



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 03:10 PM GMT

PDB ID : 3TMT
Title : IrisFP, distorted chromophore
Authors : Adam, V.; Carpentier, P.; Roy, A.; Field, M.; Bourgeois, D.
Deposited on : 2011-08-31
Resolution : 2.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

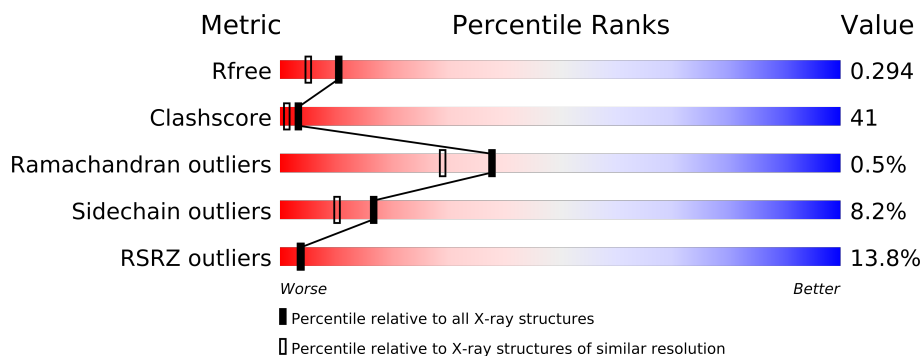
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	230	
1	B	230	
1	C	230	
1	D	230	

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	SO4	A	228	-	X
2	SO4	C	1225	-	X
2	SO4	C	1226	-	X
2	SO4	C	227	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9939 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 Green to red photoconvertible GPF-like protein EosFP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	3	4	0
			1808	1150	309	337	12			
1	B	221	Total	C	N	O	S	1	3	0
			1792	1141	305	335	11			
1	C	220	Total	C	N	O	S	1	2	0
			1779	1133	304	331	11			
1	D	221	Total	C	N	O	S	2	3	0
			1790	1140	305	333	12			

There are 44 discrepancies between the modelled and reference sequences:

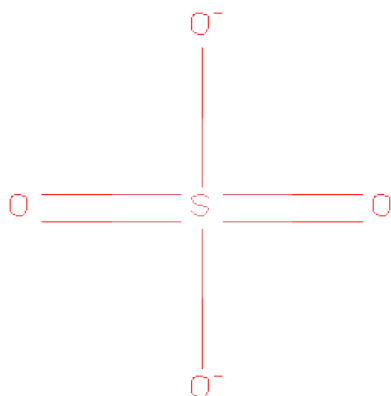
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
A	-4	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
A	-3	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
A	-2	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
A	-1	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
A	0	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
A	64	CR8	HIS	CHROMOPHORE	UNP Q5S6Z9
A	64	CR8	TYR	CHROMOPHORE	UNP Q5S6Z9
A	64	CR8	GLY	CHROMOPHORE	UNP Q5S6Z9
A	173	SER	PHE	ENGINEERED MUTATION	UNP Q5S6Z9
A	191	LEU	PHE	ENGINEERED MUTATION	UNP Q5S6Z9
B	-5	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
B	-4	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
B	-3	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
B	-2	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
B	-1	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
B	0	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
B	64	CR8	HIS	CHROMOPHORE	UNP Q5S6Z9
B	64	CR8	TYR	CHROMOPHORE	UNP Q5S6Z9
B	64	CR8	GLY	CHROMOPHORE	UNP Q5S6Z9
B	173	SER	PHE	ENGINEERED MUTATION	UNP Q5S6Z9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	191	LEU	PHE	ENGINEERED MUTATION	UNP Q5S6Z9
C	-5	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
C	-4	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
C	-3	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
C	-2	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
C	-1	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
C	0	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
C	64	CR8	HIS	CHROMOPHORE	UNP Q5S6Z9
C	64	CR8	TYR	CHROMOPHORE	UNP Q5S6Z9
C	64	CR8	GLY	CHROMOPHORE	UNP Q5S6Z9
C	173	SER	PHE	ENGINEERED MUTATION	UNP Q5S6Z9
C	191	LEU	PHE	ENGINEERED MUTATION	UNP Q5S6Z9
D	-5	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
D	-4	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
D	-3	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
D	-2	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
D	-1	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
D	0	HIS	-	EXPRESSION TAG	UNP Q5S6Z9
D	64	CR8	HIS	CHROMOPHORE	UNP Q5S6Z9
D	64	CR8	TYR	CHROMOPHORE	UNP Q5S6Z9
D	64	CR8	GLY	CHROMOPHORE	UNP Q5S6Z9
D	173	SER	PHE	ENGINEERED MUTATION	UNP Q5S6Z9
D	191	LEU	PHE	ENGINEERED MUTATION	UNP Q5S6Z9

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



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	679	Total O 679 679	0	0
3	B	555	Total O 555 555	0	0
3	C	660	Total O 660 660	0	0

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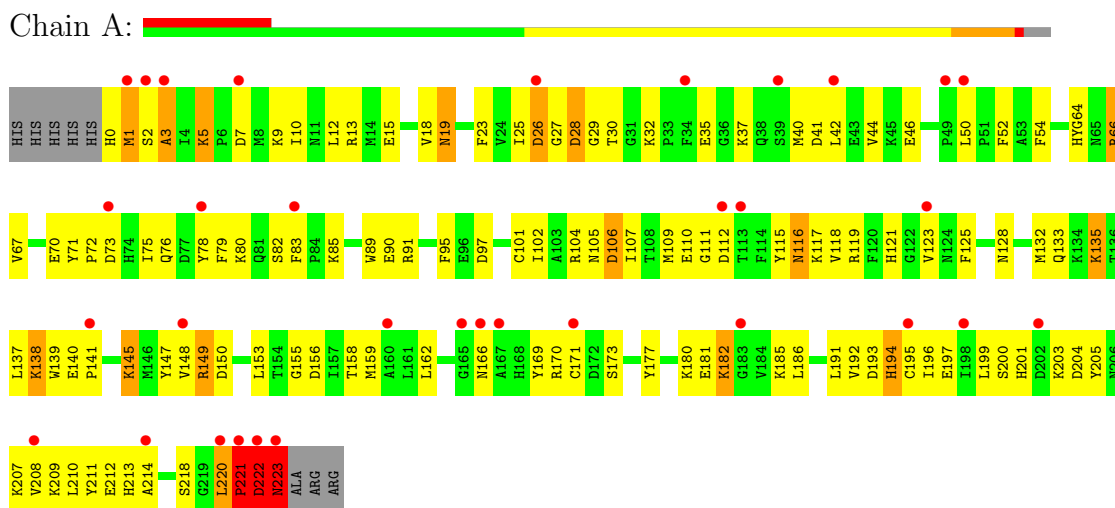
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	791	Total 791	O 791	0	0

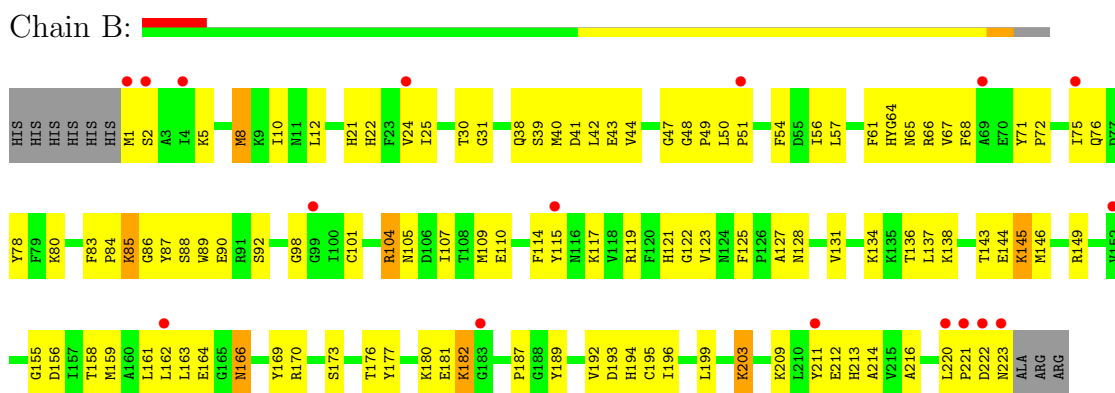
3 Residue-property plots

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.

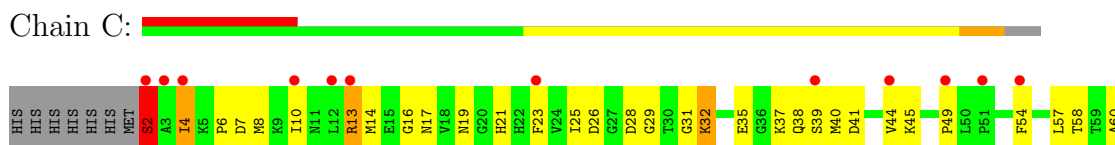
- Molecule 1: Green to red photoconvertible GPF-like protein EosFP

