



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 08:52 PM GMT

PDB ID : 3L7Z  
Title : Crystal structure of the *S. solfataricus* archaeal exosome  
Authors : Lu, C.; Ding, F.; Ke, A.  
Deposited on : 2009-12-29  
Resolution : 2.41 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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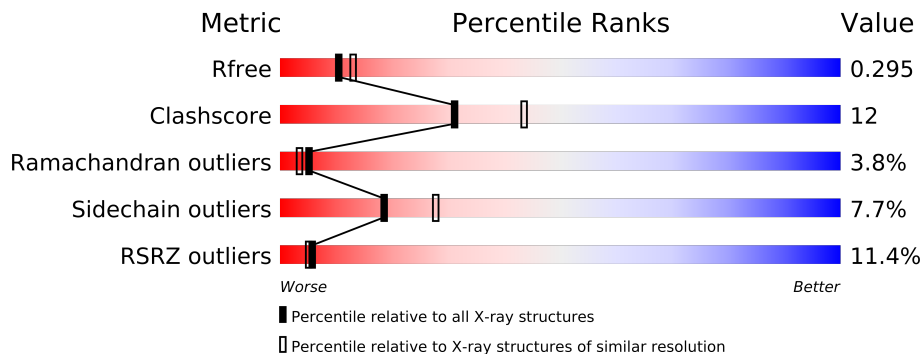
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.41 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	2496 (2.44-2.40)
Clashscore	79885	3124 (2.44-2.40)
Ramachandran outliers	78287	3067 (2.44-2.40)
Sidechain outliers	78261	3068 (2.44-2.40)
RSRZ outliers	66119	2499 (2.44-2.40)

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	271	
1	D	271	
1	G	271	
2	B	245	
2	E	245	
2	H	245	
3	C	249	
3	F	249	
3	I	249	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16393 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 Probable exosome complex exonuclease 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	0	0
			1926	1229	314	378	5			
1	D	261	Total	C	N	O	S	0	0	0
			1974	1260	321	388	5			
1	G	270	Total	C	N	O	S	0	0	0
			2082	1328	338	411	5			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	THR	GLU	engineered	UNP Q9UXC0
A	?	-	HIS	DELETION	UNP Q9UXC0
A	?	-	SER	DELETION	UNP Q9UXC0
A	?	-	ASN	DELETION	UNP Q9UXC0
A	?	-	GLY	DELETION	UNP Q9UXC0
D	96	THR	GLU	engineered	UNP Q9UXC0
D	?	-	HIS	DELETION	UNP Q9UXC0
D	?	-	SER	DELETION	UNP Q9UXC0
D	?	-	ASN	DELETION	UNP Q9UXC0
D	?	-	GLY	DELETION	UNP Q9UXC0
G	96	THR	GLU	engineered	UNP Q9UXC0
G	?	-	HIS	DELETION	UNP Q9UXC0
G	?	-	SER	DELETION	UNP Q9UXC0
G	?	-	ASN	DELETION	UNP Q9UXC0
G	?	-	GLY	DELETION	UNP Q9UXC0

- Molecule 2 is a protein called Probable exosome complex exonuclease 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	232	Total	C	N	O	S	0	0	0
			1774	1122	309	334	9			

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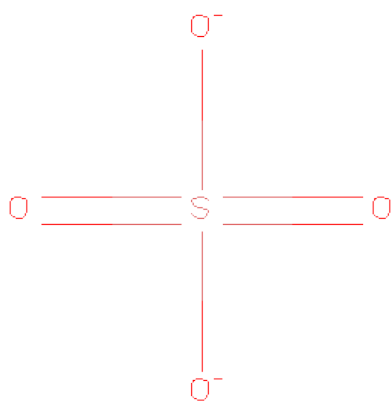
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	237	Total	C	N	O	S	0	0	0
			1832	1157	319	346	10			
2	H	234	Total	C	N	O	S	0	0	0
			1810	1142	316	342	10			

- Molecule 3 is a protein called Probable exosome complex RNA-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	222	Total	C	N	O	S	0	0	0
			1697	1096	279	319	3			
3	F	215	Total	C	N	O	S	0	0	0
			1705	1104	281	316	4			
3	I	206	Total	C	N	O	S	0	0	0
			1578	1029	250	296	3			

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



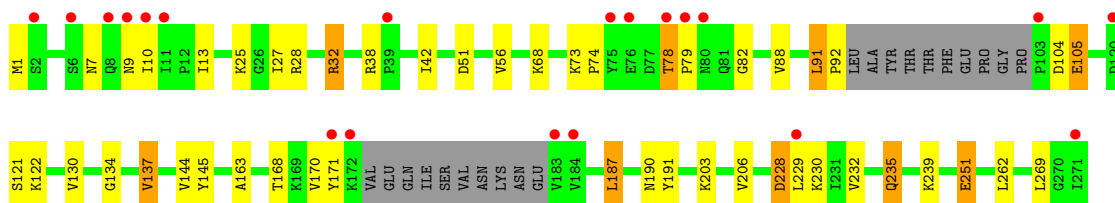
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		

### 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.

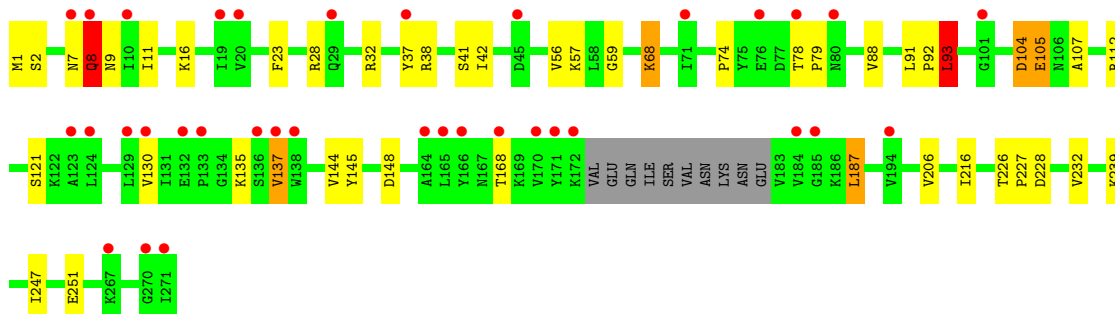
- Molecule 1: Probable exosome complex exonuclease 2

Chain A: 



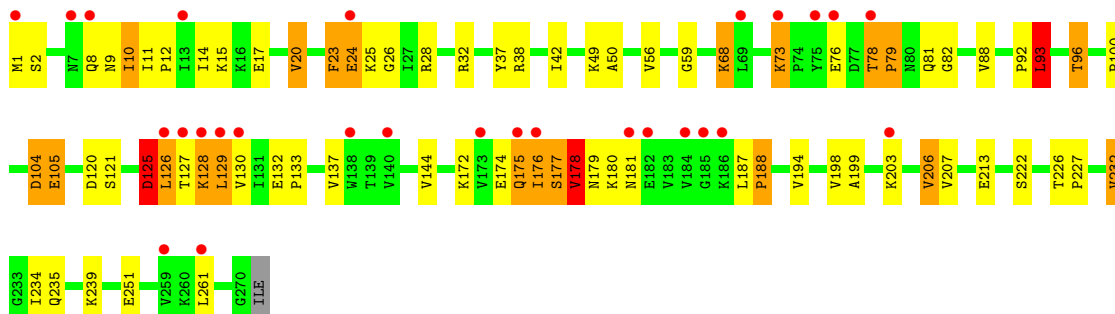
- Molecule 1: Probable exosome complex exonuclease 2

