



# Full wwPDB X-ray Structure Validation Report i

Mar 1, 2014 – 03:05 AM GMT

PDB ID : 1OJY  
Title : DECAY ACCELERATING FACTOR (CD55): THE STRUCTURE OF AN  
INTACT HUMAN COMPLEMENT REGULATOR.  
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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)

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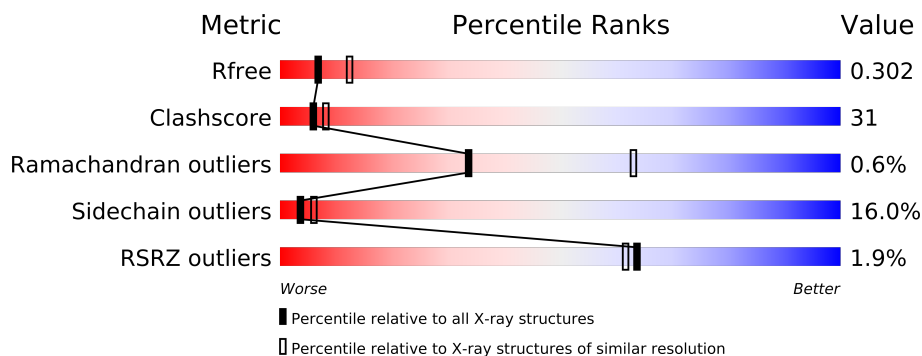
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.60 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (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 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	
1	C	254	
1	D	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
2	ACT	A	1254	-	X
2	ACT	B	1255	-	X
2	ACT	C	1256	-	X
2	ACT	D	1256	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	GOL	B	1256	X	X
3	GOL	C	1255	X	X
3	GOL	C	1258	X	X
3	GOL	D	1257	X	X
3	GOL	D	1258	X	X
3	GOL	D	1259	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8050 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	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:

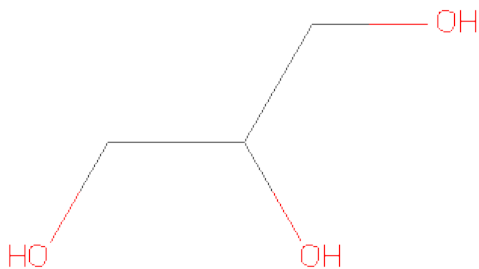
Chain	Residue	Modelled	Actual	Comment	Reference
A	48	ILE	THR	SEE REMARK 999	UNP P08174
B	48	ILE	THR	SEE REMARK 999	UNP P08174
C	48	ILE	THR	SEE REMARK 999	UNP P08174
D	48	ILE	THR	SEE REMARK 999	UNP P08174

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



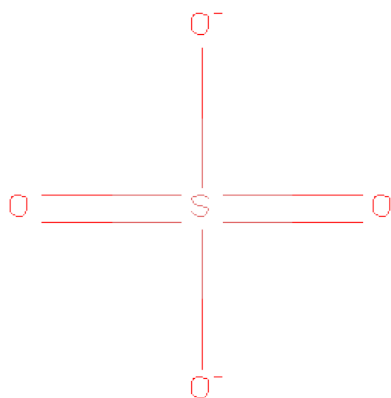
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 5 is water.

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

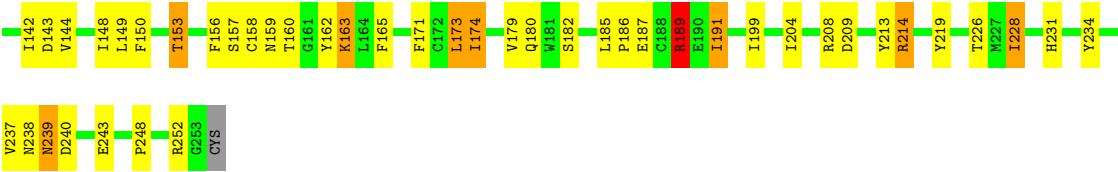
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	40	Total 40	O 40	0	0
5	C	36	Total 36	O 36	0	0
5	D	42	Total 42	O 42	0	0