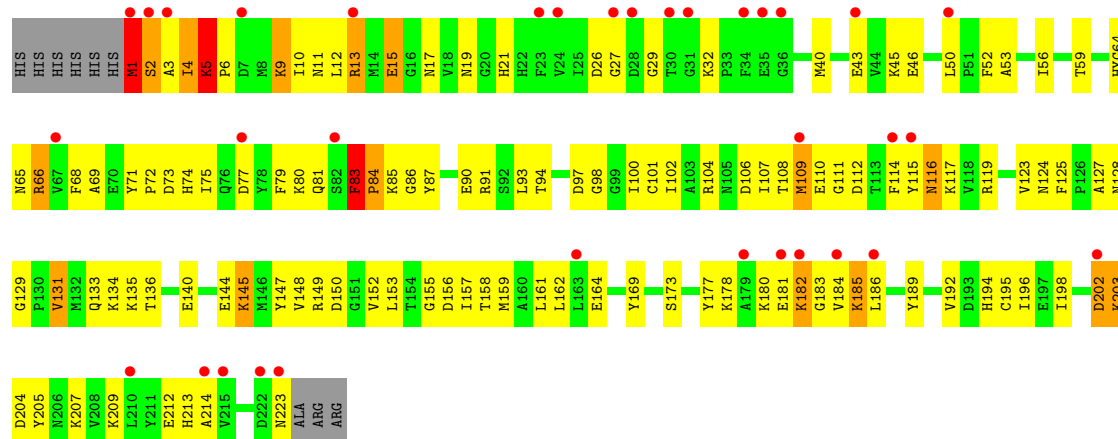


- Molecule 1: Green to red photoconvertible GPF-like protein EosFP



- Molecule 1: Green to red photoconvertible GPF-like protein EosFP





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.84Å 96.51Å 140.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.98 – 2.00 12.98 – 1.99	Depositor EDS
% Data completeness (in resolution range)	83.9 (12.98-2.00) 82.8 (12.98-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.34 (at 1.99Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.295 , 0.295 0.294 , 0.294	Depositor DCC
R_{free} test set	3263 reflections (4.97%)	DCC
Wilson B-factor (Å ²)	11.6	Xtriage
Anisotropy	2.002	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.53 , 78.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.39$	Xtriage
Outliers	9 of 74570 reflections (0.012%)	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	9939	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: CR8, 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	0.85	13/1838 (0.7%)	0.83	10/2478 (0.4%)
1	B	0.41	0/1821	0.60	0/2455
1	C	0.61	2/1805 (0.1%)	0.63	1/2434 (0.0%)
1	D	0.69	6/1819 (0.3%)	0.71	4/2452 (0.2%)
All	All	0.66	21/7283 (0.3%)	0.70	15/9819 (0.2%)

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	A	0	1
1	C	0	1
1	D	0	2
All	All	0	4

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2	SER	CB-OG	-15.59	1.22	1.42
1	A	221	PRO	CA-CB	-10.25	1.33	1.53
1	C	4	ILE	CB-CG2	-9.66	1.23	1.52
1	A	1	MET	C-O	-9.53	1.05	1.23
1	A	3	ALA	C-O	-8.81	1.06	1.23
1	D	4	ILE	CA-CB	-8.28	1.35	1.54
1	A	222	ASP	N-CA	-8.17	1.30	1.46
1	A	221	PRO	CG-CD	-8.08	1.24	1.50
1	A	1	MET	CG-SD	-7.77	1.60	1.81
1	A	221	PRO	CB-CG	-7.49	1.12	1.50
1	D	83	PHE	CE1-CZ	-7.32	1.23	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	83	PHE	CA-CB	-6.84	1.38	1.53
1	D	84	PRO	CB-CG	-6.76	1.16	1.50
1	D	84	PRO	C-O	-6.68	1.09	1.23
1	A	2	SER	CA-CB	-6.29	1.43	1.52
1	A	2	SER	C-O	-6.28	1.11	1.23
1	D	83	PHE	CG-CD1	6.02	1.47	1.38
1	A	222	ASP	CA-C	-5.45	1.38	1.52
1	A	223	ASN	C-O	5.40	1.33	1.23
1	A	3	ALA	CA-CB	5.26	1.63	1.52
1	A	2	SER	CB-OG	-5.01	1.35	1.42

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1	MET	CG-SD-CE	9.53	115.45	100.20
1	A	220	LEU	CA-CB-CG	9.19	136.44	115.30
1	A	3	ALA	N-CA-CB	8.49	121.99	110.10
1	A	2	SER	N-CA-C	7.64	131.63	111.00
1	D	5	LYS	CD-CE-NZ	6.71	127.13	111.70
1	A	221	PRO	CB-CA-C	-6.49	95.77	112.00
1	A	1	MET	CG-SD-CE	-6.10	90.44	100.20
1	A	222	ASP	CB-CG-OD2	6.09	123.78	118.30
1	A	2	SER	CA-CB-OG	-5.55	96.21	111.20
1	D	84	PRO	CA-N-CD	-5.36	104.00	111.50
1	A	221	PRO	CA-N-CD	-5.25	104.14	111.50
1	A	221	PRO	N-CD-CG	-5.17	95.44	103.20
1	C	4	ILE	CB-CA-C	-5.14	101.32	111.60
1	A	223	ASN	CB-CA-C	5.12	120.65	110.40
1	D	4	ILE	CG1-CB-CG2	5.11	122.63	111.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	221	PRO	Peptide
1	C	2	SER	Peptide
1	D	1	MET	Peptide
1	D	83	PHE	Peptide

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	1808	0	1740	153	0
1	B	1792	0	1729	139	1
1	C	1779	0	1714	144	1
1	D	1790	0	1730	144	0
2	A	20	0	0	1	0
2	B	15	0	0	5	0
2	C	25	0	0	4	0
2	D	25	0	0	1	0
3	A	679	0	0	79	5
3	B	555	0	0	67	6
3	C	660	0	0	66	3
3	D	791	0	0	68	5
All	All	9939	0	6913	574	11

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 41.

All (574) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:135:LYS:NZ	3:A:723:HOH:O	1.86	1.06
2:B:1225:SO4:O4	3:B:595:HOH:O	1.75	1.03
1:B:5:LYS:NZ	3:B:662:HOH:O	1.83	1.03
1:C:197:GLU:OE2	3:C:1385:HOH:O	1.80	0.99
1:D:212:GLU:OE1	3:D:2145:HOH:O	1.81	0.97
1:A:221:PRO:HG2	1:A:221:PRO:O	1.58	0.96
1:C:204:ASP:OD1	3:C:266:HOH:O	1.83	0.95
1:C:2:SER:HA	1:C:4:ILE:HD12	1.46	0.95
1:B:85:LYS:HD2	3:B:2780:HOH:O	1.67	0.94
1:A:70:GLU:OE1	3:A:1896:HOH:O	1.85	0.94
1:B:180:LYS:NZ	3:B:3080:HOH:O	2.01	0.93
1:A:159:MET:SD	1:A:173:SER:HB2	2.10	0.91
1:D:64:CR8:H10	3:D:1799:HOH:O	1.70	0.91
1:D:87:TYR:CZ	1:D:107:ILE:HD13	2.07	0.89
1:C:175:THR:HG23	3:C:1982:HOH:O	1.74	0.88