Chain D: 



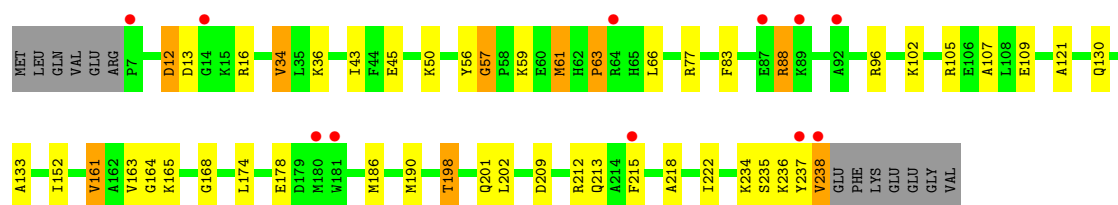
- Molecule 1: Probable exosome complex exonuclease 2

Chain G: 



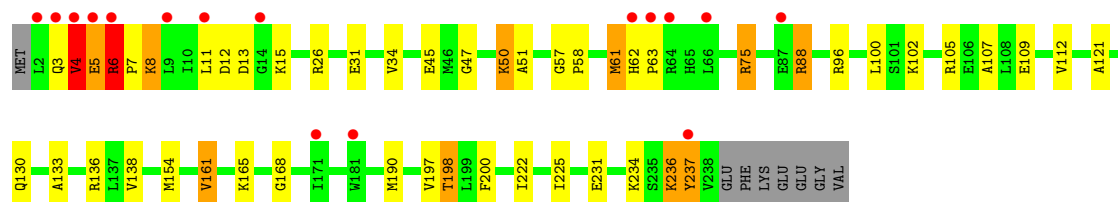
- Molecule 2: Probable exosome complex exonuclease 1

Chain B: 



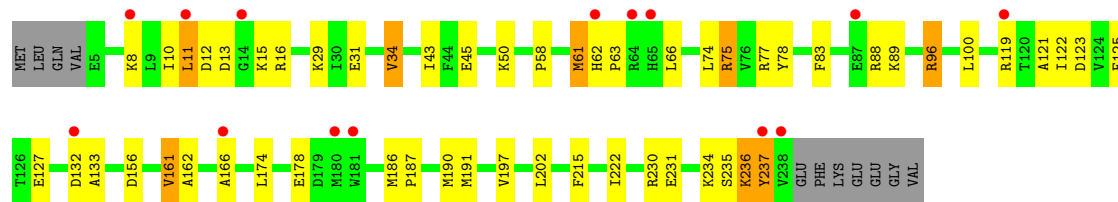
• Molecule 2: Probable exosome complex exonuclease 1

Chain E:



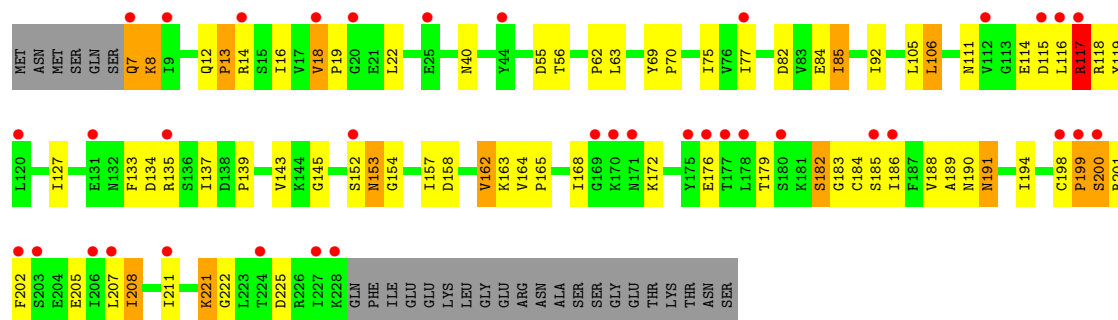
• Molecule 2: Probable exosome complex exonuclease 1

Chain H:



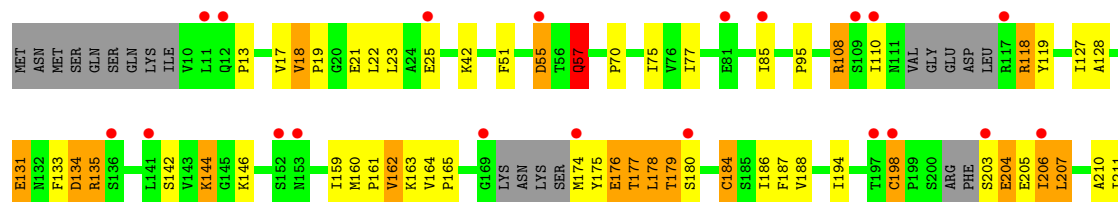
• Molecule 3: Probable exosome complex RNA-binding protein 1

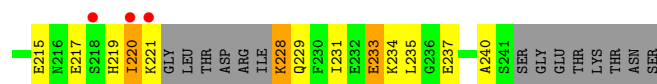
Chain C:



• Molecule 3: Probable exosome complex RNA-binding protein 1

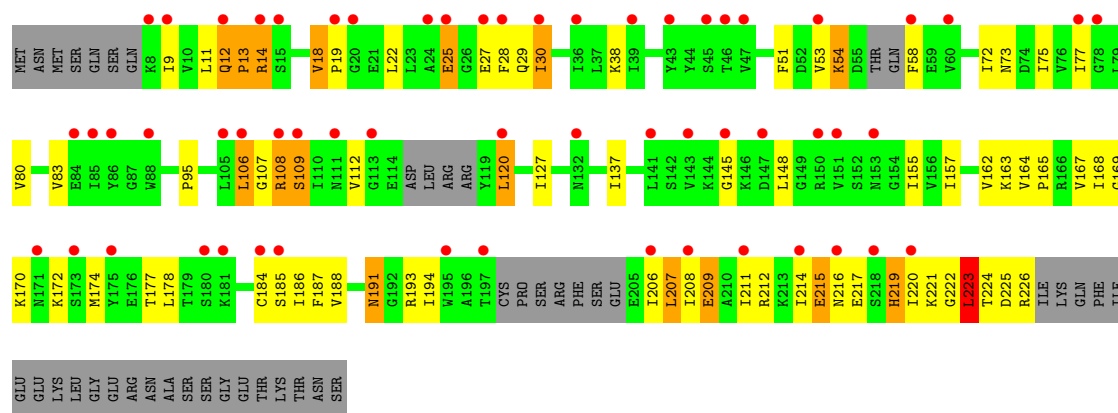
Chain F:





- Molecule 3: Probable exosome complex RNA-binding protein 1

Chain I:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.12Å 145.48Å 97.25Å 90.00° 93.79° 90.00°	Depositor
Resolution (Å)	20.00 – 2.41 20.00 – 2.41	Depositor EDS
% Data completeness (in resolution range)	92.4 (20.00-2.41) 92.4 (20.00-2.41)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.4.0066	Depositor
R, $R_{free}$	0.263 , 0.289 0.264 , 0.295	Depositor DCC
$R_{free}$ test set	7505 reflections (11.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.7	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 43.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 74262 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	16393	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.34	0/1952	0.54	0/2646
1	D	0.32	0/2004	0.53	1/2724 (0.0%)
1	G	0.35	0/2114	0.60	0/2873
2	B	0.35	0/1802	0.56	0/2439
2	E	0.37	0/1859	0.59	1/2512 (0.0%)
2	H	0.36	0/1838	0.57	0/2484
3	C	0.37	0/1732	0.62	0/2362
3	F	0.37	0/1737	0.58	0/2351
3	I	0.38	0/1609	0.62	0/2188
All	All	0.36	0/16647	0.58	2/22579 (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	G	0	2
2	H	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	236	LYS	N-CA-C	-5.37	96.49	111.00
1	D	93	LEU	CA-CB-CG	5.25	127.38	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	125	ASP	Peptide
1	G	76	GLU	Peptide
2	H	11	LEU	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	1926	0	1997	29	0
1	D	1974	0	2008	28	0
1	G	2082	0	2151	65	0
2	B	1774	0	1801	36	0
2	E	1832	0	1882	34	0
2	H	1810	0	1850	49	0
3	C	1697	0	1667	54	0
3	F	1705	0	1733	54	0
3	I	1578	0	1555	76	0
4	B	5	0	0	0	0
4	E	5	0	0	0	0
4	H	5	0	0	0	0
All	All	16393	0	16644	388	0

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 12.

All (388) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:221:LYS:HB3	3:I:222:GLY:HA2	1.21	1.18
3:I:224:THR:HB	3:I:225:ASP:HB3	1.25	1.18
3:C:221:LYS:HG3	3:C:222:GLY:HA2	1.28	1.14
2:H:236:LYS:O	2:H:237:TYR:CD2	2.02	1.12
3:I:208:ILE:N	3:I:209:GLU:HB3	1.67	1.10
1:G:125:ASP:HB3	1:G:127:THR:HA	1.34	1.09
3:I:224:THR:HB	3:I:225:ASP:CB	1.83	1.08
1:G:127:THR:CB	1:G:128:LYS:HB2	1.86	1.05
2:H:237:TYR:HD2	3:I:219:HIS:CD2	1.76	1.02