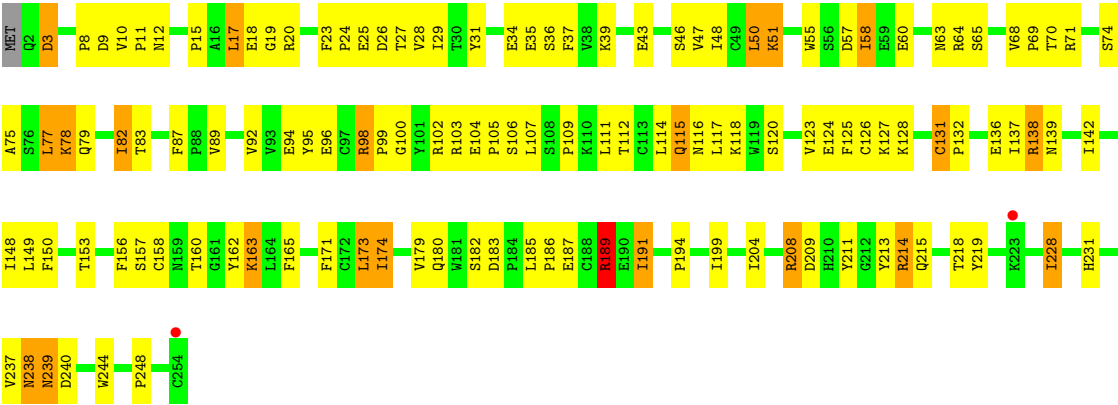






● Molecule 1: COMPLEMENT DECAy-ACCELERATING FACTOR

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 2.58Å)	Xtriage
Refinement program	TNT 5F	Depositor
R, $R_{free}$	0.000 , (Not available) 0.251 , 0.302	Depositor DCC
$R_{free}$ test set	1715 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.2	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 25.2	EDS
Estimated twinning fraction	0.000 for -h,-l,-k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 34514 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8050	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, 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	0.37	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(°)	Ideal(°)
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 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	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

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 31.