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:76:GLN:OE1	3:B:242:HOH:O	1.92	0.87
1:A:153:LEU:HB2	3:A:2117:HOH:O	1.73	0.87
1:B:50:LEU:O	1:B:134:LYS:NZ	2.08	0.87
1:B:137:LEU:O	3:B:284:HOH:O	1.92	0.86
1:B:85:LYS:HD3	1:B:181:GLU:HB2	1.57	0.86
1:A:0:HIS:HA	3:A:3332:HOH:O	1.75	0.86
2:B:1224:SO4:O2	3:B:2277:HOH:O	1.95	0.85
1:A:186:LEU:HD22	3:A:2117:HOH:O	1.77	0.84
1:C:104:ARG:HG3	1:C:119:ARG:HB2	1.61	0.82
1:B:10:ILE:HD12	3:B:312:HOH:O	1.76	0.82
1:D:148:VAL:HG22	3:D:2062:HOH:O	1.77	0.82
1:A:72:PRO:O	3:A:846:HOH:O	1.95	0.82
1:A:220:LEU:HB3	1:A:221:PRO:HB3	1.61	0.82
1:A:182:LYS:HB2	3:A:2689:HOH:O	1.78	0.82
1:C:112:ASP:OD1	3:C:292:HOH:O	1.98	0.81
2:C:1226:SO4:O2	3:C:2751:HOH:O	1.98	0.81
1:C:2:SER:CB	1:C:4:ILE:H	1.94	0.80
1:C:2:SER:CA	1:C:4:ILE:H	1.93	0.80
1:C:159:MET:SD	1:C:173:SER:HB3	2.21	0.80
2:B:227:SO4:O2	3:B:241:HOH:O	1.97	0.80
1:A:109:MET:O	3:A:2045:HOH:O	1.98	0.80
1:C:25:ILE:O	3:C:791:HOH:O	2.00	0.80
1:D:83:PHE:CE2	1:D:86:GLY:HA2	2.16	0.80
1:A:72:PRO:HG2	1:A:75:ILE:HG13	1.62	0.80
1:B:75:ILE:HD12	3:B:3176:HOH:O	1.81	0.79
1:B:180:LYS:O	3:B:962:HOH:O	1.98	0.79
1:D:27:GLY:O	3:D:904:HOH:O	2.00	0.79
1:A:76:GLN:NE2	3:A:530:HOH:O	1.81	0.79
1:D:223:ASN:O	3:D:1975:HOH:O	2.00	0.79
1:C:116:ASN:O	3:C:2138:HOH:O	2.00	0.79
1:C:77:ASP:HB2	3:C:3204:HOH:O	1.83	0.79
1:C:85:LYS:HG2	1:C:181:GLU:HG2	1.62	0.79
2:C:1224:SO4:O1	3:C:1898:HOH:O	2.00	0.78
1:A:73:ASP:OD1	3:A:1925:HOH:O	2.00	0.78
1:B:110:GLU:OE2	3:B:740:HOH:O	2.00	0.78
1:C:222:ASP:N	1:C:222:ASP:OD2	2.17	0.78
1:A:80:LYS:NZ	3:A:1784:HOH:O	2.00	0.78
1:D:73:ASP:OD2	3:D:563:HOH:O	2.02	0.77
1:D:128:ASN:O	3:D:1940:HOH:O	2.01	0.77
1:A:106[A]:ASP:OD1	3:A:3046:HOH:O	2.03	0.77
1:C:91:ARG:NH2	3:C:2773:HOH:O	2.16	0.77
1:B:104:ARG:HG2	3:B:2118:HOH:O	1.84	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:85:LYS:NZ	1:A:181:GLU:OE1	2.18	0.76
1:A:194:HIS:HB3	1:A:212:GLU:OE1	1.84	0.76
1:A:110:GLU:HB2	1:A:115:TYR:CE1	2.20	0.76
1:A:209:LYS:HG3	3:A:260:HOH:O	1.86	0.75
1:D:64:CR8:H23	1:D:212:GLU:HB2	1.68	0.75
1:B:49:PRO:HB2	3:B:2124:HOH:O	1.84	0.75
1:B:203:LYS:O	3:B:267:HOH:O	2.05	0.75
1:C:83:PHE:O	3:C:3135:HOH:O	2.03	0.75
1:A:106[B]:ASP:OD2	3:A:515:HOH:O	2.05	0.75
1:C:130:PRO:O	3:C:1876:HOH:O	2.04	0.75
1:D:64:CR8:C23	1:D:212:GLU:HB2	2.17	0.75
1:C:117:LYS:HE3	1:C:119:ARG:CZ	2.17	0.75
1:A:37:LYS:HE2	3:A:2795:HOH:O	1.86	0.75
1:D:202:ASP:OD2	1:D:207:LYS:HB2	1.87	0.75
1:C:121:HIS:NE2	3:C:466:HOH:O	2.20	0.75
1:A:66:ARG:HD2	1:A:192:VAL:HG11	1.69	0.74
1:C:161:LEU:HD12	1:C:169:TYR:HD2	1.52	0.74
1:B:30:THR:HB	3:B:2029:HOH:O	1.87	0.74
2:B:1225:SO4:O3	3:B:3330:HOH:O	2.06	0.73
1:C:85:LYS:HE2	3:C:3104:HOH:O	1.88	0.73
2:A:227:SO4:O3	3:A:1682:HOH:O	2.05	0.73
1:A:196:ILE:HG12	3:A:2116:HOH:O	1.87	0.73
1:A:185:LYS:HE3	3:A:3326:HOH:O	1.88	0.73
1:C:7:ASP:OD1	3:C:2148:HOH:O	2.06	0.73
1:A:199:LEU:O	3:A:738:HOH:O	2.06	0.73
1:B:199:LEU:O	3:B:299:HOH:O	2.04	0.73
1:D:10:ILE:HB	3:D:1432:HOH:O	1.88	0.73
1:B:220:LEU:O	3:B:2154:HOH:O	2.05	0.73
1:B:117:LYS:NZ	3:B:2103:HOH:O	2.22	0.73
1:D:45:LYS:HD3	3:D:3229:HOH:O	1.86	0.73
1:D:162:LEU:HD21	3:D:2141:HOH:O	1.87	0.73
1:C:64:CR8:H8	1:C:66:ARG:NH2	2.05	0.72
1:A:201:HIS:NE2	3:A:1805:HOH:O	2.22	0.72
1:D:13:ARG:HG2	3:D:3130:HOH:O	1.89	0.72
1:D:181:GLU:OE2	3:D:683:HOH:O	2.06	0.72
1:C:2:SER:HB2	3:C:762:HOH:O	1.88	0.72
1:D:135:LYS:HE2	3:D:951:HOH:O	1.88	0.71
1:C:2:SER:HB3	1:C:4:ILE:H	1.54	0.71
1:C:170:ARG:NH1	3:C:314:HOH:O	2.24	0.71
1:D:93:LEU:HB2	1:D:101:CYS:HB2	1.72	0.71
1:A:135:LYS:HB2	3:A:2678:HOH:O	1.89	0.71
1:D:195[A]:CYS:SG	1:D:213:HIS:HB3	2.31	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:11:ASN:OD1	3:D:904:HOH:O	2.09	0.70
1:B:222:ASP:OD2	3:B:1363:HOH:O	2.10	0.70
1:A:10:ILE:HD13	3:A:3119:HOH:O	1.89	0.70
1:C:6:PRO:O	3:C:447:HOH:O	2.08	0.70
1:B:209:LYS:NZ	3:B:1429:HOH:O	2.23	0.70
1:C:70:GLU:OE1	3:C:577:HOH:O	2.09	0.70
2:D:1226:SO4:O3	3:D:3132:HOH:O	2.08	0.70
1:A:222:ASP:C	1:A:222:ASP:OD1	2.29	0.70
1:A:148:VAL:O	3:A:294:HOH:O	2.10	0.69
1:A:28:ASP:N	1:A:28:ASP:OD1	2.26	0.69
1:D:56:ILE:HG12	3:D:809:HOH:O	1.89	0.69
1:C:202:ASP:OD2	1:C:207:LYS:HB2	1.92	0.69
1:C:31:GLY:HA3	1:C:68:PHE:CE2	2.28	0.69
1:B:50:LEU:HD22	3:B:2976:HOH:O	1.93	0.69
1:A:203:LYS:NZ	3:A:722:HOH:O	2.17	0.69
1:D:53:ALA:O	3:D:809:HOH:O	2.10	0.69
1:C:149:ARG:NH1	3:C:1745:HOH:O	2.25	0.69
1:D:128:ASN:O	3:D:2781:HOH:O	2.11	0.68
1:C:165:GLY:N	3:C:1379:HOH:O	2.25	0.68
1:C:174:ARG:HG2	1:D:124:ASN:ND2	2.09	0.68
1:C:80:LYS:O	3:C:3135:HOH:O	2.12	0.68
1:B:67:VAL:HG11	1:B:83:PHE:CE1	2.29	0.68
1:A:110:GLU:HB2	1:A:115:TYR:HE1	1.57	0.67
1:A:91:ARG:NH1	3:A:353:HOH:O	2.27	0.67
1:D:87:TYR:CE1	1:D:107:ILE:HD13	2.30	0.67
1:D:26:ASP:HB2	1:D:45:LYS:HE3	1.75	0.67
1:C:95:PHE:CD2	1:C:171:CYS:HB2	2.30	0.67
1:C:97:ASP:OD2	3:C:1981:HOH:O	2.12	0.67
1:B:72:PRO:HG2	1:B:75:ILE:HG13	1.76	0.67
1:C:87:TYR:CZ	1:C:107:ILE:HD12	2.29	0.67
2:C:1226:SO4:O2	3:C:948:HOH:O	2.13	0.67
1:B:64:CR8:O3	3:B:270:HOH:O	2.12	0.67
1:C:49:PRO:HA	3:C:248:HOH:O	1.95	0.67
1:C:83:PHE:HB3	1:C:84:PRO:HA	1.77	0.67
1:A:35:GLU:OE1	3:A:268:HOH:O	2.13	0.67
1:B:24:VAL:HG12	3:B:2066:HOH:O	1.94	0.67
1:A:104:ARG:NH1	1:B:122:GLY:O	2.28	0.67
1:D:136:THR:HG21	1:D:161:LEU:HD13	1.76	0.66
1:A:71:TYR:HB3	3:A:846:HOH:O	1.93	0.66
1:C:158:THR:HG23	1:C:170:ARG:CZ	2.25	0.66
1:C:2:SER:C	1:C:4:ILE:H	1.99	0.66
1:C:64:CR8:O25	3:C:2773:HOH:O	2.14	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:64:CR8:O3	3:A:458:HOH:O	2.13	0.66
1:C:117:LYS:HE3	1:C:119:ARG:NH1	2.11	0.66
1:B:90:GLU:OE1	3:B:1686:HOH:O	2.13	0.66
1:C:96:GLU:OE2	1:C:170:ARG:N	2.27	0.65
1:B:144:GLU:OE2	1:B:177:TYR:OH	2.14	0.65
1:A:7:ASP:O	3:A:965:HOH:O	2.14	0.65
1:C:220:LEU:O	3:C:2633:HOH:O	2.14	0.65
1:A:180:LYS:O	3:A:797:HOH:O	2.14	0.65
1:B:189:TYR:CE2	1:D:140:GLU:HB3	2.32	0.65
1:D:147:TYR:CE2	3:D:2129:HOH:O	2.50	0.65
1:C:10:ILE:HD11	1:C:68:PHE:CZ	2.33	0.64
1:D:150:ASP:HA	3:D:1857:HOH:O	1.97	0.64
1:B:78:TYR:HE2	3:B:2201:HOH:O	1.79	0.64
1:D:149:ARG:HG3	3:D:2175:HOH:O	1.97	0.64
1:A:112:ASP:HB3	3:A:3122:HOH:O	1.96	0.64
1:C:58:THR:CG2	3:C:2054:HOH:O	2.45	0.64
1:C:26:ASP:OD1	3:C:791:HOH:O	2.15	0.64
1:A:64:CR8:C14	3:A:1929:HOH:O	2.45	0.64
1:A:194:HIS:CB	1:A:212:GLU:OE1	2.45	0.64
1:A:64:CR8:H23	1:A:212:GLU:HB2	1.79	0.64
3:C:269:HOH:O	1:D:98:GLY:HA3	1.97	0.64
1:B:87:TYR:CZ	1:B:107:ILE:HD13	2.33	0.64
1:D:15:GLU:HG3	1:D:119:ARG:CZ	2.29	0.63
1:D:72:PRO:HG2	1:D:75:ILE:HD12	1.78	0.63
1:B:223:ASN:O	3:B:2653:HOH:O	2.14	0.63
1:D:186:LEU:HD22	3:D:2062:HOH:O	1.98	0.63
1:C:174:ARG:NH1	3:C:252:HOH:O	2.30	0.63
1:A:150:ASP:OD2	3:A:253:HOH:O	2.14	0.63
1:D:4:ILE:HD11	1:D:83:PHE:HB2	1.80	0.63
1:A:90:GLU:OE2	1:A:104:ARG:NE	2.28	0.62
1:C:151:GLY:N	3:C:283:HOH:O	2.09	0.62
3:C:482:HOH:O	1:D:127:ALA:HB2	1.98	0.62
1:C:2:SER:HB3	1:C:4:ILE:N	2.14	0.62
1:D:109:MET:HE2	1:D:114:PHE:CE1	2.33	0.62
1:C:196:ILE:HG21	3:C:3179:HOH:O	1.98	0.62
1:C:184:VAL:O	3:C:2627:HOH:O	2.16	0.61
1:B:182:LYS:HE3	3:B:1625:HOH:O	2.00	0.61
3:A:2622:HOH:O	1:B:22:HIS:HB2	2.01	0.61
1:C:16:GLY:HA3	1:C:23:PHE:CE1	2.34	0.61
1:A:110:GLU:HG3	3:A:3041:HOH:O	1.99	0.61
1:A:46:GLU:OE2	3:A:838:HOH:O	2.16	0.61
1:A:133:GLN:HB2	3:A:2678:HOH:O	2.00	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:64:CR8:H8	1:B:66:ARG:NH1	2.16	0.61
1:D:19:ASN:ND2	3:D:241:HOH:O	2.13	0.61
1:A:138:LYS:HE2	1:A:162:LEU:HD22	1.83	0.60
1:D:40:MET:HB2	3:D:1799:HOH:O	2.01	0.60
1:B:199:LEU:HD12	1:B:209:LYS:HG2	1.82	0.60
1:D:59:THR:HG23	3:D:273:HOH:O	2.02	0.60
1:C:174:ARG:NH2	3:C:269:HOH:O	2.11	0.60
1:A:210:LEU:HB2	3:A:2777:HOH:O	2.02	0.60
1:D:77:ASP:OD2	1:D:80:LYS:HD2	2.00	0.60
1:B:56:ILE:HA	3:B:2791:HOH:O	2.02	0.60
1:C:8:MET:O	1:C:31:GLY:N	2.29	0.60
1:B:25:ILE:HD12	1:B:61:PHE:HZ	1.66	0.60
1:C:133:GLN:OE1	3:C:836:HOH:O	2.17	0.59
1:A:78:TYR:O	1:A:82:SER:OG	2.16	0.59
1:C:111:GLY:O	3:C:721:HOH:O	2.17	0.59
1:D:147:TYR:HA	3:D:2132:HOH:O	2.02	0.59
1:C:31:GLY:HA3	1:C:68:PHE:HE2	1.67	0.59
1:C:203:LYS:HB3	3:C:1848:HOH:O	2.03	0.59
1:C:145:LYS:O	1:C:155:GLY:HA2	2.03	0.59