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:237:TYR:CD2	3:I:219:HIS:NE2	2.28	1.02
3:C:117:ARG:HD3	3:C:118:ARG:H	1.22	1.00
2:H:237:TYR:CD2	3:I:219:HIS:CD2	2.50	1.00
1:G:127:THR:HB	1:G:128:LYS:CB	1.92	0.99
1:D:7:ASN:CA	1:D:8:GLN:HB2	1.92	0.98
3:I:224:THR:HB	3:I:225:ASP:CA	1.93	0.98
1:G:127:THR:HB	1:G:128:LYS:HB2	0.99	0.96
3:I:224:THR:CB	3:I:225:ASP:HB3	1.96	0.96
3:F:134:ASP:CG	3:F:135:ARG:H	1.69	0.94
1:G:1:MET:N	2:H:77:ARG:HH12	1.65	0.94
1:A:235:GLN:HE22	2:B:201:GLN:HE21	1.16	0.93
3:I:221:LYS:CB	3:I:222:GLY:HA2	2.01	0.90
3:F:178:LEU:O	3:F:180:SER:N	2.05	0.88
3:I:221:LYS:HB3	3:I:222:GLY:CA	2.06	0.85
3:I:53:VAL:HG22	3:I:54:LYS:H	1.40	0.84
1:G:174:GLU:O	1:G:175:GLN:HB2	1.76	0.84
1:G:1:MET:H1	2:H:77:ARG:HH12	1.22	0.83
2:B:88:ARG:HH11	2:B:88:ARG:CG	1.92	0.82
1:G:126:LEU:O	1:G:129:LEU:HG	1.78	0.82
2:B:59:LYS:NZ	1:G:96:THR:HG22	1.93	0.82
1:G:125:ASP:CB	1:G:127:THR:HA	2.08	0.82
3:I:18:VAL:HG22	3:I:19:PRO:HD2	1.63	0.81
2:E:45:GLU:HG2	2:E:50:LYS:HG3	1.61	0.80
3:C:221:LYS:CG	3:C:222:GLY:HA2	2.12	0.79
3:F:75:ILE:HG12	3:F:187:PHE:HZ	1.48	0.79
3:I:208:ILE:N	3:I:209:GLU:CB	2.46	0.79
1:G:73:LYS:HE2	1:G:73:LYS:H	1.48	0.78
3:C:18:VAL:HG22	3:C:19:PRO:HD2	1.64	0.78
3:I:224:THR:HB	3:I:225:ASP:HA	1.64	0.77
2:E:88:ARG:HH11	2:E:88:ARG:HG2	1.49	0.77
3:F:134:ASP:CG	3:F:135:ARG:N	2.40	0.75
3:I:222:GLY:O	3:I:223:LEU:HB3	1.86	0.75
3:C:198:CYS:SG	3:C:205:GLU:HB3	2.27	0.75
1:G:127:THR:OG1	1:G:188:PRO:CB	2.35	0.74
3:I:108:ARG:O	3:I:109:SER:HB2	1.88	0.74
3:C:85:ILE:HG12	3:I:137:ILE:HG22	1.67	0.74
3:F:18:VAL:HG22	3:F:19:PRO:HD2	1.69	0.74
1:D:130:VAL:HA	1:D:137:VAL:HG23	1.68	0.74
3:F:220:ILE:HG22	3:F:221:LYS:H	1.52	0.73
3:F:75:ILE:HD11	3:F:127:ILE:HG22	1.71	0.73
3:C:205:GLU:HG2	3:C:205:GLU:O	1.89	0.72
3:C:75:ILE:H	3:C:190:ASN:HD22	1.36	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:72:ILE:O	3:I:73:ASN:HB2	1.88	0.72
3:C:221:LYS:HG3	3:C:222:GLY:CA	2.16	0.72
2:B:59:LYS:HZ1	1:G:96:THR:HG22	1.53	0.71
1:A:1:MET:HG2	2:B:77:ARG:HG3	1.71	0.71
1:G:1:MET:N	2:H:77:ARG:NH1	2.39	0.71
3:F:203:SER:O	3:F:204:GLU:HB2	1.90	0.71
1:G:176:ILE:O	1:G:177:SER:O	2.08	0.70
3:C:184:CYS:CB	3:C:185:SER:HA	2.20	0.70
2:H:11:LEU:HB3	2:H:12:ASP:HB2	1.74	0.70
1:A:228:ASP:O	1:A:229:LEU:HB2	1.90	0.70
2:E:88:ARG:HH11	2:E:88:ARG:CG	2.04	0.70
3:I:53:VAL:HA	3:I:58:PHE:HA	1.72	0.70
1:G:127:THR:OG1	1:G:188:PRO:HB3	1.93	0.69
3:C:157:ILE:HD12	3:C:194:ILE:HD11	1.73	0.69
2:E:161:VAL:HG22	2:E:222:ILE:HG13	1.76	0.68
2:B:63:PRO:HG2	2:B:66:LEU:HD12	1.75	0.68
3:F:204:GLU:HG3	3:F:205:GLU:H	1.58	0.67
3:I:208:ILE:H	3:I:209:GLU:HB3	1.53	0.67
3:I:188:VAL:HA	3:I:194:ILE:HG22	1.76	0.67
3:I:216:ASN:O	3:I:219:HIS:CE1	2.48	0.67
1:D:121:SER:HA	1:D:232:VAL:HG21	1.77	0.67
2:H:161:VAL:HG22	2:H:222:ILE:HG13	1.75	0.67
3:F:159:ILE:HG21	3:F:211:ILE:HG22	1.75	0.66
1:A:91:LEU:N	1:A:92:PRO:HD2	2.10	0.66
1:A:91:LEU:HD11	1:A:145:TYR:HD2	1.60	0.66
3:C:152:SER:O	3:C:153:ASN:HB3	1.94	0.66
2:E:75:ARG:HG2	2:E:75:ARG:HH11	1.59	0.66
1:G:127:THR:OG1	1:G:188:PRO:HB2	1.94	0.66
2:B:88:ARG:HH11	2:B:88:ARG:HG2	1.62	0.65
3:I:217:GLU:HA	3:I:219:HIS:HE1	1.60	0.65
2:H:11:LEU:CA	2:H:12:ASP:HB2	2.26	0.65
1:D:88:VAL:HG22	1:D:144:VAL:HB	1.79	0.64
2:H:75:ARG:HG2	2:H:75:ARG:HH11	1.62	0.64
3:C:199:PRO:HB2	3:C:200:SER:HA	1.79	0.64
2:H:236:LYS:O	2:H:237:TYR:CG	2.50	0.64
1:G:127:THR:H	1:G:128:LYS:HB3	1.62	0.64
1:D:104:ASP:O	1:D:105:GLU:HB2	1.98	0.63
3:C:117:ARG:CD	3:C:118:ARG:H	2.05	0.63
3:I:211:ILE:O	3:I:215:GLU:HB2	1.98	0.63
2:B:88:ARG:HH11	2:B:88:ARG:HG3	1.64	0.63
3:C:182:SER:HB2	3:C:183:GLY:HA3	1.81	0.62
3:I:217:GLU:HA	3:I:219:HIS:CE1	2.35	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:75:ILE:H	3:C:190:ASN:ND2	1.97	0.62
1:G:92:PRO:O	1:G:93:LEU:HD12	1.98	0.62
1:G:121:SER:HA	1:G:232:VAL:HG21	1.80	0.62
3:F:75:ILE:HG12	3:F:187:PHE:CZ	2.34	0.62
3:I:174:MET:HE2	3:I:214:ILE:HD12	1.80	0.62
3:I:207:LEU:C	3:I:209:GLU:HB3	2.20	0.62
2:H:11:LEU:HA	2:H:12:ASP:HB2	1.80	0.62
2:B:105:ARG:O	2:B:109:GLU:HG2	2.00	0.61
3:I:208:ILE:H	3:I:209:GLU:CB	2.11	0.61
3:I:53:VAL:HG22	3:I:54:LYS:N	2.13	0.61