All (478) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:189:ARG:HB3	1:B:189:ARG:HH11	1.16	1.11
1:D:157:SER:HA	3:D:1257:GOL:H12	1.33	1.05
1:A:223:LYS:HA	1:A:223:LYS:HE3	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:HH21	1:B:20:ARG:HG2	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	Distance(Å)	Clash(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:NH2	1:B:20:ARG:HG2	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:CB	1:B:189:ARG:HH11	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:HG12	1:A:237:VAL:O	1.87	0.75
1:C:102:ARG:HG3	1:C:102:ARG:HH11	1.50	0.75
1:D:102:ARG:HH11	1:D:102:ARG:HG3	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:D:18:GLU:HG3	1:D:19:GLY:CA	2.18	0.73
1:B:80:PRO:HG2	1:B:84:GLN:OE1	1.89	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:165:PHE:CZ	1:A:189:ARG:HD2	2.26	0.71
1:D:69:PRO:HD3	1:D:87:PHE:CE1	2.24	0.71
1:A:77:LEU:HD13	1:A:95:TYR:CE2	2.26	0.71
1:B:77:LEU:HD13	1:B:95:TYR:CE2	2.26	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:187:GLU:OE1	1:B:189:ARG:NH2	2.24	0.70
1:B:20:ARG:CG	1:B:20:ARG:HH21	2.03	0.70
1:B:23:PHE:CD2	1:B:55:TRP:HZ2	2.10	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:214:ARG:NH1	1:C:238:ASN:ND2	2.40	0.69
1:D:18:GLU:CG	1:D:19:GLY:HA2	2.22	0.69
1:A:191:ILE:HD12	1:A:237:VAL:HG11	1.74	0.69
1:C:29:ILE:HD13	1:C:55:TRP:CH2	2.27	0.69
1:C:12:ASN:C	1:C:34:GLU:HG3	2.11	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:D:171:PHE:HB3	1:D:173:LEU:HD11	1.75	0.68
1:A:34:GLU:O	1:A:37:PHE:HB2	1.93	0.68
1:A:115:GLN:OE1	1:A:115:GLN:N	2.27	0.68
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:OE1	1:B:115:GLN:N	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:D:165:PHE:CD1	1:D:189:ARG:HG2	2.29	0.67
1:C:187:GLU:OE1	1:C:189:ARG:NE	2.27	0.67
1:D:102:ARG:NH1	1:D:102:ARG:HG3	2.09	0.67
1:C:109:PRO:HA	1:C:125:PHE:CD1	2.29	0.67
1:D:189:ARG:HG3	1:D:189:ARG:HH21	1.60	0.67
1:B:133:ASN:OD1	1:B:134:PRO:HD2	1.95	0.67
1:A:214:ARG:NH2	1:C:160:THR:CG2	2.59	0.66
1:D:163:LYS:HB2	1:D:191:ILE:CD1	2.25	0.66
1:C:189:ARG:HH21	1:C:189:ARG:HG3	1.60	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:D:189:ARG:HG3	1:D:189:ARG:NH2	2.10	0.65
1:A:198:GLN:NE2	5:A:2017:HOH:O	2.30	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:173:LEU:HD22	1:D:182:SER:HB3	1.79	0.64
1:D:27:THR:HG22	1:D:29:ILE:HD12	1.77	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
1:A:7:PRO:CG	1:A:29:ILE:HD13	2.27	0.63
1:D:77:LEU:O	1:D:82:ILE:HD12	1.99	0.63
1:D:12:ASN:O	1:D:34:GLU:HG3	1.99	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:C:77:LEU:O	1:C:82:ILE:HD12	1.99	0.62
1:A:23:PHE:HB3	1:A:27:THR:HG21	1.82	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:C:107:LEU:HD12	1:C:124:GLU:C	2.20	0.62
1:A:7:PRO:HG3	1:A:29:ILE:CD1	2.29	0.62
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:159:ASN:ND2	5:A:2015:HOH:O	2.28	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:B:81:TYR:CD2	1:B:93:VAL:HG12	2.36	0.61