1:A:220:LEU:HD23	1:A:223:ASN:HD21	1.67	0.59
1:A:67:VAL:HG23	1:A:80:LYS:HG2	1.85	0.59
1:B:80:LYS:NZ	3:B:245:HOH:O	2.34	0.59
1:D:156:ASP:N	3:D:2129:HOH:O	2.36	0.59
1:C:184:VAL:O	3:C:257:HOH:O	2.16	0.59
1:B:72:PRO:HD2	3:B:3176:HOH:O	2.03	0.59
1:A:158:THR:HG23	1:A:170:ARG:NH1	2.18	0.59
1:D:125:PHE:CE1	1:D:131:VAL:HG21	2.38	0.58
1:D:110:GLU:HB2	1:D:115:TYR:CE1	2.38	0.58
1:C:40:MET:HB2	3:C:2069:HOH:O	2.03	0.58
1:C:66:ARG:HG2	1:C:79:PHE:CE1	2.38	0.58
1:B:144:GLU:CD	1:B:146:MET:HE1	2.22	0.58
1:A:197:GLU:HG3	3:A:2704:HOH:O	2.03	0.58
3:A:654:HOH:O	1:C:221:PRO:HG3	2.03	0.58
1:D:108:THR:HB	3:D:244:HOH:O	2.04	0.58
1:C:2:SER:C	1:C:4:ILE:N	2.55	0.57
1:C:136:THR:HG21	1:C:161:LEU:HD13	1.84	0.57
1:A:54:PHE:CZ	1:A:208:VAL:HG21	2.38	0.57
1:B:89:TRP:NE1	1:B:105:ASN:HB3	2.18	0.57
1:D:1:MET:HB3	3:D:1063:HOH:O	2.04	0.57
1:C:125:PHE:CE1	1:C:131:VAL:HG21	2.39	0.57
1:B:12:LEU:C	1:B:12:LEU:HD23	2.24	0.57
1:B:64:CR8:C23	1:B:212:GLU:HB2	2.35	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:13:ARG:NH1	3:A:2674:HOH:O	2.37	0.57
1:A:23:PHE:CE2	1:A:52:PHE:HZ	2.23	0.56
1:A:64:CR8:H8	1:A:66:ARG:CZ	2.34	0.56
1:B:220:LEU:CD2	1:B:221:PRO:HA	2.34	0.56
1:A:140:GLU:HB3	1:C:189:TYR:CE2	2.40	0.56
1:C:4:ILE:O	1:C:4:ILE:HG22	1.90	0.56
1:A:7:ASP:OD1	3:A:3171:HOH:O	2.17	0.56
1:A:140:GLU:HB3	1:A:141:PRO:HD2	1.86	0.56
1:C:79:PHE:HE2	1:C:177:TYR:CD1	2.23	0.56
1:A:37:LYS:HE3	1:A:213:HIS:CE1	2.41	0.56
1:B:193:ASP:O	1:B:214:ALA:HA	2.06	0.56
1:B:44:VAL:HG12	3:B:833:HOH:O	2.04	0.56
1:C:25:ILE:HG12	1:C:44:VAL:HG22	1.87	0.56
1:A:123:VAL:HB	1:B:90:GLU:HB3	1.87	0.56
1:A:118:VAL:O	1:A:119:ARG:NH2	2.37	0.56
1:D:203:LYS:HD2	3:D:2762:HOH:O	2.06	0.56
1:B:158:THR:HG23	1:B:170:ARG:CZ	2.36	0.56
1:C:49:PRO:HB3	1:C:204:ASP:HB3	1.88	0.56
1:C:7:ASP:OD1	1:C:32:LYS:NZ	2.36	0.56
1:B:71:TYR:O	3:B:2162:HOH:O	2.18	0.56
1:A:125:PHE:HB2	1:A:132:MET:HE3	1.89	0.55
1:B:30:THR:HG23	3:B:288:HOH:O	2.06	0.55
1:B:145:LYS:O	1:B:155:GLY:HA2	2.06	0.55
1:B:156:ASP:HB3	3:D:1813:HOH:O	2.06	0.55
1:C:40:MET:HE3	1:C:64:CR8:H10	1.89	0.55
1:C:13:ARG:HA	3:C:791:HOH:O	2.06	0.55
1:B:181:GLU:HG2	1:B:182:LYS:O	2.07	0.55
1:D:29:GLY:HA2	3:D:1759:HOH:O	2.05	0.55
1:B:84:PRO:HB3	1:B:109:MET:CE	2.37	0.55
1:A:210:LEU:HD13	3:A:2777:HOH:O	2.06	0.55
1:B:66:ARG:HB2	3:B:1907:HOH:O	2.05	0.55
1:B:144:GLU:OE2	1:B:146:MET:HE1	2.07	0.55
1:B:66:ARG:N	3:B:1907:HOH:O	2.20	0.54
1:D:161:LEU:HB2	1:D:169:TYR:HB3	1.89	0.54
1:A:30:THR:O	3:A:2120:HOH:O	2.18	0.54
1:D:13:ARG:NH1	3:D:2258:HOH:O	2.40	0.54
1:D:32:LYS:HE2	3:D:2176:HOH:O	2.08	0.54
1:C:136:THR:CG2	1:C:161:LEU:HD13	2.38	0.54
1:A:149:ARG:NH2	1:C:96:GLU:OE1	2.40	0.54
1:A:32:LYS:HG2	3:A:3171:HOH:O	2.06	0.54
1:A:207:LYS:HG2	3:A:247:HOH:O	2.08	0.54
1:B:76:GLN:N	3:B:1415:HOH:O	2.41	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:101:CYS:HA	1:B:121:HIS:O	2.07	0.54
1:C:32:LYS:HB3	1:C:35:GLU:HB2	1.90	0.54
1:C:58:THR:HG22	3:C:2054:HOH:O	2.05	0.54
1:C:161:LEU:HD12	1:C:169:TYR:CD2	2.38	0.53
1:D:111:GLY:HA3	3:D:1406:HOH:O	2.07	0.53
1:A:19:ASN:ND2	3:A:1806:HOH:O	1.91	0.53
1:C:130:PRO:HG3	3:C:506:HOH:O	2.08	0.53
1:A:149:ARG:NH2	3:A:496:HOH:O	2.05	0.53
1:D:3:ALA:HA	3:D:1778:HOH:O	2.08	0.53
1:D:65:ASN:HD22	1:D:68:PHE:HE1	1.57	0.53
1:C:123:VAL:HG12	1:D:90:GLU:OE2	2.09	0.53
1:D:157:ILE:HB	1:D:173:SER:HB3	1.90	0.53
1:D:136:THR:CG2	1:D:161:LEU:HD13	2.38	0.53
1:C:58:THR:HG23	3:C:2054:HOH:O	2.06	0.53
1:A:46:GLU:HG2	3:A:751:HOH:O	2.09	0.53
1:A:125:PHE:HB2	1:A:132:MET:CE	2.39	0.53
1:A:128:ASN:OD1	3:A:2169:HOH:O	2.18	0.53
1:B:119:ARG:NH1	3:B:1952:HOH:O	2.27	0.52
1:D:64:CR8:H8	1:D:194:HIS:CE1	2.45	0.52
1:B:196:ILE:HB	1:B:212:GLU:HG2	1.90	0.52
1:D:72:PRO:HB2	1:D:74:HIS:CE1	2.45	0.52
1:D:69:ALA:O	1:D:80:LYS:NZ	2.42	0.52
1:D:9:LYS:HB3	3:D:2761:HOH:O	2.09	0.52
1:B:166:ASN:HB2	3:B:1984:HOH:O	2.08	0.52
1:A:197:GLU:HB2	3:A:917:HOH:O	2.08	0.52
1:B:162:LEU:HD21	3:B:719:HOH:O	2.10	0.52
1:C:38:GLN:NE2	3:C:1637:HOH:O	2.05	0.52
1:B:182:LYS:N	3:B:1814:HOH:O	2.42	0.52
1:B:48:GLY:O	3:B:930:HOH:O	2.18	0.52
1:D:156:ASP:HB2	3:D:1836:HOH:O	2.11	0.51
1:D:125:PHE:CD1	1:D:131:VAL:HG21	2.46	0.51
1:A:101:CYS:HA	1:A:121:HIS:O	2.10	0.51
1:C:49:PRO:CB	1:C:204:ASP:HB3	2.40	0.51
1:B:67:VAL:CG1	1:B:83:PHE:HE1	2.23	0.51
1:D:145:LYS:O	1:D:155:GLY:HA2	2.10	0.51
1:A:3:ALA:O	1:A:5:LYS:HE3	2.11	0.51
1:A:23:PHE:CE2	1:A:52:PHE:CZ	2.98	0.51
1:C:197:GLU:O	1:C:210:LEU:HD12	2.10	0.51
1:A:111:GLY:O	3:A:711:HOH:O	2.19	0.51
1:A:204:ASP:O	1:A:205:TYR:HB2	2.09	0.51
1:B:12:LEU:HB3	1:B:40:MET:HE2	1.93	0.51
1:A:207:LYS:HE3	3:A:1348:HOH:O	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:204:ASP:O	1:D:205:TYR:HB2	2.10	0.51
1:D:72:PRO:HB2	1:D:74:HIS:ND1	2.25	0.51
1:A:83:PHE:HB3	1:A:109:MET:HE2	1.93	0.50
1:B:110:GLU:CG	1:B:115:TYR:CE1	2.94	0.50
1:B:159:MET:SD	1:B:173:SER:HB2	2.52	0.50
1:D:152:VAL:HA	3:D:256:HOH:O	2.10	0.50
1:D:178:LYS:HD3	3:D:2991:HOH:O	2.10	0.50
1:C:136:THR:HG23	3:C:1876:HOH:O	2.12	0.50
1:A:112:ASP:HA	3:A:711:HOH:O	2.11	0.50
1:A:218:SER:HB2	3:A:465:HOH:O	2.11	0.50
1:C:14:MET:HA	1:C:118:VAL:O	2.11	0.50
1:B:195:CYS:SG	1:B:213:HIS:HB3	2.51	0.50
1:D:5:LYS:HB3	1:D:6:PRO:HD2	1.93	0.50
1:A:64:CR8:C23	1:A:212:GLU:HB2	2.41	0.50
1:A:40:MET:HB2	1:A:64:CR8:H10	1.94	0.50
1:D:209:LYS:HE2	3:D:2744:HOH:O	2.12	0.50
1:B:51:PRO:HA	1:B:134:LYS:HZ2	1.77	0.50
1:A:137:LEU:HD12	1:A:162:LEU:HG	1.93	0.50
1:A:25:ILE:HG12	1:A:44:VAL:HG22	1.94	0.50
1:B:136:THR:HG21	1:B:161:LEU:HD13	1.93	0.50
1:D:66:ARG:NH2	3:D:252:HOH:O	2.44	0.50
1:C:39:SER:HA	1:C:210:LEU:O	2.11	0.49
1:B:85:LYS:HB2	3:B:235:HOH:O	2.12	0.49
1:D:13:ARG:NH2	3:D:642:HOH:O	2.44	0.49
1:C:144:GLU:HA	1:C:157:ILE:HG12	1.94	0.49
1:B:41:ASP:OD1	1:B:209:LYS:HE3	2.11	0.49
1:C:17:ASN:HA	1:C:21:HIS:O	2.12	0.49
1:C:37:LYS:HD3	1:C:211:TYR:OH	2.11	0.49
1:C:104:ARG:CG	1:C:119:ARG:HB2	2.39	0.49
1:A:107:ILE:N	1:A:107:ILE:HD12	2.28	0.49
1:C:64:CR8:H8	1:C:66:ARG:HH22	1.77	0.49
1:C:57:LEU:O	1:C:60:ALA:HB3	2.12	0.49
1:A:26:ASP:O	1:A:42:LEU:HA	2.13	0.49
1:C:91:ARG:HB2	3:C:1982:HOH:O	2.11	0.49
1:C:93:LEU:HB2	1:C:101:CYS:HB2	1.94	0.49
1:D:129:GLY:O	1:D:133:GLN:HB2	2.13	0.49
1:D:50:LEU:HD13	1:D:52:PHE:CZ	2.47	0.49
1:D:2:SER:HB2	3:D:1966:HOH:O	2.13	0.49
1:B:220:LEU:HG	3:D:2778:HOH:O	2.11	0.49
1:B:21:HIS:CE1	1:B:47:GLY:O	2.66	0.49
1:C:182:LYS:HD2	3:C:2403:HOH:O	2.12	0.49
1:A:0:HIS:CA	3:A:3332:HOH:O	2.48	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:138:LYS:HE2	1:A:162:LEU:CD2	2.42	0.48
1:B:145:LYS:HD3	1:D:158:THR:HB	1.94	0.48
1:B:68:PHE:HB3	3:B:884:HOH:O	2.13	0.48
1:C:89:TRP:CE2	1:C:105:ASN:HB3	2.47	0.48
1:B:67:VAL:HG11	1:B:83:PHE:HE1	1.75	0.48
1:B:145:LYS:N	1:B:145:LYS:HD2	2.28	0.48
1:C:98:GLY:HA2	3:C:1946:HOH:O	2.12	0.48
1:D:182:LYS:HD3	3:D:725:HOH:O	2.12	0.48
1:D:83:PHE:CD2	1:D:86:GLY:HA2	2.48	0.48
1:B:163:LEU:HD11	1:B:169:TYR:HB2	1.96	0.48
1:D:110:GLU:HG2	3:D:2083:HOH:O	2.12	0.48
1:B:31:GLY:HA3	1:B:68:PHE:CE1	2.48	0.48
1:D:185:LYS:HB2	3:D:1964:HOH:O	2.14	0.48
1:A:37:LYS:HB2	3:A:1983:HOH:O	2.13	0.48
1:C:14:MET:HG2	3:C:3175:HOH:O	2.12	0.48
1:A:32:LYS:HD2	3:A:1983:HOH:O	2.14	0.48
1:C:66:ARG:NH1	1:C:177:TYR:OH	2.43	0.48
1:C:111:GLY:HA3	3:C:2235:HOH:O	2.14	0.48
1:A:95:PHE:CD1	1:A:171:CYS:HB2	2.49	0.48
1:B:182:LYS:HB2	3:B:1814:HOH:O	2.13	0.48
1:D:149:ARG:NH1	3:D:1852:HOH:O	2.46	0.48
1:C:54:PHE:CE2	1:C:208:VAL:HG11	2.48	0.48
1:D:104:ARG:HG3	1:D:119:ARG:HB2	1.95	0.48
1:D:153:LEU:HA	3:D:2062:HOH:O	2.13	0.47
1:A:13:ARG:CZ	3:A:2674:HOH:O	2.62	0.47
1:A:27:GLY:HA2	1:A:41:ASP:O	2.13	0.47
1:D:94:THR:HG23	1:D:100:ILE:CD1	2.44	0.47
1:A:145:LYS:O	1:A:155:GLY:HA2	2.14	0.47
1:A:67:VAL:O	1:A:80:LYS:HE3	2.13	0.47
1:B:84:PRO:HB3	1:B:109:MET:HE1	1.96	0.47
1:C:202:ASP:HB2	2:C:1226:SO4:O1	2.14	0.47
1:D:198:ILE:HD13	1:D:205:TYR:HE2	1.78	0.47
1:D:69:ALA:HA	1:D:214:ALA:HB3	1.96	0.47
1:C:10:ILE:N	1:C:29:GLY:O	2.45	0.47
1:B:123:VAL:HG22	3:B:2050:HOH:O	2.13	0.47
1:B:149:ARG:HD2	3:B:1995:HOH:O	2.14	0.47
1:C:73:ASP:OD2	3:C:2686:HOH:O	2.19	0.47
