIS
1	D	239	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	79	GLN
1	A	85	ASN
1	A	159	ASN
1	A	198	GLN
1	A	201	ASN
1	A	222	ASN
1	A	231	HIS
1	A	239	ASN
1	B	2	GLN
1	B	54	GLN
1	B	79	GLN
1	B	85	ASN
1	B	159	ASN
1	B	198	GLN
1	B	222	ASN
1	B	231	HIS
1	B	239	ASN
1	C	84	GLN
1	C	85	ASN
1	C	159	ASN
1	C	205	GLN
1	C	238	ASN
1	C	239	ASN
1	D	84	GLN
1	D	85	ASN
1	D	159	ASN
1	D	205	GLN
1	D	238	ASN

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Mol	Chain	Res	Type
1	D	239	ASN

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

13 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	GOL	D	1259	-	5,5,5	4.54	5 (100%)	5,5,5	5.73	3 (60%)
3	GOL	D	1257	-	5,5,5	4.51	5 (100%)	5,5,5	5.72	3 (60%)
4	SO4	C	1254	-	4,4,4	0.37	0	6,6,6	0.74	0
4	SO4	D	1255	-	4,4,4	0.37	0	6,6,6	0.74	0
3	GOL	C	1255	-	5,5,5	4.49	5 (100%)	5,5,5	5.72	3 (60%)
2	ACT	B	1255	-	3,3,3	1.20	1 (33%)	3,3,3	0.77	0
3	GOL	D	1258	-	5,5,5	4.50	5 (100%)	5,5,5	5.75	3 (60%)
2	ACT	C	1256	-	3,3,3	1.15	0	3,3,3	0.73	0
2	ACT	D	1256	-	3,3,3	1.15	0	3,3,3	0.74	0
2	ACT	A	1254	-	3,3,3	1.20	1 (33%)	3,3,3	0.78	0
4	SO4	C	1257	-	4,4,4	0.40	0	6,6,6	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	GOL	B	1256	-	5,5,5	4.51	5 (100%)	5,5,5	5.72	3 (60%)
3	GOL	C	1258	-	5,5,5	4.46	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
3	GOL	D	1259	-	-	2/4/4/4	-
3	GOL	D	1257	-	-	3/4/4/4	-
3	GOL	C	1255	-	-	2/4/4/4	-
3	GOL	D	1258	-	-	3/4/4/4	-
3	GOL	B	1256	-	-	3/4/4/4	-
3	GOL	C	1258	-	-	2/4/4/4	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1259	GOL	C3-C2	-7.41	1.21	1.51
3	D	1258	GOL	C3-C2	-7.33	1.21	1.51
3	B	1256	GOL	C3-C2	-7.33	1.21	1.51
3	D	1257	GOL	C3-C2	-7.32	1.21	1.51
3	C	1255	GOL	C3-C2	-7.29	1.21	1.51
3	C	1258	GOL	C3-C2	-7.19	1.22	1.51
3	B	1256	GOL	O1-C1	4.69	1.62	1.42
3	D	1257	GOL	O1-C1	4.66	1.62	1.42
3	C	1258	GOL	O1-C1	4.57	1.61	1.42
3	C	1255	GOL	O1-C1	4.55	1.61	1.42
3	D	1258	GOL	O1-C1	4.52	1.61	1.42
3	D	1259	GOL	O1-C1	4.46	1.61	1.42
3	C	1258	GOL	O3-C3	3.50	1.57	1.42
3	C	1255	GOL	O3-C3	3.50	1.57	1.42
3	B	1256	GOL	O3-C3	3.48	1.57	1.42
3	D	1258	GOL	O3-C3	3.46	1.57	1.42
3	D	1257	GOL	O3-C3	3.42	1.56	1.42
3	D	1259	GOL	O3-C3	3.37	1.56	1.42
3	D	1259	GOL	C1-C2	-2.91	1.39	1.51
3	D	1259	GOL	O2-C2	-2.86	1.34	1.43
3	D	1258	GOL	C1-C2	-2.78	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1255	GOL	O2-C2	-2.76	1.35	1.43
3	D	1257	GOL	O2-C2	-2.75	1.35	1.43
3	D	1258	GOL	O2-C2	-2.73	1.35	1.43
3	C	1258	GOL	C1-C2	-2.72	1.40	1.51
3	C	1255	GOL	C1-C2	-2.67	1.40	1.51
3	C	1258	GOL	O2-C2	-2.67	1.35	1.43
3	D	1257	GOL	C1-C2	-2.67	1.40	1.51
3	B	1256	GOL	C1-C2	-2.64	1.40	1.51
3	B	1256	GOL	O2-C2	-2.64	1.35	1.43
2	B	1255	ACT	O-C	2.02	1.31	1.22
2	A	1254	ACT	O-C	2.01	1.31	1.22