1:A:29:ILE:HD12	1:A:55:TRP:CH2	2.35	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: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:C:116:ASN:ND2	1:C:118:LYS:HD2	2.19	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:D:77:LEU:HD13	1:D:95:TYR:CE2	2.40	0.57
1:A:111:LEU:HD22	1:A:120:SER:O	2.05	0.57
1:A:161:GLY:C	1:A:191:ILE:HG13	2.25	0.57
1:D:17:LEU:HB2	1:D:18:GLU:HA	1.87	0.56
1:C:77:LEU:HD13	1:C:95:TYR:CE2	2.40	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:A:95:TYR:CE1	1:A:111:LEU:HD12	2.40	0.56
1:A:183:ASP:N	1:A:183:ASP:OD1	2.37	0.56
1:D:18:GLU:CA	1:D:20:ARG:H	2.18	0.56
1:B:183:ASP:OD1	1:B:183:ASP:N	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:C:82:ILE:CG2	1:C:83:THR:HG23	2.37	0.55
1:A:239:ASN:HD22	1:B:105:PRO:HG3	1.71	0.55
1:C:69:PRO:CG	1:C:77:LEU:HD21	2.34	0.55
1:A:227:MET:HE3	5:A:2025:HOH:O	2.06	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:C:106:SER:O	1:C:107:LEU:HD23	2.08	0.54
1:D:106:SER:O	1:D:107:LEU:HD23	2.08	0.54
1:C:29:ILE:O	1:C:46:SER:HB2	2.08	0.54
1:A:231:HIS:HD2	1:C:143:ASP:OD2	1.91	0.54
1:C:144:VAL:O	5:C:2017:HOH:O	2.18	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:C:17:LEU:HB2	1:C:18:GLU:CB	2.38	0.54
1:B:73:ASN:O	1:B:98:ARG:HD2	2.07	0.54
1:C:25:GLU:O	1:C:26:ASP:HB2	2.07	0.53
1:A:73:ASN:O	1:A:98:ARG:HD2	2.07	0.53
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:239:ASN:O	1:B:240:ASP:HB2	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:211:TYR:CE2	1:B:217:VAL:HG12	2.44	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:C:29:ILE:HD13	1:C:55:TRP:HH2	1.72	0.52
1:A:160:THR:O	1:C:214:ARG:NH1	2.43	0.52
1:A:102:ARG:HE	1:A:127:LYS:HE3	1.73	0.52
1:D:17:LEU:CA	1:D:18:GLU:HB2	2.40	0.52
1:A:239:ASN:O	1:A:240:ASP:HB2	2.08	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:D:189:ARG:CG	1:D:189:ARG:HH21	2.23	0.52
1:C:189:ARG:HH21	1:C:189:ARG:CG	2.23	0.52
1:B:123:VAL:HG22	5:B:2019:HOH:O	2.10	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:CA	1:A:223:LYS:HE3	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: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:B:175:SER:N	1:B:178:SER:O	2.36	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:C:124:GLU:OE2	1:C:124:GLU:N	2.44	0.50
1:B:145:PRO:HD2	5:B:2028:HOH:O	2.10	0.50
1:C:204:ILE:HB	5:C:2027:HOH:O	2.11	0.50
1:D:89:VAL:CG2	1:D:117:LEU:HD23	2.41	0.50
1:D:37:PHE:HA	1:D:63:ASN:O	2.12	0.50
1:A:165:PHE:CE1	1:A:189:ARG:HD2	2.47	0.50
1:B:237:VAL:O	1:B:237:VAL:CG1	2.60	0.50
1:D:17:LEU:HB2	1:D:18:GLU:CA	2.41	0.50
1:B:77:LEU:HD13	1:B:95:TYR:CZ	2.46	0.50
1:A:159:ASN:ND2	1:C:234:TYR:CE1	2.80	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:191:ILE:HG21	1:B:237:VAL:HG13	1.94	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: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:D:18:GLU:HA	1:D:20:ARG:N	2.28	0.49
1:C:162:TYR:HD2	1:C:189:ARG:O	1.94	0.49
1:A:39:LYS:HG2	1:A:39:LYS:O	2.12	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:D:156:PHE:CD1	1:D:186:PRO:HG3	2.48	0.49
1:B:39:LYS:O	1:B:39:LYS:HG2	2.12	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:77:LEU:HB3	1:B:82:ILE:HD12	1.96	0.48