1:A:220:LEU:HD23	1:A:223:ASN:ND2	2.30	0.47
1:B:220:LEU:C	3:B:2749:HOH:O	2.53	0.47
1:B:66:ARG:NH2	3:B:256:HOH:O	2.47	0.47
1:D:32:LYS:HZ2	1:D:32:LYS:HG2	1.64	0.47
1:B:143:THR:H	1:D:145:LYS:NZ	2.12	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:185:LYS:HE3	1:D:185:LYS:HB3	1.54	0.47
1:A:220:LEU:HB3	1:A:221:PRO:CB	2.38	0.47
1:C:202:ASP:HB3	3:C:1902:HOH:O	2.14	0.47
1:A:12:LEU:HD23	1:A:13:ARG:N	2.30	0.47
1:D:32:LYS:HE3	3:D:1880:HOH:O	2.15	0.47
1:D:66:ARG:HG2	1:D:79:PHE:CE1	2.50	0.47
1:B:21:HIS:HE1	1:B:47:GLY:O	1.97	0.46
1:B:98:GLY:HA3	3:B:234:HOH:O	2.14	0.46
1:C:206:ASN:OD1	3:C:248:HOH:O	2.20	0.46
1:D:10:ILE:N	3:D:2761:HOH:O	2.49	0.46
1:C:90:GLU:C	3:C:1982:HOH:O	2.52	0.46
1:D:117:LYS:HD3	3:D:2052:HOH:O	2.16	0.46
1:C:90:GLU:OE2	1:D:19:ASN:HA	2.16	0.46
1:B:12:LEU:HB3	1:B:40:MET:CE	2.45	0.46
1:A:18:VAL:HB	1:A:52:PHE:CE2	2.51	0.46
1:D:117:LYS:HE2	3:D:1998:HOH:O	2.14	0.46
1:A:13:ARG:HG3	3:A:645:HOH:O	2.16	0.46
1:B:39[A]:SER:OG	1:B:211:TYR:HD1	1.98	0.46
1:B:39[B]:SER:OG	1:B:211:TYR:HD1	1.98	0.46
1:A:102:ILE:HD12	1:A:102:ILE:C	2.36	0.46
1:B:143:THR:H	1:D:145:LYS:HZ1	1.63	0.46
1:A:32:LYS:HE2	3:A:555:HOH:O	2.16	0.46
1:A:42:LEU:HD11	1:A:210:LEU:HD22	1.98	0.46
1:D:45:LYS:HD2	3:D:1721:HOH:O	2.15	0.46
1:B:220:LEU:HD22	1:B:221:PRO:HA	1.96	0.46
1:A:54:PHE:CE1	1:A:208:VAL:HG21	2.50	0.46
1:B:89:TRP:CE2	1:B:105:ASN:HB3	2.51	0.46
1:C:76:GLN:NE2	1:C:81:GLN:HG3	2.29	0.46
1:B:88[A]:SER:OG	3:B:2907:HOH:O	2.08	0.46
1:C:2:SER:OG	1:C:4:ILE:HB	2.16	0.46
1:D:85:LYS:HE2	3:D:2966:HOH:O	2.16	0.46
1:A:147:TYR:CZ	1:A:149:ARG:HD2	2.50	0.46
1:D:56:ILE:CG1	3:D:809:HOH:O	2.56	0.46
1:A:35:GLU:HB3	3:A:2017:HOH:O	2.16	0.45
1:D:91:ARG:O	1:D:102:ILE:HA	2.16	0.45
1:D:85:LYS:HD2	1:D:181:GLU:OE2	2.16	0.45
1:A:90:GLU:HB3	1:B:123:VAL:HB	1.99	0.45
1:D:156:ASP:CG	3:D:2129:HOH:O	2.55	0.45
1:A:12:LEU:C	1:A:12:LEU:HD23	2.37	0.45
1:B:146:MET:HE3	3:B:876:HOH:O	2.16	0.45
1:D:85:LYS:HD2	1:D:181:GLU:HB2	1.98	0.45
1:B:64:CR8:H23	1:B:212:GLU:HB2	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:196:ILE:HG22	3:C:2981:HOH:O	2.15	0.45
1:D:180:LYS:HD2	1:D:180:LYS:HA	1.84	0.45
1:D:116:ASN:N	1:D:116:ASN:ND2	2.64	0.45
1:B:76:GLN:HB3	1:B:187:PRO:HA	1.98	0.45
1:B:64:CR8:C14	3:B:1781:HOH:O	2.64	0.45
1:D:153:LEU:HB3	1:D:177:TYR:HB2	1.97	0.45
1:A:85:LYS:HD3	1:A:181:GLU:OE2	2.17	0.45
1:B:146:MET:CE	3:B:876:HOH:O	2.65	0.45
1:A:13:ARG:HD2	1:A:13:ARG:HA	1.77	0.45
1:D:159:MET:SD	1:D:173:SER:HB2	2.57	0.45
1:B:164:GLU:O	3:B:934:HOH:O	2.21	0.45
1:C:105:ASN:CG	1:C:118:VAL:HG22	2.37	0.45
1:C:202:ASP:CB	3:C:1902:HOH:O	2.65	0.45
1:A:195[A]:CYS:SG	1:A:213:HIS:HB3	2.57	0.45
1:D:147:TYR:HE2	3:D:2129:HOH:O	1.93	0.45
1:A:89:TRP:CE2	1:A:105:ASN:HB3	2.52	0.45
1:C:112:ASP:OD2	3:C:1997:HOH:O	2.21	0.44
1:D:45:LYS:C	1:D:46:GLU:HG3	2.37	0.44
1:A:37:LYS:CE	3:A:2795:HOH:O	2.55	0.44
1:D:53:ALA:N	1:D:134:LYS:HG2	2.32	0.44
1:B:65:ASN:OD1	1:B:67:VAL:HG22	2.17	0.44
1:C:13:ARG:HB2	3:C:2138:HOH:O	2.15	0.44
1:A:37:LYS:NZ	3:A:510:HOH:O	2.11	0.44
1:D:9:LYS:HD3	1:D:112:ASP:OD2	2.18	0.44
1:B:83:PHE:HB3	1:B:84:PRO:HA	1.98	0.44
1:A:208:VAL:HG12	3:A:2777:HOH:O	2.16	0.44
1:C:124:ASN:N	3:D:653:HOH:O	2.50	0.44
1:D:66:ARG:HG3	1:D:66:ARG:O	2.18	0.44
1:A:66:ARG:CZ	1:A:66:ARG:HB2	2.47	0.44
1:B:144:GLU:CD	1:B:146:MET:CE	2.86	0.44
1:C:105:ASN:HA	1:C:117:LYS:O	2.18	0.44
1:C:121:HIS:HB3	1:D:102:ILE:HD11	1.99	0.44
1:A:13:ARG:NH1	3:A:2360:HOH:O	2.50	0.44
1:D:81:GLN:HG3	3:D:2057:HOH:O	2.17	0.44
1:D:164:GLU:O	3:D:1362:HOH:O	2.21	0.44
1:D:66:ARG:HD2	1:D:192:VAL:HG11	1.99	0.44
1:C:192:VAL:HG12	1:C:193:ASP:O	2.18	0.44
1:A:110:GLU:CG	3:A:3041:HOH:O	2.63	0.44
1:A:28:ASP:OD2	3:A:946:HOH:O	2.20	0.44
1:B:87:TYR:CE1	1:B:107:ILE:HD13	2.53	0.43
1:A:125:PHE:CB	1:A:132:MET:HE2	2.48	0.43
1:A:135:LYS:HD2	3:A:2678:HOH:O	2.17	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:0:HIS:NE2	1:A:83:PHE:O	2.41	0.43
1:D:119:ARG:HA	1:D:119:ARG:HD3	1.74	0.43
1:D:43:GLU:HG2	1:D:45:LYS:HE2	2.00	0.43
1:D:29:GLY:CA	3:D:1432:HOH:O	2.67	0.43
1:B:83:PHE:CZ	1:B:114:PHE:HE1	2.36	0.43
1:B:123:VAL:HG13	3:B:2050:HOH:O	2.17	0.43
1:D:117:LYS:HG3	1:D:119:ARG:HH22	1.82	0.43
1:D:196:ILE:HB	1:D:212:GLU:HG2	2.00	0.43
1:A:67:VAL:CG2	1:A:80:LYS:HG2	2.48	0.43
1:A:5:LYS:HD2	3:A:711:HOH:O	2.18	0.43
1:C:38:GLN:HB2	3:C:1637:HOH:O	2.18	0.43
3:A:289:HOH:O	1:B:127:ALA:HB3	2.19	0.43
1:B:110:GLU:HG2	1:B:115:TYR:CE1	2.52	0.43
1:B:84:PRO:HB3	1:B:109:MET:HE2	2.01	0.43
1:A:137:LEU:HD11	3:A:3243:HOH:O	2.17	0.43
1:B:8:MET:HG3	3:B:2240:HOH:O	2.17	0.43
1:D:144:GLU:HB3	1:D:192:VAL:HB	2.01	0.43
1:D:15:GLU:HG3	1:D:119:ARG:NH1	2.33	0.43
1:D:131:VAL:HB	3:D:233:HOH:O	2.18	0.43
1:D:183:GLY:O	1:D:184:VAL:C	2.55	0.43
1:D:87:TYR:CZ	1:D:107:ILE:CD1	2.93	0.43
1:D:43:GLU:OE1	1:D:207:LYS:HG2	2.18	0.43
1:A:200:SER:HB3	3:A:1386:HOH:O	2.19	0.43
1:A:72:PRO:HB3	3:A:1589:HOH:O	2.19	0.43
1:A:123:VAL:HG12	1:B:90:GLU:OE2	2.19	0.43
1:C:130:PRO:C	3:C:1876:HOH:O	2.55	0.42
1:D:9:LYS:HE3	1:D:112:ASP:OD2	2.19	0.42
1:A:10:ILE:N	1:A:29:GLY:O	2.49	0.42
1:B:51:PRO:HA	1:B:134:LYS:NZ	2.34	0.42
1:D:13:ARG:NH2	3:D:3051:HOH:O	2.51	0.42
1:B:196:ILE:HB	1:B:212:GLU:CG	2.49	0.42
1:D:145:LYS:HG3	1:D:189:TYR:OH	2.19	0.42
1:B:170:ARG:HB3	1:B:170:ARG:CZ	2.49	0.42
1:D:12:LEU:HD23	1:D:12:LEU:C	2.39	0.42
1:B:22:HIS:CE1	3:B:2211:HOH:O	2.72	0.42
1:A:166:ASN:ND2	3:A:3220:HOH:O	2.10	0.42
1:B:137:LEU:HD22	3:B:2796:HOH:O	2.19	0.42
1:C:134:LYS:NZ	3:C:630:HOH:O	2.53	0.42
1:A:116:ASN:N	1:A:116:ASN:ND2	2.67	0.42
1:B:136:THR:CG2	1:B:161:LEU:HD13	2.49	0.42
1:C:217:HIS:ND1	1:C:223:ASN:HB3	2.34	0.42
1:B:38:GLN:NE2	3:B:323:HOH:O	2.07	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:85:LYS:NZ	3:B:704:HOH:O	2.16	0.42
1:B:92:SER:O	1:B:173:SER:HA	2.20	0.42
1:C:205:TYR:N	1:C:205:TYR:CD1	2.88	0.42
1:C:83:PHE:CB	1:C:84:PRO:HA	2.45	0.42
1:A:15:GLU:OE2	3:A:569:HOH:O	2.21	0.42
1:C:49:PRO:HB3	1:C:204:ASP:CB	2.50	0.42
1:C:89:TRP:HB2	3:C:1982:HOH:O	2.20	0.42
1:B:89:TRP:HA	1:B:176:THR:O	2.20	0.42
1:A:193:ASP:O	1:A:214:ALA:HA	2.19	0.42
1:A:139:TRP:CZ3	1:A:159:MET:HB3	2.55	0.42
1:A:97:ASP:OD1	1:A:169:TYR:OH	2.31	0.42
1:B:125:PHE:CE1	1:B:131:VAL:HG21	2.55	0.42
1:A:64:CR8:H2	1:A:196:ILE:HB	2.00	0.41
1:B:220:LEU:HB3	1:D:195[A]:CYS:SG	2.60	0.41
1:D:135:LYS:NZ	3:D:3105:HOH:O	2.13	0.41
1:C:54:PHE:CD2	3:C:2054:HOH:O	2.72	0.41
1:C:196:ILE:HB	1:C:212:GLU:CG	2.50	0.41
1:A:79:PHE:HE1	1:A:177:TYR:CD1	2.37	0.41
1:C:41:ASP:OD1	1:C:209:LYS:HG3	2.19	0.41
1:C:89:TRP:HA	3:C:2085:HOH:O	2.19	0.41
2:B:227:SO4:O3	3:B:2729:HOH:O	2.21	0.41
1:B:220:LEU:HA	1:B:221:PRO:HA	1.74	0.41
1:B:203:LYS:HD3	3:B:3325:HOH:O	2.21	0.41
1:A:199:LEU:HD11	1:A:211:TYR:HB2	2.03	0.41
1:C:126:PRO:HB3	3:D:2175:HOH:O	2.18	0.41
1:C:148:VAL:HG11	1:C:186:LEU:HD13	2.02	0.41
1:D:5:LYS:HD3	1:D:5:LYS:N	2.35	0.41
1:A:156:ASP:HA	1:A:173:SER:O	2.21	0.41
1:A:66:ARG:NE	1:A:194:HIS:HE1	2.17	0.41
1:B:194:HIS:HB3	1:B:212:GLU:OE1	2.20	0.41
1:A:50:LEU:HD13	1:A:52:PHE:CE1	2.55	0.41
1:C:217:HIS:CE1	1:C:219:GLY:HA2	2.55	0.41
1:B:83:PHE:CE2	1:B:86:GLY:HA2	2.56	0.41
1:B:203:LYS:HE3	3:B:2516:HOH:O	2.20	0.41
1:A:203:LYS:HB3	3:A:806:HOH:O	2.19	0.41
1:A:204:ASP:O	3:A:264:HOH:O	2.21	0.41
1:C:90:GLU:HB3	1:D:123:VAL:HB	2.02	0.41
1:D:135:LYS:NZ	3:D:2684:HOH:O	2.47	0.41
1:C:163:LEU:HD11	1:C:169:TYR:HB2	2.03	0.41
1:C:102:ILE:HD12	1:C:102:ILE:C	2.42	0.41
1:B:5:LYS:H	1:B:8:MET:HE1	1.86	0.40
1:A:64:CR8:H8	1:A:66:ARG:NH1	2.36	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:71:TYR:HA	1:D:72:PRO:HD3	1.81	0.40
1:D:66:ARG:CZ	1:D:66:ARG:HB2	2.50	0.40
1:C:60:ALA:O	1:C:118:VAL:HG11	2.21	0.40
1:C:26:ASP:OD2	1:C:45:LYS:HG3	2.21	0.40
1:D:97:ASP:OD1	1:D:169:TYR:OH	2.31	0.40
1:B:43:GLU:HG3	3:B:3206:HOH:O	2.20	0.40
1:C:137:LEU:HD23	1:C:137:LEU:HA	1.75	0.40
1:A:111:GLY:HA2	3:A:681:HOH:O	2.21	0.40
1:B:192:VAL:HA	1:B:216:ALA:HA	2.02	0.40
1:D:17:ASN:HA	1:D:21:HIS:O	2.21	0.40
1:B:64:CR8:H6	1:B:212:GLU:OE1	2.21	0.40
1:B:54:PHE:HB2	3:B:421:HOH:O	2.20	0.40
1:D:94:THR:HG23	1:D:100:ILE:HD13	2.04	0.40