3:I:174:MET:CE	3:I:214:ILE:HD12	2.29	0.61
1:D:105:GLU:HG2	2:E:102:LYS:HD2	1.83	0.61
2:E:58:PRO:HB2	3:F:95:PRO:HB3	1.82	0.61
3:I:164:VAL:HB	3:I:165:PRO:HD3	1.82	0.60
1:D:7:ASN:CA	1:D:8:GLN:CB	2.70	0.60
2:E:4:VAL:HG13	2:E:4:VAL:O	2.02	0.59
1:A:122:LYS:O	1:A:190:ASN:ND2	2.33	0.59
3:C:199:PRO:N	3:C:200:SER:HB2	2.17	0.59
1:G:1:MET:H1	2:H:77:ARG:NH1	1.95	0.59
3:F:188:VAL:HA	3:F:194:ILE:HG22	1.83	0.59
1:A:121:SER:HA	1:A:232:VAL:HG21	1.84	0.59
1:G:17:GLU:O	1:G:20:VAL:HG12	2.02	0.59
1:G:1:MET:H2	2:H:77:ARG:HH12	1.48	0.59
1:A:74:PRO:HB2	1:A:79:PRO:HA	1.85	0.59
3:I:157:ILE:HD12	3:I:194:ILE:HD11	1.84	0.59
3:F:144:LYS:O	3:F:144:LYS:HG2	2.02	0.59
2:E:6:ARG:HB3	2:E:7:PRO:HA	1.85	0.58
1:D:226:THR:HB	1:D:227:PRO:HD2	1.84	0.58
3:F:161:PRO:O	3:F:162:VAL:HB	2.03	0.58
1:G:8:GLN:C	1:G:10:ILE:H	2.07	0.58
2:H:123:ASP:HB3	2:H:125:PHE:CE1	2.38	0.58
3:I:224:THR:CB	3:I:225:ASP:CB	2.68	0.58
1:D:91:LEU:C	1:D:93:LEU:H	2.06	0.58
2:H:16:ARG:HD3	2:H:178:GLU:OE2	2.03	0.58
1:G:226:THR:HB	1:G:227:PRO:HD2	1.86	0.57
1:A:91:LEU:HD11	1:A:145:TYR:CD2	2.39	0.57
1:A:28:ARG:NH1	1:A:206:VAL:HG13	2.20	0.57
3:C:117:ARG:HD3	3:C:118:ARG:N	2.07	0.57
2:E:4:VAL:O	2:E:5:GLU:HB2	2.05	0.57
2:E:105:ARG:O	2:E:109:GLU:HG2	2.05	0.57
2:H:63:PRO:HG2	2:H:66:LEU:HD12	1.85	0.57
1:G:23:PHE:O	1:G:25:LYS:N	2.38	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:176:GLU:O	3:F:178:LEU:N	2.38	0.57
1:G:172:LYS:HE3	1:G:174:GLU:HB3	1.87	0.57
1:D:104:ASP:O	1:D:105:GLU:CB	2.54	0.56
3:C:62:PRO:HB2	3:C:162:VAL:HG21	1.88	0.56
2:B:16:ARG:HD3	2:B:178:GLU:OE2	2.05	0.56
2:B:61:MET:HG2	2:B:121:ALA:HB2	1.88	0.56
1:A:130:VAL:HA	1:A:137:VAL:HG23	1.87	0.56
1:G:82:GLY:HA3	1:G:129:LEU:HB3	1.86	0.56
3:F:77:ILE:HG22	3:F:127:ILE:HG23	1.86	0.56
2:E:107:ALA:HB1	2:E:198:THR:HG23	1.88	0.56
1:D:1:MET:HG3	1:D:2:SER:H	1.72	0.55
1:A:42:ILE:HG12	1:A:56:VAL:HG22	1.87	0.55
2:H:11:LEU:CB	2:H:12:ASP:HB2	2.35	0.55
3:F:118:ARG:H	3:F:118:ARG:CD	2.20	0.55
3:C:188:VAL:HA	3:C:194:ILE:HG22	1.89	0.55
2:H:61:MET:HG2	2:H:121:ALA:HB2	1.89	0.55
1:D:91:LEU:HD11	1:D:145:TYR:HD2	1.72	0.54
3:F:194:ILE:HD11	3:F:211:ILE:HD13	1.88	0.54
1:G:82:GLY:HA2	1:G:137:VAL:HG13	1.89	0.54
3:F:159:ILE:HG21	3:F:211:ILE:CG2	2.37	0.54
2:E:26:ARG:HD2	2:E:47:GLY:HA3	1.88	0.54
1:G:127:THR:CB	1:G:128:LYS:CB	2.67	0.54
3:C:176:GLU:HA	3:C:179:THR:HB	1.88	0.54
1:A:88:VAL:HG22	1:A:144:VAL:HB	1.90	0.54
1:G:28:ARG:HD3	1:G:213:GLU:OE2	2.08	0.54
3:C:184:CYS:CB	3:C:185:SER:CA	2.86	0.54
2:E:3:GLN:O	2:E:4:VAL:HB	2.08	0.54
2:E:62:HIS:CB	2:E:63:PRO:HD3	2.38	0.53
1:A:51:ASP:HB3	1:A:168:THR:HG23	1.90	0.53
3:F:118:ARG:HD2	3:F:118:ARG:H	1.73	0.53
3:F:210:ALA:HB2	3:F:235:LEU:HD21	1.91	0.53
3:I:162:VAL:HG12	3:I:163:LYS:HD2	1.91	0.53
2:B:238:VAL:HA	3:C:16:ILE:HG13	1.91	0.53
1:D:68:LYS:HG2	2:H:88:ARG:HB2	1.91	0.53
3:F:17:VAL:HG21	3:F:23:LEU:HD21	1.90	0.52
2:B:161:VAL:HG22	2:B:222:ILE:HG13	1.91	0.52
2:B:209:ASP:O	2:B:213:GLN:HG3	2.09	0.52
3:C:199:PRO:HB2	3:C:200:SER:CA	2.39	0.52
2:H:45:GLU:HG2	2:H:50:LYS:HG3	1.92	0.52
3:I:225:ASP:O	3:I:226:ARG:HB2	2.10	0.52
3:I:53:VAL:CG2	3:I:54:LYS:H	2.17	0.52
1:A:91:LEU:N	1:A:92:PRO:CD	2.72	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:190:MET:HG2	2:B:222:ILE:HD13	1.92	0.52
2:H:58:PRO:HB2	3:I:95:PRO:HB3	1.92	0.52
3:I:174:MET:O	3:I:177:THR:HG22	2.09	0.52
3:C:205:GLU:C	3:C:207:LEU:H	2.14	0.51
1:G:125:ASP:HB3	1:G:126:LEU:CA	2.40	0.51
3:F:220:ILE:HG22	3:F:221:LYS:N	2.23	0.51
1:A:163:ALA:HA	1:A:269:LEU:HD21	1.91	0.51
3:C:164:VAL:HG11	3:C:190:ASN:HA	1.92	0.51
1:D:91:LEU:HD13	2:H:127:GLU:HG3	1.93	0.51
3:I:212:ARG:CA	3:I:215:GLU:HB2	2.40	0.51
1:G:82:GLY:HA3	1:G:129:LEU:HD12	1.93	0.51
2:B:234:LYS:C	2:B:236:LYS:H	2.12	0.51
3:I:221:LYS:CB	3:I:222:GLY:CA	2.78	0.51
3:I:174:MET:O	3:I:178:LEU:HD12	2.10	0.51
2:E:61:MET:HG2	2:E:121:ALA:HB2	1.93	0.51
2:E:231:GLU:HA	2:E:234:LYS:HB2	1.92	0.51
2:B:45:GLU:HG2	2:B:50:LYS:HG3	1.92	0.51
1:D:41:SER:HB3	1:D:57:LYS:HB2	1.92	0.51
3:F:177:THR:HB	3:F:179:THR:OG1	2.10	0.50
3:C:14:ARG:HG2	3:C:14:ARG:O	2.10	0.50
1:A:235:GLN:NE2	2:B:201:GLN:HE21	1.96	0.50
2:E:190:MET:HG2	2:E:222:ILE:HD13	1.94	0.50