1:B:74:SER:OG	5:B:2016:HOH:O	2.10	0.48
1:C:138:ARG:O	1:C:139:ASN:HB2	2.14	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:210:HIS:CD2	5:A:2021:HOH:O	2.66	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:D:68:VAL:HA	1:D:87:PHE:HE1	1.79	0.48
1:C:68:VAL:HA	1:C: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:D:183:ASP:O	2:D:1256:ACT:OXT	2.32	0.47
1:C:128:LYS:HD3	1:C:150:PHE:O	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:69:PRO:HD3	1:B:87:PHE:CE1	2.49	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:A:69:PRO:HD3	1:A:87:PHE:CE1	2.50	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:D:109:PRO:HA	1:D:125:PHE:CG	2.50	0.46
1:C:156:PHE:CE1	1:C:186:PRO:HD3	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:209:ASP:OD2	1:C:209:ASP:N	2.48	0.46
1:C:174:ILE:O	1:C:174:ILE:HD13	2.15	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:HD3	1:D:138:ARG:HA	1.40	0.46
1:D:174:ILE:O	1:D:174:ILE:HD13	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:D:15:PRO:HD3	3:D:1258:GOL:H12	1.96	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: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:D:15:PRO:CD	3:D:1258:GOL:C1	2.94	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
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:B:7:PRO:HD3	1:B:23:PHE:HE2	1.75	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:7:PRO:HG2	1:A:29:ILE:HD13	1.99	0.45
1:B:40:ILE:HG13	1:B:61:PHE:O	2.16	0.45
1:C:104:GLU:O	1:C:107:LEU:N	2.40	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:B:10:VAL:CG2	1:B:31:TYR:CE1	3.00	0.45
1:D:237:VAL:CG1	1:D:237:VAL:O	2.65	0.44
1:A:165:PHE:CE2	1:A:189:ARG:NH2	2.85	0.44
1:B:191:ILE:CD1	1:B:240:ASP:HA	2.48	0.44
1:A:252:ARG:HH12	1:D:208:ARG:HE	1.65	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:C:123:VAL:O	1:C:125:PHE:HD2	2.00	0.44
1:A:107:LEU:HB3	1:A:123:VAL:HG21	1.99	0.44
1:A:99:PRO:HA	1:A:100:GLY:HA2	1.54	0.44
1:B:77:LEU:HG	1:B:81:TYR:HB2	1.99	0.44
1:A:40:ILE:HG13	1:A:61:PHE:O	2.16	0.44
1:B:138:ARG:HA	1:B:138:ARG:HD3	1.42	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:A:102:ARG:HH11	1:A:127:LYS:HE3	1.82	0.44
1:B:24:PRO:HB2	5:B:2005:HOH:O	2.17	0.44
1:D:109:PRO:CA	1:D:125:PHE:CD1	3.00	0.43
1:C:204:ILE:CB	5:C:2027:HOH:O	2.66	0.43
1:C:134:PRO:O	2:C:1256:ACT:H3	2.17	0.43
1:C:15:PRO:HA	1:C:31:TYR:HA	2.00	0.43
1:B:250:GLU:HG2	1:B:251:CYS:N	2.32	0.43
1:C:18:GLU:HA	1:C:20:ARG:H	1.83	0.43
1:B:92:VAL:HA	1:B:111:LEU:O	2.18	0.43
1:D:17:LEU:N	1:D:18:GLU:HB2	2.33	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:194:PRO:O	1:D:244:TRP:NE1	2.50	0.43
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:C:3:ASP:OD2	1:C:24:PRO:HA	2.19	0.43
1:B:116:ASN:ND2	1:B:118:LYS:HB2	2.34	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:C:214:ARG:HD2	1:C:214:ARG:HA	1.43	0.43
1:C:134:PRO:HA	2:C:1256:ACT:H2	1.99	0.43
1:A:252:ARG:HH12	1:D:208:ARG:HH21	1.66	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:7:PRO:HG2	1:B:29:ILE:HD13	1.98	0.43
1:A:219:TYR:CD1	1:A:249:PRO:HD2	2.54	0.43