All (11) 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:128:ASN:ND2	3:B:322:HOH:O[3_554]	1.89	0.31
3:A:3106:HOH:O	3:D:2715:HOH:O[4_445]	1.99	0.21
3:B:2380:HOH:O	3:D:2944:HOH:O[3_554]	2.02	0.18
3:A:453:HOH:O	3:B:301:HOH:O[3_554]	2.04	0.16
3:C:1436:HOH:O	3:D:2068:HOH:O[2_555]	2.05	0.15
3:B:2134:HOH:O	3:C:638:HOH:O[2_554]	2.06	0.14
1:C:41:ASP:OD2	3:A:752:HOH:O[4_555]	2.07	0.13
3:A:710:HOH:O	3:D:2307:HOH:O[3_554]	2.07	0.13
3:A:308:HOH:O	3:B:522:HOH:O[3_554]	2.08	0.12
3:B:771:HOH:O	3:B:1414:HOH:O[3_554]	2.09	0.11
3:C:552:HOH:O	3:D:2030:HOH:O[2_555]	2.15	0.05

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	223/230 (97%)	210 (94%)	11 (5%)	2 (1%)	25 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	221/230 (96%)	218 (99%)	3 (1%)	0	100	100
1	C	219/230 (95%)	211 (96%)	8 (4%)	0	100	100
1	D	221/230 (96%)	212 (96%)	7 (3%)	2 (1%)	25	14
All	All	884/920 (96%)	851 (96%)	29 (3%)	4 (0%)	38	29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	PRO
1	A	222	ASP
1	D	84	PRO
1	D	131	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	194/197 (98%)	174 (90%)	20 (10%)	10	5
1	B	192/197 (98%)	180 (94%)	12 (6%)	25	18
1	C	190/197 (96%)	174 (92%)	16 (8%)	16	9
1	D	192/197 (98%)	177 (92%)	15 (8%)	18	11
All	All	768/788 (98%)	705 (92%)	63 (8%)	17	10