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1255	GOL	O3-C3-C2	10.51	160.60	110.20
3	D	1259	GOL	O3-C3-C2	10.46	160.35	110.20
3	D	1258	GOL	O3-C3-C2	10.45	160.29	110.20
3	D	1257	GOL	O3-C3-C2	10.44	160.26	110.20
3	B	1256	GOL	O3-C3-C2	10.44	160.25	110.20
3	C	1258	GOL	O3-C3-C2	10.42	160.17	110.20
3	D	1258	GOL	O2-C2-C3	6.69	138.60	109.12
3	D	1259	GOL	O2-C2-C3	6.60	138.19	109.12
3	D	1257	GOL	O2-C2-C3	6.53	137.90	109.12
3	C	1258	GOL	O2-C2-C3	6.53	137.89	109.12
3	B	1256	GOL	O2-C2-C3	6.53	137.87	109.12
3	C	1255	GOL	O2-C2-C3	6.42	137.41	109.12
3	D	1257	GOL	O1-C1-C2	3.36	126.29	110.20
3	B	1256	GOL	O1-C1-C2	3.34	126.23	110.20
3	D	1258	GOL	O1-C1-C2	3.33	126.14	110.20
3	C	1255	GOL	O1-C1-C2	3.32	126.13	110.20
3	C	1258	GOL	O1-C1-C2	3.30	126.01	110.20
3	D	1259	GOL	O1-C1-C2	3.21	125.59	110.20

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1256	GOL	O1-C1-C2-C3
3	B	1256	GOL	C1-C2-C3-O3
3	C	1255	GOL	O1-C1-C2-C3
3	D	1257	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	D	1257	GOL	O2-C2-C3-O3
3	D	1258	GOL	O2-C2-C3-O3
3	D	1257	GOL	C1-C2-C3-O3
3	D	1258	GOL	O1-C1-C2-C3
3	D	1258	GOL	C1-C2-C3-O3
3	D	1259	GOL	O1-C1-C2-C3
3	D	1259	GOL	C1-C2-C3-O3
3	C	1258	GOL	O1-C1-C2-O2
3	C	1258	GOL	O2-C2-C3-O3
3	B	1256	GOL	O2-C2-C3-O3
3	C	1255	GOL	O2-C2-C3-O3

There are no ring outliers.

10 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1259	GOL	1	0
3	D	1257	GOL	4	0
4	C	1254	SO4	2	0
3	C	1255	GOL	1	0
2	B	1255	ACT	5	0
3	D	1258	GOL	5	0
2	C	1256	ACT	3	0
2	D	1256	ACT	2	0
2	A	1254	ACT	4	0
3	C	1258	GOL	3	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	252/254 (99%)	0.03	7 (2%)	53	46	19, 37, 60, 75	0
1	B	253/254 (99%)	0.05	8 (3%)	47	40	23, 38, 59, 72	0
1	C	253/254 (99%)	0.11	7 (2%)	53	46	18, 39, 59, 73	0
1	D	253/254 (99%)	-0.06	3 (1%)	79	76	19, 37, 56, 70	0
All	All	1011/1016 (99%)	0.03	25 (2%)	57	51	18, 38, 59, 75	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	5.3
1	D	254	CYS	4.4
1	B	254	CYS	3.3
1	A	34	GLU	3.1
1	D	223	LYS	3.0
1	C	102	ARG	2.8
1	A	2	GLN	2.8
1	A	18	GLU	2.8
1	B	177	SER	2.8
1	C	114	LEU	2.7
1	B	238	ASN	2.5
1	C	123	VAL	2.4
1	B	165	PHE	2.3
1	D	73	ASN	2.2
1	A	16	ALA	2.2
1	B	105	PRO	2.2
1	C	238	ASN	2.2
1	C	80	PRO	2.1
1	B	80	PRO	2.1
1	B	240	ASP	2.1
1	C	172	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	238	ASN	2.1
1	A	237	VAL	2.0
1	A	6	LEU	2.0
1	B	20	ARG	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 monosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	GOL	D	1257	6/6	0.65	0.43	53,54,55,55	0
3	GOL	C	1258	6/6	0.74	0.44	44,45,46,46	0
3	GOL	D	1258	6/6	0.75	0.42	72,73,73,73	0
2	ACT	A	1254	4/4	0.81	0.33	42,42,43,43	0
3	GOL	B	1256	6/6	0.84	0.26	49,49,49,50	0
2	ACT	D	1256	4/4	0.87	0.25	49,49,49,50	0
2	ACT	C	1256	4/4	0.88	0.27	45,45,45,45	0
3	GOL	D	1259	6/6	0.88	0.25	54,55,56,56	0
2	ACT	B	1255	4/4	0.90	0.27	40,41,41,41	0
3	GOL	C	1255	6/6	0.90	0.31	45,46,46,46	0
4	SO4	C	1257	5/5	0.91	0.28	76,76,76,76	0
4	SO4	D	1255	5/5	0.96	0.12	43,43,43,43	0
4	SO4	C	1254	5/5	0.98	0.10	44,45,45,45	0

6.5 Other polymers ⓘ

There are no such residues in this entry.