1:A:250:GLU:HG2	1:A:251:CYS:N	2.34	0.43
1:D:15:PRO:HA	1:D:31:TYR:HA	2.00	0.43
1:A:18:GLU:N	1:A:19:GLY:HA2	2.33	0.43
1:C:109:PRO:HB3	1:C:125:PHE:CD1	2.54	0.42
1:D:109:PRO:HB3	1:D:125:PHE:CD1	2.54	0.42
1:C:173:LEU:O	1:C:179:VAL:HA	2.19	0.42
1:C:159:ASN:ND2	3:C:1255:GOL:H12	2.34	0.42
1:D:70:THR:HA	5:D:2011:HOH:O	2.17	0.42
1:C:103:ARG:NH2	1:C:125:PHE:HB2	2.34	0.42
1:C:237:VAL:CG1	1:C:237:VAL:O	2.62	0.42
1:C:138:ARG:HA	1:C:138:ARG:HD3	1.40	0.42
1:A:103:ARG:O	1:A:105:PRO:HD3	2.19	0.42
1:D:158:CYS:H	3:D:1257:GOL:C2	2.33	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: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:C:23:PHE:N	1:C:23:PHE:CD2	2.88	0.42
1:A:130:SER:HA	1:A:149:LEU:HA	2.01	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:A:88:PRO:HD2	1:A:91:THR:OG1	2.19	0.42
1:D:111:LEU:HA	1:D:111:LEU:HD23	1.86	0.42
1:A:165:PHE:CD2	1:A:189:ARG:CZ	3.03	0.42
1:D:75:ALA:HB1	1:D:96:GLU:O	2.20	0.42
1:D:25:GLU:OE2	1:D:51:LYS:HD2	2.19	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:C:75:ALA:HB1	1:C: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
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: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:25:GLU:O	1:A:26:ASP:HB2	2.20	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:HA	1:B:185:LEU:HD12	1.86	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:B:82:ILE:HG23	1:B:83:THR:HG23	2.02	0.41
1:D:160:THR:CG2	1:D:213:TYR:CE2	3.02	0.41
1:A:239:ASN:ND2	1:B:105:PRO:HG3	2.34	0.41
1:A:23:PHE:CD2	1:A:55:TRP:HZ2	2.38	0.41
1:D:131:CYS:O	1:D:148:ILE:HD12	2.21	0.41
1:D:48:ILE:HG23	1:D:50:LEU:HD13	2.02	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:156:PHE:CD1	1:D:186:PRO:HD3	2.56	0.41
1:D:28:VAL:HG22	1:D:48:ILE:HB	2.02	0.41
1:C:109:PRO:CA	1:C:125:PHE:CD1	3.00	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:C:131:CYS:O	1:C:148:ILE:HD12	2.21	0.41
1:C:111:LEU:HA	1:C:111:LEU:HD23	1.86	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: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
1:C:123:VAL:O	1:C:125:PHE:CD2	2.74	0.40
1:D:89:VAL:HG22	1:D:117:LEU:HD23	2.02	0.40
1:C:204:ILE:N	5:C:2027:HOH:O	2.04	0.40
1:C:89:VAL:HG22	1:C:117:LEU:HD23	2.02	0.40
1:C:156:PHE:CD1	1:C:186:PRO:HD3	2.56	0.40
1:C:1:MET:N	1:C:2:GLN:HB3	2.37	0.40
1:A:252:ARG:HH22	1:D:208:ARG:HE	1.69	0.40
1:D:74:SER:O	1:D:98:ARG:HB2	2.21	0.40
1:B:159:ASN:ND2	5:B:2030:HOH:O	2.48	0.40
1:B:150:PHE:HA	1:B:172:CYS:SG	2.62	0.40
1:C:171:PHE:HB3	1:C:173:LEU:HD13	2.00	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:86:TYR:HB2	5:C:2007:HOH:O	2.21	0.40
1:A:150:PHE:HA	1:A:172:CYS:SG	2.62	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
1:A:201:ASN:ND2	1:A:225:PHE:CE2	2.90	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)
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%)	43	72
1	B	251/254 (99%)	230 (92%)	20 (8%)	1 (0%)	43	72
1	C	251/254 (99%)	228 (91%)	21 (8%)	2 (1%)	27	53
1	D	251/254 (99%)	227 (90%)	22 (9%)	2 (1%)	27	53
All	All	1003/1016 (99%)	912 (91%)	85 (8%)	6 (1%)	33	63