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	LYS
1	A	9	LYS
1	A	19	ASN
1	A	26	ASP
1	A	28	ASP
1	A	66	ARG
1	A	106[A]	ASP

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Mol	Chain	Res	Type
1	A	106[B]	ASP
1	A	116	ASN
1	A	117	LYS
1	A	135	LYS
1	A	138	LYS
1	A	145	LYS
1	A	149	ARG
1	A	182	LYS
1	A	191	LEU
1	A	194	HIS
1	A	222	ASP
1	A	223	ASN
1	B	1	MET
1	B	2	SER
1	B	8	MET
1	B	42	LEU
1	B	57	LEU
1	B	85	LYS
1	B	104	ARG
1	B	138	LYS
1	B	145	LYS
1	B	166	ASN
1	B	182	LYS
1	B	203	LYS
1	C	13	ARG
1	C	19	ASN
1	C	28	ASP
1	C	32	LYS
1	C	67	VAL
1	C	85	LYS
1	C	100	ILE
1	C	110	GLU
1	C	116	ASN
1	C	145	LYS
1	C	174	ARG
1	C	182	LYS
1	C	196	ILE
1	C	205	TYR
1	C	209	LYS
1	C	222	ASP
1	D	1	MET
1	D	2	SER

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Mol	Chain	Res	Type
1	D	5	LYS
1	D	9	LYS
1	D	13	ARG
1	D	15	GLU
1	D	66	ARG
1	D	106	ASP
1	D	109	MET
1	D	116	ASN
1	D	145	LYS
1	D	182	LYS
1	D	185	LYS
1	D	202	ASP
1	D	203	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	76	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	CR8	A	64	1	27,27,28	3.76	8 (29%)	29,37,39	1.90	8 (27%)
1	CR8	B	64	1	27,27,28	3.64	7 (25%)	29,37,39	1.93	7 (24%)
1	CR8	C	64	1	27,27,28	3.55	9 (33%)	29,37,39	2.21	10 (34%)
1	CR8	D	64	1	27,27,28	3.77	7 (25%)	29,37,39	2.35	6 (20%)

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
1	CR8	A	64	1	-	0/9/25/26	0/3/3/3
1	CR8	B	64	1	-	0/9/25/26	0/3/3/3
1	CR8	C	64	1	-	0/9/25/26	0/3/3/3
1	CR8	D	64	1	-	0/9/25/26	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	64	CR8	O19-C	17.19	1.23	1.11
1	A	64	CR8	O19-C	16.97	1.23	1.11
1	B	64	CR8	O19-C	16.28	1.22	1.11
1	C	64	CR8	O19-C	15.63	1.22	1.11
1	B	64	CR8	C8-C7	5.87	1.49	1.36
1	A	64	CR8	C8-C7	5.79	1.49	1.36
1	D	64	CR8	C8-C7	5.28	1.47	1.36
1	C	64	CR8	C8-C7	5.26	1.47	1.36
1	B	64	CR8	C4-C1	-3.15	1.38	1.46
1	D	64	CR8	C4-C1	-3.15	1.38	1.46
1	C	64	CR8	C2-C1	-3.12	1.39	1.46
1	B	64	CR8	C2-C1	-3.07	1.39	1.46
1	A	64	CR8	C4-C1	-2.91	1.39	1.46
1	D	64	CR8	C2-C1	-2.90	1.39	1.46
1	C	64	CR8	C21-N22	-2.85	1.34	1.38
1	A	64	CR8	C2-C1	-2.71	1.39	1.46
1	B	64	CR8	C9-C8	2.67	1.48	1.39
1	C	64	CR8	C4-C1	-2.62	1.40	1.46
1	A	64	CR8	C9-C8	2.61	1.48	1.39
1	D	64	CR8	C9-C8	2.60	1.48	1.39
1	C	64	CR8	C9-C12	-2.51	1.36	1.40
1	C	64	CR8	C9-N15	-2.48	1.33	1.39
1	D	64	CR8	C21-N22	-2.46	1.35	1.38
1	C	64	CR8	C9-C8	2.35	1.47	1.39
1	C	64	CR8	C12-N13	-2.25	1.31	1.36
1	A	64	CR8	C21-N22	-2.23	1.35	1.38
1	A	64	CR8	C20-C21	2.23	1.51	1.49
1	D	64	CR8	C9-C12	-2.18	1.37	1.40
1	A	64	CR8	C9-C12	-2.13	1.37	1.40
1	B	64	CR8	C5-C4	2.07	1.40	1.35
1	B	64	CR8	C21-N22	-2.06	1.35	1.38