1:G:92:PRO:HG3	1:G:100:PRO:HB3	1.94	0.50
3:C:179:THR:HG23	3:C:184:CYS:CB	2.42	0.50
3:F:184:CYS:HB2	3:F:186:ILE:HD11	1.94	0.50
1:D:74:PRO:HB2	1:D:79:PRO:HA	1.94	0.50
1:G:49:LYS:O	1:G:68:LYS:HE3	2.12	0.50
3:C:157:ILE:HG21	3:C:211:ILE:HG21	1.95	0.49
1:D:104:ASP:H	1:D:107:ALA:HB3	1.76	0.49
2:H:237:TYR:HB2	3:I:220:ILE:HD13	1.94	0.49
2:E:88:ARG:NH1	2:E:88:ARG:CG	2.71	0.49
2:B:186:MET:HE2	2:B:202:LEU:HD13	1.94	0.49
2:B:59:LYS:HZ3	1:G:96:THR:HG22	1.74	0.49
2:B:56:TYR:CD2	1:G:96:THR:HG23	2.47	0.49
2:B:164:GLY:HA3	2:B:174:LEU:HD21	1.95	0.49
1:G:194:VAL:HB	1:G:261:LEU:HD23	1.94	0.49
3:F:108:ARG:NH1	3:F:110:ILE:H	2.10	0.49
3:I:224:THR:CB	3:I:225:ASP:HA	2.35	0.49
3:I:145:GLY:H	3:I:148:LEU:HD12	1.77	0.49
2:H:34:VAL:HG21	2:H:43:ILE:HG13	1.94	0.49
3:F:204:GLU:HG3	3:F:205:GLU:N	2.25	0.49
2:E:4:VAL:O	2:E:5:GLU:CB	2.61	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:91:LEU:HD11	1:D:145:TYR:CD2	2.47	0.49
3:I:80:VAL:HG21	3:I:120:LEU:HD13	1.94	0.49
3:F:75:ILE:HD12	3:F:128:ALA:O	2.13	0.49
3:C:186:ILE:HG13	3:C:194:ILE:HD13	1.94	0.49
3:I:14:ARG:HB3	3:I:51:PHE:O	2.13	0.49
2:H:190:MET:HB3	2:H:197:VAL:HA	1.95	0.49
3:C:154:GLY:O	1:G:14:ILE:HD11	2.12	0.48
1:G:125:ASP:CG	1:G:127:THR:HG23	2.34	0.48
3:F:178:LEU:C	3:F:180:SER:H	2.09	0.48
3:C:157:ILE:HB	3:C:194:ILE:HG13	1.96	0.48
2:E:237:TYR:O	2:E:237:TYR:CG	2.66	0.48
1:G:38:ARG:HD2	1:G:59:GLY:HA3	1.94	0.48
2:H:186:MET:HE2	2:H:202:LEU:HD13	1.96	0.48
3:C:106:LEU:HD11	3:C:119:TYR:CZ	2.49	0.48
3:C:201:ARG:HA	3:C:202:PHE:HA	1.67	0.48
2:H:237:TYR:C	3:I:220:ILE:HD11	2.34	0.47
3:I:211:ILE:HA	3:I:214:ILE:HG22	1.95	0.47
2:E:31:GLU:HG3	2:E:34:VAL:HG13	1.95	0.47
3:I:208:ILE:HA	3:I:211:ILE:HG22	1.96	0.47
2:E:8:LYS:HG2	2:E:11:LEU:HD23	1.95	0.47
2:E:161:VAL:HG13	2:E:225:ILE:HD12	1.95	0.47
3:I:223:LEU:HG	3:I:224:THR:HG23	1.95	0.47
3:I:29:GLN:CA	3:I:30:ILE:HB	2.45	0.47
1:G:1:MET:H2	2:H:77:ARG:NH1	2.08	0.47
2:B:50:LYS:HB2	2:B:130:GLN:HB2	1.95	0.47
1:A:79:PRO:HB2	1:A:134:GLY:HA2	1.96	0.47
1:A:25:LYS:HE2	1:A:27:ILE:HG21	1.97	0.47
3:C:168:ILE:HG22	3:C:172:LYS:HA	1.97	0.47
1:D:38:ARG:HD2	1:D:59:GLY:HA3	1.97	0.47
3:F:142:SER:HB2	3:F:144:LYS:HD2	1.97	0.47
1:G:199:ALA:HB3	1:G:206:VAL:HG12	1.97	0.47
3:F:217:GLU:C	3:F:219:HIS:H	2.18	0.46
2:B:88:ARG:CG	2:B:88:ARG:NH1	2.63	0.46
3:C:7:GLN:O	3:C:8:LYS:HG3	2.15	0.46
1:G:121:SER:HB3	1:G:232:VAL:HG11	1.97	0.46
1:G:12:PRO:HB2	1:G:15:LYS:HB2	1.97	0.46
3:I:77:ILE:HD11	3:I:193:ARG:HB3	1.97	0.46
2:H:230:ARG:HG2	3:I:18:VAL:HG11	1.97	0.46
3:F:221:LYS:HD3	3:F:228:LYS:HE3	1.98	0.46
3:I:224:THR:CB	3:I:225:ASP:CA	2.74	0.46
1:A:32:ARG:CZ	1:A:38:ARG:HG3	2.46	0.46
3:I:184:CYS:O	3:I:186:ILE:N	2.49	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:51:ALA:HB3	2:E:138:VAL:HG12	1.98	0.46
3:C:205:GLU:CG	3:C:205:GLU:O	2.63	0.46
3:F:110:ILE:HG21	3:F:119:TYR:CE2	2.51	0.46
3:F:164:VAL:N	3:F:165:PRO:HD2	2.31	0.46
3:F:23:LEU:HD22	3:F:51:PHE:CD1	2.51	0.45
2:H:78:TYR:CE2	2:H:100:LEU:HD12	2.52	0.45
3:I:106:LEU:HB3	3:I:107:GLY:H	1.35	0.45
3:I:28:PHE:CD2	3:I:58:PHE:HE2	2.35	0.45
1:G:8:GLN:C	1:G:10:ILE:N	2.68	0.45
3:I:29:GLN:HA	3:I:30:ILE:HB	1.96	0.45
1:G:24:GLU:C	1:G:26:GLY:N	2.70	0.45
1:G:42:ILE:HG12	1:G:56:VAL:HG22	1.99	0.45
3:F:70:PRO:HB2	3:F:133:PHE:CD2	2.50	0.45
2:B:107:ALA:HB1	2:B:198:THR:HG23	1.97	0.45
3:F:108:ARG:HH12	3:F:110:ILE:H	1.63	0.45
2:H:237:TYR:O	3:I:220:ILE:HD11	2.17	0.45
2:E:50:LYS:HD3	2:E:130:GLN:CD	2.36	0.45
1:G:32:ARG:CZ	1:G:38:ARG:HG3	2.47	0.45
3:I:77:ILE:HG22	3:I:127:ILE:HG12	1.98	0.45
3:C:105:LEU:HD23	3:C:143:VAL:HG21	1.98	0.45
3:C:69:TYR:HA	3:C:70:PRO:HD3	1.79	0.45
3:C:92:ILE:O	3:C:191:ASN:ND2	2.44	0.45
1:G:132:GLU:HA	1:G:133:PRO:HD3	1.84	0.45
2:H:234:LYS:O	2:H:236:LYS:N	2.40	0.45
1:G:104:ASP:O	1:G:105:GLU:HB2	2.17	0.45
3:I:219:HIS:N	3:I:219:HIS:ND1	2.64	0.45
3:I:157:ILE:HB	3:I:194:ILE:HG13	1.99	0.45
1:D:42:ILE:HG12	1:D:56:VAL:HG22	1.98	0.45
2:H:10:ILE:HD13	2:H:166:ALA:HB3	2.00	0.44
3:F:131:GLU:HG3	3:F:142:SER:HB3	1.98	0.44
2:E:6:ARG:HB3	2:E:7:PRO:CA	2.47	0.44
2:E:11:LEU:HB3	2:E:12:ASP:H	1.65	0.44
2:B:165:LYS:HE3	2:B:168:GLY:HA2	1.98	0.44