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%)	3	5
1	B	224/225 (100%)	183 (82%)	41 (18%)	2	4
1	C	224/225 (100%)	190 (85%)	34 (15%)	4	7
1	D	224/225 (100%)	193 (86%)	31 (14%)	5	9
All	All	895/900 (99%)	752 (84%)	143 (16%)	3	6

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

Some 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

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Mol	Chain	Res	Type
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
1	D	239	ASN

### 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

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$
2	ACT	A	1254	-	1,3,3	0.55	0	0,3,3	0.00	-
2	ACT	B	1255	-	1,3,3	0.53	0	0,3,3	0.00	-
3	GOL	B	1256	-	5,5,5	4.52	5 (100%)	5,5,5	5.69	3 (60%)
4	SO4	C	1254	-	4,4,4	0.60	0	6,6,6	0.71	0
3	GOL	C	1255	-	5,5,5	4.50	5 (100%)	5,5,5	5.69	3 (60%)
2	ACT	C	1256	-	1,3,3	0.67	0	0,3,3	0.00	-
4	SO4	C	1257	-	4,4,4	0.67	0	6,6,6	0.69	0
3	GOL	C	1258	-	5,5,5	4.47	5 (100%)	5,5,5	5.68	3 (60%)
4	SO4	D	1255	-	4,4,4	0.61	0	6,6,6	0.71	0
2	ACT	D	1256	-	1,3,3	0.67	0	0,3,3	0.00	-
3	GOL	D	1257	-	5,5,5	4.52	5 (100%)	5,5,5	5.69	3 (60%)
3	GOL	D	1258	-	5,5,5	4.51	5 (100%)	5,5,5	5.72	3 (60%)
3	GOL	D	1259	-	5,5,5	4.55	5 (100%)	5,5,5	5.70	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	ACT	A	1254	-	-	0/0/0/0	0/0/0/0
2	ACT	B	1255	-	-	0/0/0/0	0/0/0/0
3	GOL	B	1256	-	-	0/4/4/4	0/0/0/0
4	SO4	C	1254	-	-	0/0/0/0	0/0/0/0
3	GOL	C	1255	-	-	0/4/4/4	0/0/0/0
2	ACT	C	1256	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1257	-	-	0/0/0/0	0/0/0/0
3	GOL	C	1258	-	-	0/4/4/4	0/0/0/0
4	SO4	D	1255	-	-	0/0/0/0	0/0/0/0
2	ACT	D	1256	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	1257	-	-	0/4/4/4	0/0/0/0
3	GOL	D	1258	-	-	0/4/4/4	0/0/0/0
3	GOL	D	1259	-	-	0/4/4/4	0/0/0/0

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1259	GOL	C3-C2	-7.53	1.21	1.52
3	D	1258	GOL	C3-C2	-7.46	1.21	1.52
3	B	1256	GOL	C3-C2	-7.45	1.21	1.52
3	D	1257	GOL	C3-C2	-7.44	1.21	1.52
3	C	1255	GOL	C3-C2	-7.41	1.21	1.52
3	C	1258	GOL	C3-C2	-7.31	1.22	1.52
3	B	1256	GOL	O1-C1	4.56	1.62	1.42
3	D	1257	GOL	O1-C1	4.53	1.62	1.42
3	C	1258	GOL	O1-C1	4.44	1.61	1.42
3	C	1255	GOL	O1-C1	4.42	1.61	1.42
3	D	1258	GOL	O1-C1	4.40	1.61	1.42
3	D	1259	GOL	O1-C1	4.34	1.61	1.42
3	C	1258	GOL	O3-C3	3.41	1.57	1.42
3	C	1255	GOL	O3-C3	3.41	1.57	1.42
3	B	1256	GOL	O3-C3	3.39	1.57	1.42
3	D	1258	GOL	O3-C3	3.36	1.57	1.42
3	D	1257	GOL	O3-C3	3.33	1.56	1.42
3	D	1259	GOL	O3-C3	3.28	1.56	1.42
3	D	1259	GOL	C1-C2	-3.06	1.39	1.52
3	D	1258	GOL	C1-C2	-2.93	1.40	1.52
3	C	1258	GOL	C1-C2	-2.87	1.40	1.52
3	C	1255	GOL	C1-C2	-2.82	1.40	1.52
3	D	1257	GOL	C1-C2	-2.82	1.40	1.52
3	B	1256	GOL	C1-C2	-2.79	1.40	1.52
3	D	1259	GOL	O2-C2	-2.79	1.34	1.43
3	C	1255	GOL	O2-C2	-2.69	1.35	1.43
3	D	1257	GOL	O2-C2	-2.68	1.35	1.43
3	D	1258	GOL	O2-C2	-2.66	1.35	1.43
3	C	1258	GOL	O2-C2	-2.61	1.35	1.43
3	B	1256	GOL	O2-C2	-2.58	1.35	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1255	GOL	O3-C3-C2	10.43	160.60	109.71