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	64	CR8	C20-C16-C14	-6.95	103.72	111.18
1	C	64	CR8	C20-C16-C14	-5.98	104.76	111.18
1	D	64	CR8	C9-C12-N13	5.46	111.08	104.65
1	D	64	CR8	C12-N13-C14	-5.31	104.93	111.94
1	C	64	CR8	C9-C12-N13	5.20	110.78	104.65
1	C	64	CR8	C12-N13-C14	-5.11	105.19	111.94
1	B	64	CR8	C9-C12-N13	4.68	110.16	104.65
1	A	64	CR8	C12-N13-C14	-4.57	105.90	111.94
1	B	64	CR8	C12-N13-C14	-4.49	106.01	111.94
1	A	64	CR8	C9-C12-N13	4.42	109.85	104.65
1	D	64	CR8	C2-C6-C7	-3.50	118.87	121.92
1	A	64	CR8	C20-C16-C14	-2.98	107.99	111.18
1	C	64	CR8	C4-C5-C7	-2.94	119.36	121.92
1	B	64	CR8	C20-C16-C14	-2.92	108.05	111.18
1	A	64	CR8	C21-C20-C16	-2.92	107.26	113.19
1	B	64	CR8	C20-C21-C23	-2.91	125.48	130.62
1	B	64	CR8	C9-C8-C7	-2.86	122.45	128.63
1	D	64	CR8	C20-C21-C23	-2.75	125.77	130.62
1	C	64	CR8	C9-C8-C7	-2.63	122.95	128.63
1	D	64	CR8	C9-C8-C7	-2.55	123.12	128.63
1	A	64	CR8	C9-C8-C7	-2.42	123.40	128.63
1	A	64	CR8	C20-C21-C23	-2.39	126.39	130.62
1	C	64	CR8	C20-C21-C23	-2.25	126.64	130.62
1	C	64	CR8	C6-C7-C5	2.23	120.27	115.23
1	C	64	CR8	C2-C6-C7	-2.23	119.98	121.92
1	C	64	CR8	C21-C20-C16	-2.17	108.78	113.19
1	A	64	CR8	C17-N13-C12	2.15	128.33	124.24
1	B	64	CR8	C2-C6-C7	-2.14	120.06	121.92
1	C	64	CR8	C17-N13-C14	2.14	129.63	126.62
1	A	64	CR8	C4-C1-C2	2.04	120.25	116.66
1	B	64	CR8	C17-N13-C12	2.01	128.06	124.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

17 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	1224	-	4,4,4	0.10	0	6,6,6	0.13	0
2	SO4	A	1225	-	4,4,4	0.21	0	6,6,6	0.15	0
2	SO4	A	227	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	A	228	-	4,4,4	0.18	0	6,6,6	0.12	0
2	SO4	B	1224	-	4,4,4	0.16	0	6,6,6	0.08	0
2	SO4	B	1225	-	4,4,4	0.25	0	6,6,6	0.11	0
2	SO4	B	227	-	4,4,4	0.25	0	6,6,6	0.32	0
2	SO4	C	1224	-	4,4,4	0.16	0	6,6,6	0.14	0
2	SO4	C	1225	-	4,4,4	0.15	0	6,6,6	0.16	0
2	SO4	C	1226	-	4,4,4	0.25	0	6,6,6	0.11	0
2	SO4	C	1227	-	4,4,4	0.20	0	6,6,6	0.09	0
2	SO4	C	227	-	4,4,4	0.17	0	6,6,6	0.07	0
2	SO4	D	1225	-	4,4,4	0.28	0	6,6,6	0.10	0
2	SO4	D	1226	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	D	1227	-	4,4,4	0.28	0	6,6,6	0.11	0
2	SO4	D	227	-	4,4,4	0.20	0	6,6,6	0.13	0
2	SO4	D	228	-	4,4,4	0.25	0	6,6,6	0.10	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	1224	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1225	-	-	0/0/0/0	0/0/0/0
2	SO4	A	227	-	-	0/0/0/0	0/0/0/0
2	SO4	A	228	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1224	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1225	-	-	0/0/0/0	0/0/0/0
2	SO4	B	227	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1224	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	C	1225	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1226	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1227	-	-	0/0/0/0	0/0/0/0
2	SO4	C	227	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1225	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1226	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1227	-	-	0/0/0/0	0/0/0/0
2	SO4	D	227	-	-	0/0/0/0	0/0/0/0
2	SO4	D	228	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	222/230 (96%)	1.26	33 (14%) 3 3	12, 20, 30, 38	2 (0%)
1	B	221/230 (96%)	1.04	17 (7%) 13 12	11, 18, 26, 40	1 (0%)
1	C	220/230 (95%)	1.34	40 (18%) 2 2	14, 21, 30, 37	2 (0%)
1	D	221/230 (96%)	1.33	34 (15%) 3 3	13, 22, 34, 49	3 (1%)
All	All	884/920 (96%)	1.24	124 (14%) 4 3	11, 20, 31, 49	8 (0%)

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2	SER	5.2
1	B	1	MET	4.6
1	D	115	TYR	3.7
1	D	3	ALA	3.6
1	A	222	ASP	3.5
1	D	24	VAL	3.5
1	C	2	SER	3.4
1	C	3	ALA	3.4
1	C	81	GLN	3.3
1	A	3	ALA	3.2
1	A	166	ASN	3.2
1	C	150	ASP	3.1
1	C	86	GLY	3.1
1	D	186	LEU	3.1
1	C	223	ASN	3.1
1	C	83	PHE	3.0
1	A	198	ILE	3.0
1	D	184	VAL	3.0
1	C	10	ILE	3.0
1	D	1	MET	3.0
1	B	69	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	49	PRO	2.9
1	A	165	GLY	2.9
1	A	171	CYS	2.8
1	C	182	LYS	2.8
1	D	7	ASP	2.8
1	D	27	GLY	2.8
1	C	118	VAL	2.7
1	D	13	ARG	2.7
1	A	183	GLY	2.7
1	D	182	LYS	2.7
1	C	23	PHE	2.7
1	D	50	LEU	2.7
1	A	214	ALA	2.6
1	D	181	GLU	2.6
1	A	221	PRO	2.6
1	C	221	PRO	2.6
1	C	12	LEU	2.6
1	B	2	SER	2.6
1	D	34	PHE	2.6
1	A	123	VAL	2.6
1	C	184	VAL	2.6
1	A	148	VAL	2.6
1	C	214	ALA	2.6
1	D	67	VAL	2.6
1	A	7	ASP	2.5
1	B	222	ASP	2.5
1	D	23	PHE	2.5
1	A	167	ALA	2.5
1	B	162	LEU	2.5
1	B	183	GLY	2.5
1	A	220	LEU	2.5
1	A	202	ASP	2.5
1	A	42	LEU	2.5
1	C	107	ILE	2.5
1	D	43	GLU	2.4
1	C	220	LEU	2.4
1	B	223	ASN	2.4
1	A	49	PRO	2.4
1	D	109	MET	2.4
1	C	84	PRO	2.4
1	D	222	ASP	2.4
1	D	30	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	179	ALA	2.4
1	C	151	GLY	2.4
1	A	50	LEU	2.3
1	A	195[A]	CYS	2.3
1	A	112	ASP	2.3
1	B	211	TYR	2.3
1	C	186	LEU	2.3
1	D	77	ASP	2.3
1	D	36	GLY	2.3
1	A	73	ASP	2.3
1	D	82	SER	2.3
1	B	115	TYR	2.3
1	B	221	PRO	2.3
1	A	113	THR	2.3
1	A	39[A]	SER	2.2
1	D	214	ALA	2.2
1	A	34	PHE	2.2
1	D	114	PHE	2.2
1	C	93	LEU	2.2
1	B	152	VAL	2.2
1	D	223	ASN	2.2
1	C	13	ARG	2.2
1	A	78	TYR	2.2
1	C	54	PHE	2.2
1	D	202	ASP	2.2
1	B	4	ILE	2.2
1	D	163	LEU	2.2
1	C	69	ALA	2.2
1	C	211	TYR	2.2
1	B	75	ILE	2.2
1	A	208	VAL	2.2
1	A	83	PHE	2.1
1	A	141	PRO	2.1
1	C	64	CR8	2.1
1	D	31	GLY	2.1
1	A	160	ALA	2.1
1	C	183	GLY	2.1
1	A	223	ASN	2.1
1	B	51	PRO	2.1
1	C	44	VAL	2.1
1	C	130	PRO	2.1
1	A	2	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	220	LEU	2.1
1	C	202	ASP	2.1
1	C	222	ASP	2.1
1	D	215	VAL	2.1
1	B	99	GLY	2.1
1	A	26	ASP	2.1
1	D	35	GLU	2.0
1	D	210	LEU	2.0
1	B	24	VAL	2.0
1	C	136	THR	2.0
1	C	4	ILE	2.0
1	A	1	MET	2.0
1	D	28	ASP	2.0
1	C	92	SER	2.0
1	C	125	PHE	2.0
1	C	51	PRO	2.0
1	C	204	ASP	2.0
1	C	198	ILE	2.0
1	C	39	SER	2.0

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

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	CR8	C	64	25/26	0.21	0.55	6,17,24,32	0
1	CR8	B	64	25/26	0.18	-0.11	11,17,21,23	0
1	CR8	A	64	25/26	0.18	-0.31	9,18,26,34	0
1	CR8	D	64	25/26	0.18	-0.31	11,19,25,27	0

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	C	227	5/5	0.33	10.79	36,38,55,74	0
2	SO4	C	1225	5/5	0.33	5.97	23,23,39,51	0
2	SO4	C	1226	5/5	0.32	3.02	25,25,29,40	5
2	SO4	A	228	5/5	0.30	2.57	31,34,54,59	0
2	SO4	B	1224	5/5	0.34	1.72	34,40,51,62	0
2	SO4	D	1226	5/5	0.32	1.43	29,36,44,51	5
2	SO4	D	1225	5/5	0.26	1.39	29,30,35,37	0
2	SO4	B	1225	5/5	0.22	1.22	8,13,20,27	5
2	SO4	D	227	5/5	0.29	1.22	32,35,45,55	0
2	SO4	A	1224	5/5	0.20	0.78	21,30,35,46	0
2	SO4	D	228	5/5	0.20	0.56	28,28,33,41	0
2	SO4	B	227	5/5	0.21	0.40	17,26,28,42	0
2	SO4	A	1225	5/5	0.27	-0.12	11,11,22,35	5
2	SO4	D	1227	5/5	0.28	-0.31	18,27,33,39	5
2	SO4	C	1224	5/5	0.21	-0.32	22,27,39,49	0
2	SO4	C	1227	5/5	0.19	-1.70	24,27,39,45	5
2	SO4	A	227	5/5	0.13	-4.05	29,30,36,38	0

6.5 Other polymers ⓘ

There are no such residues in this entry.