1:G:222:SER:O	1:G:234:ILE:HA	2.17	0.44
1:G:82:GLY:HA2	1:G:137:VAL:CG1	2.48	0.44
1:D:32:ARG:CZ	1:D:38:ARG:HG3	2.48	0.44
3:C:77:ILE:HG22	3:C:127:ILE:HG12	1.99	0.44
2:H:156:ASP:HB3	2:H:191:MET:HB3	2.00	0.44
1:G:28:ARG:NH2	1:G:207:VAL:O	2.39	0.44
3:C:84:GLU:HG2	3:C:85:ILE:H	1.83	0.44
1:G:12:PRO:C	1:G:14:ILE:H	2.21	0.44
3:F:25:GLU:HG2	3:F:42:LYS:HG2	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:29:GLN:N	3:I:30:ILE:HB	2.33	0.44
1:G:78:THR:HA	1:G:79:PRO:HD3	1.52	0.44
3:F:219:HIS:HB2	3:F:220:ILE:HD12	2.00	0.44
1:A:251:GLU:OE2	2:B:212:ARG:NH2	2.51	0.44
1:A:168:THR:HB	1:A:187:LEU:CD2	2.48	0.43
1:G:127:THR:CA	1:G:128:LYS:CB	2.97	0.43
3:I:224:THR:OG1	3:I:225:ASP:HB3	2.16	0.43
3:C:205:GLU:C	3:C:207:LEU:N	2.71	0.43
2:B:34:VAL:HG21	2:B:43:ILE:HG13	1.99	0.43
1:G:88:VAL:HG22	1:G:144:VAL:HB	1.99	0.43
1:A:228:ASP:HB2	1:A:230:LYS:HB2	1.99	0.43
3:F:217:GLU:C	3:F:219:HIS:N	2.71	0.43
3:F:198:CYS:HB3	3:F:205:GLU:HB3	1.99	0.43
2:E:112:VAL:HA	2:E:154:MET:HG2	1.99	0.43
1:A:105:GLU:HG2	2:B:102:LYS:HD2	2.01	0.43
3:I:107:GLY:O	3:I:108:ARG:HB2	2.19	0.43
2:H:62:HIS:CB	2:H:63:PRO:HD3	2.48	0.43
2:H:29:LYS:HB3	2:H:45:GLU:HB2	1.99	0.43
2:E:197:VAL:HG11	2:E:200:PHE:HD1	1.84	0.43
1:G:127:THR:H	1:G:128:LYS:CB	2.31	0.43
1:D:121:SER:CA	1:D:232:VAL:HG21	2.46	0.43
3:I:169:GLY:HA2	3:I:170:LYS:CG	2.48	0.43
3:I:168:ILE:C	3:I:174:MET:HB2	2.39	0.43
3:I:187:PHE:O	3:I:194:ILE:HA	2.19	0.43
3:F:186:ILE:HD12	3:F:207:LEU:HD11	2.01	0.43
2:E:100:LEU:HD21	2:E:136:ARG:CZ	2.49	0.43
2:H:8:LYS:HE3	2:H:11:LEU:HD23	2.00	0.43
1:G:28:ARG:CZ	1:G:206:VAL:HG22	2.48	0.43
3:F:75:ILE:HD11	3:F:127:ILE:CG2	2.45	0.42
3:F:18:VAL:HG12	3:F:21:GLU:HB2	2.00	0.42
3:C:208:ILE:O	3:C:211:ILE:HG22	2.18	0.42
1:G:178:VAL:HG12	1:G:179:ASN:H	1.84	0.42
3:C:116:LEU:C	3:C:117:ARG:HG3	2.39	0.42
2:H:96:ARG:O	2:H:100:LEU:HG	2.19	0.42
3:I:11:LEU:HB2	3:I:12:GLN:HE21	1.83	0.42
3:C:12:GLN:HA	3:C:13:PRO:HD3	1.88	0.42
3:F:206:ILE:O	3:F:206:ILE:HG23	2.18	0.42
3:I:167:VAL:HG12	3:I:167:VAL:O	2.19	0.42
1:G:198:VAL:HG22	1:G:207:VAL:HG22	2.00	0.42
3:I:167:VAL:HA	3:I:214:ILE:HD13	2.01	0.42
2:B:163:VAL:HB	2:B:218:ALA:HB2	2.01	0.42
3:C:82:ASP:OD1	2:H:119:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:82:GLY:HA3	1:G:129:LEU:CD1	2.49	0.42
3:C:164:VAL:HB	3:C:165:PRO:HD3	2.02	0.42
2:H:10:ILE:HG23	2:H:11:LEU:O	2.19	0.42
2:B:236:LYS:HE3	3:C:63:LEU:HB3	2.00	0.42
3:F:57:GLN:HE21	3:F:57:GLN:HB3	1.63	0.42
3:I:9:ILE:HG23	3:I:25:GLU:OE2	2.19	0.42
2:B:83:PHE:HB2	1:G:50:ALA:HB2	2.02	0.42
3:I:211:ILE:O	3:I:215:GLU:CB	2.68	0.42
1:D:112:ARG:HH22	2:E:96:ARG:NH1	2.18	0.42
1:D:168:THR:HB	1:D:187:LEU:HD22	2.00	0.41
3:C:16:ILE:HD12	3:C:63:LEU:HD11	2.02	0.41
1:D:11:ILE:HG21	1:D:216:ILE:CG2	2.50	0.41
2:H:74:LEU:HD23	2:H:122:ILE:HB	2.02	0.41
2:B:57:GLY:HA2	2:B:152:ILE:HD11	2.02	0.41
2:H:231:GLU:HA	2:H:234:LYS:HB2	2.02	0.41
1:D:121:SER:HA	1:D:232:VAL:CG2	2.48	0.41
1:G:121:SER:CA	1:G:232:VAL:HG21	2.49	0.41
2:H:31:GLU:HG3	2:H:34:VAL:HG13	2.02	0.41
2:H:162:ALA:HA	2:H:187:PRO:HA	2.02	0.41
3:C:111:ASN:HB2	3:C:114:GLU:HG3	2.02	0.41
1:A:1:MET:CG	2:B:77:ARG:HG3	2.44	0.41
3:I:13:PRO:HB2	3:I:14:ARG:H	1.72	0.41
2:B:234:LYS:C	2:B:236:LYS:N	2.74	0.41
3:F:17:VAL:HG21	3:F:23:LEU:CD2	2.51	0.41
3:F:179:THR:HG23	3:F:186:ILE:HG12	2.01	0.41
3:F:110:ILE:HG21	3:F:119:TYR:HE2	1.84	0.41
1:D:68:LYS:HD3	2:H:83:PHE:HA	2.02	0.41
3:C:189:ALA:C	3:C:191:ASN:H	2.24	0.41
2:H:236:LYS:C	2:H:237:TYR:CD2	2.87	0.41
1:A:78:THR:HA	1:A:79:PRO:HD3	1.91	0.41
1:A:51:ASP:CB	1:A:168:THR:HG23	2.51	0.41
3:F:163:LYS:HD2	3:F:215:GLU:OE2	2.21	0.41
3:C:137:ILE:HG22	3:F:85:ILE:HG21	2.03	0.41
3:I:191:ASN:HA	3:I:191:ASN:HD22	1.64	0.41
2:H:190:MET:HG2	2:H:222:ILE:HD13	2.03	0.41
2:B:36:LYS:HD3	2:B:36:LYS:HA	1.92	0.41
1:A:82:GLY:HA2	1:A:137:VAL:HG22	2.03	0.40
1:A:170:VAL:HG12	1:A:171:TYR:N	2.36	0.40
1:D:23:PHE:HE1	1:D:28:ARG:HG2	1.86	0.40
3:F:233:GLU:O	3:F:237:GLU:HB3	2.20	0.40
2:E:165:LYS:HE3	2:E:168:GLY:HA2	2.04	0.40
3:C:133:PHE:CD1	3:C:139:PRO:HG3	2.56	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:4:VAL:CG1	2:E:4:VAL:O	2.69	0.40