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1259	GOL	O3-C3-C2	10.38	160.35	109.71
3	D	1258	GOL	O3-C3-C2	10.37	160.29	109.71
3	D	1257	GOL	O3-C3-C2	10.36	160.26	109.71
3	B	1256	GOL	O3-C3-C2	10.36	160.25	109.71
3	C	1258	GOL	O3-C3-C2	10.34	160.17	109.71
3	D	1258	GOL	O2-C2-C3	6.67	138.60	108.22
3	D	1259	GOL	O2-C2-C3	6.58	138.19	108.22
3	D	1257	GOL	O2-C2-C3	6.52	137.90	108.22
3	C	1258	GOL	O2-C2-C3	6.51	137.89	108.22
3	B	1256	GOL	O2-C2-C3	6.51	137.87	108.22
3	C	1255	GOL	O2-C2-C3	6.41	137.41	108.22
3	D	1257	GOL	O1-C1-C2	3.40	126.29	109.71
3	B	1256	GOL	O1-C1-C2	3.39	126.23	109.71
3	D	1258	GOL	O1-C1-C2	3.37	126.14	109.71
3	C	1255	GOL	O1-C1-C2	3.36	126.13	109.71
3	C	1258	GOL	O1-C1-C2	3.34	126.01	109.71
3	D	1259	GOL	O1-C1-C2	3.25	125.59	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%)	0.02	5 (1%) 62 60	19, 37, 60, 75	0
1	B	253/254 (99%)	0.05	5 (1%) 62 60	23, 38, 59, 72	0
1	C	253/254 (99%)	0.11	6 (2%) 56 53	18, 39, 59, 73	0
1	D	253/254 (99%)	-0.07	2 (0%) 83 85	19, 37, 56, 70	0
All	All	1011/1016 (99%)	0.03	18 (1%) 64 64	18, 38, 59, 75	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	5.0
1	D	254	CYS	4.2
1	B	254	CYS	3.3
1	B	238	ASN	3.1
1	A	34	GLU	3.1
1	D	223	LYS	3.0
1	C	114	LEU	2.8
1	C	123	VAL	2.7
1	B	177	SER	2.6
1	C	102	ARG	2.6
1	A	2	GLN	2.6
1	A	238	ASN	2.4
1	A	18	GLU	2.3
1	B	105	PRO	2.2
1	C	113	CYS	2.2
1	C	70	THR	2.1
1	B	165	PHE	2.1
1	A	237	VAL	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(Å <sup>2</sup> )	Q<0.9
2	ACT	A	1254	4/4	0.37	11.54	42,42,43,43	0
3	GOL	D	1258	6/6	0.47	8.99	72,73,73,73	0
3	GOL	C	1258	6/6	0.42	6.04	44,45,46,46	0
3	GOL	D	1257	6/6	0.42	6.01	53,54,55,55	0
2	ACT	B	1255	4/4	0.27	4.97	40,41,41,41	0
3	GOL	C	1255	6/6	0.32	4.77	45,46,46,46	0
3	GOL	B	1256	6/6	0.27	4.11	49,49,49,50	0
2	ACT	D	1256	4/4	0.26	2.97	49,49,49,50	0
2	ACT	C	1256	4/4	0.24	2.83	45,45,45,45	0
4	SO4	C	1257	5/5	0.25	1.25	76,76,76,76	0
3	GOL	D	1259	6/6	0.23	0.85	54,55,56,56	0
4	SO4	D	1255	5/5	0.13	-1.35	43,43,43,43	0
4	SO4	C	1254	5/5	0.10	-1.55	44,45,45,45	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.