There are no symmetry-related clashes.

## 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	245/271 (90%)	229 (94%)	12 (5%)	4 (2%)	14	18
1	D	257/271 (95%)	242 (94%)	10 (4%)	5 (2%)	12	14
1	G	268/271 (99%)	238 (89%)	13 (5%)	17 (6%)	2	1
2	B	230/245 (94%)	212 (92%)	12 (5%)	6 (3%)	8	7
2	E	235/245 (96%)	219 (93%)	9 (4%)	7 (3%)	7	5
2	H	232/245 (95%)	215 (93%)	12 (5%)	5 (2%)	10	10
3	C	220/249 (88%)	184 (84%)	24 (11%)	12 (6%)	3	1
3	F	205/249 (82%)	169 (82%)	24 (12%)	12 (6%)	2	1
3	I	198/249 (80%)	163 (82%)	24 (12%)	11 (6%)	3	1
All	All	2090/2295 (91%)	1871 (90%)	140 (7%)	79 (4%)	5	3

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	GLU
2	B	13	ASP
3	C	8	LYS
3	C	182	SER
1	D	8	GLN
1	D	78	THR
2	E	4	VAL
2	E	5	GLU
2	E	13	ASP
2	E	236	LYS

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Mol	Chain	Res	Type
3	F	162	VAL
3	F	177	THR
3	F	179	THR
3	F	204	GLU
3	F	220	ILE
1	G	23	PHE
1	G	105	GLU
1	G	126	LEU
1	G	175	GLN
1	G	177	SER
2	H	13	ASP
2	H	236	LYS
2	H	237	TYR
3	I	13	PRO
3	I	108	ARG
3	I	112	VAL
3	I	185	SER
3	I	206	ILE
3	I	209	GLU
3	I	223	LEU
1	A	10	ILE
3	C	13	PRO
3	C	117	ARG
3	C	208	ILE
1	D	16	LYS
1	D	105	GLU
3	F	13	PRO
3	F	57	GLN
1	G	24	GLU
1	G	78	THR
1	G	93	LEU
1	G	128	LYS
1	G	180	LYS
3	I	54	LYS
2	B	12	ASP
2	B	235	SER
3	C	40	ASN
3	C	115	ASP
3	C	145	GLY
3	C	200	SER
2	E	57	GLY
3	F	55	ASP

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Mol	Chain	Res	Type
3	F	160	MET
3	F	240	ALA
1	G	2	SER
1	G	79	PRO
1	G	176	ILE
2	H	235	SER
3	I	109	SER
2	B	57	GLY
2	B	133	ALA
2	B	237	TYR
3	C	134	ASP
3	C	153	ASN
2	E	133	ALA
3	F	108	ARG
1	G	10	ILE
3	I	172	LYS
1	A	78	THR
3	C	199	PRO
2	E	6	ARG
3	F	206	ILE
2	H	133	ALA
1	G	9	ASN
3	I	30	ILE
1	G	188	PRO
1	G	178	VAL
1	A	91	LEU
1	D	92	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	218/239 (91%)	202 (93%)	16 (7%)	20	30
1	D	217/239 (91%)	202 (93%)	15 (7%)	22	33
1	G	237/239 (99%)	215 (91%)	22 (9%)	13	18
2	B	187/205 (91%)	177 (95%)	10 (5%)	32	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	197/205 (96%)	186 (94%)	11 (6%)	30	44
2	H	194/205 (95%)	184 (95%)	10 (5%)	32	49
3	C	180/222 (81%)	165 (92%)	15 (8%)	16	23
3	F	190/222 (86%)	168 (88%)	22 (12%)	8	10
3	I	167/222 (75%)	150 (90%)	17 (10%)	11	15
All	All	1787/1998 (89%)	1649 (92%)	138 (8%)	18	28

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	9	ASN
1	A	13	ILE
1	A	32	ARG
1	A	68	LYS
1	A	73	LYS
1	A	104	ASP
1	A	137	VAL
1	A	187	LEU
1	A	191	TYR
1	A	203	LYS
1	A	228	ASP
1	A	235	GLN
1	A	239	LYS
1	A	251	GLU
1	A	262	LEU
2	B	12	ASP
2	B	34	VAL
2	B	61	MET
2	B	63	PRO
2	B	88	ARG
2	B	96	ARG
2	B	161	VAL
2	B	198	THR
2	B	215	PHE
2	B	238	VAL
3	C	7	GLN
3	C	18	VAL
3	C	22	LEU
3	C	55	ASP

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Mol	Chain	Res	Type
3	C	56	THR
3	C	85	ILE
3	C	106	LEU
3	C	117	ARG
3	C	135	ARG
3	C	158	ASP
3	C	162	VAL
3	C	163	LYS
3	C	191	ASN
3	C	221	LYS
3	C	225	ASP
1	D	8	GLN
1	D	9	ASN
1	D	37	TYR
1	D	68	LYS
1	D	93	LEU
1	D	104	ASP
1	D	135	LYS
1	D	137	VAL
1	D	148	ASP
1	D	187	LEU
1	D	206	VAL
1	D	228	ASP
1	D	239	LYS
1	D	247	ILE
1	D	251	GLU
2	E	4	VAL
2	E	6	ARG
2	E	8	LYS
2	E	15	LYS
2	E	50	LYS
2	E	61	MET
2	E	75	ARG
2	E	88	ARG
2	E	161	VAL
2	E	198	THR
2	E	237	TYR
3	F	18	VAL
3	F	22	LEU
3	F	55	ASP
3	F	57	GLN
3	F	118	ARG

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Mol	Chain	Res	Type
3	F	131	GLU
3	F	134	ASP
3	F	135	ARG
3	F	144	LYS
3	F	146	LYS
3	F	174	MET
3	F	175	TYR
3	F	176	GLU
3	F	178	LEU
3	F	184	CYS
3	F	198	CYS
3	F	207	LEU
3	F	228	LYS
3	F	229	GLN
3	F	231	ILE
3	F	233	GLU
3	F	234	LYS
1	G	11	ILE
1	G	20	VAL
1	G	37	TYR
1	G	68	LYS
1	G	73	LYS
1	G	81	GLN
1	G	93	LEU
1	G	96	THR
1	G	104	ASP
1	G	120	ASP
1	G	125	ASP
1	G	129	LEU
1	G	130	VAL
1	G	178	VAL
1	G	181	ASN
1	G	187	LEU
1	G	203	LYS
1	G	206	VAL
1	G	232	VAL
1	G	235	GLN
1	G	239	LYS
1	G	251	GLU
2	H	15	LYS
2	H	34	VAL
2	H	61	MET

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Mol	Chain	Res	Type
2	H	75	ARG
2	H	89	LYS
2	H	96	ARG
2	H	132	ASP
2	H	161	VAL
2	H	174	LEU
2	H	215	PHE
3	I	12	GLN
3	I	14	ARG
3	I	18	VAL
3	I	22	LEU
3	I	25	GLU
3	I	27	GLU
3	I	38	LYS
3	I	75	ILE
3	I	83	VAL
3	I	106	LEU
3	I	120	LEU
3	I	155	ILE
3	I	191	ASN
3	I	207	LEU
3	I	215	GLU
3	I	219	HIS
3	I	223	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	235	GLN
1	A	249	GLN
3	C	7	GLN
3	C	190	ASN
1	D	235	GLN
3	F	57	GLN
1	G	9	ASN
1	G	235	GLN
2	H	130	GLN
3	I	12	GLN
3	I	190	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 ⓘ

3 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	$\# Z  > 2$
4	SO4	B	246	-	4,4,4	0.15	0	6,6,6	0.19	0
4	SO4	E	246	-	4,4,4	0.27	0	6,6,6	0.23	0
4	SO4	H	246	-	4,4,4	0.21	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
4	SO4	B	246	-	-	0/0/0/0	0/0/0/0
4	SO4	E	246	-	-	0/0/0/0	0/0/0/0
4	SO4	H	246	-	-	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, 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	251/271 (92%)	0.24	20 (7%) 12 11	25, 42, 77, 91	0
1	D	261/271 (96%)	0.76	35 (13%) 4 3	28, 57, 112, 137	0
1	G	270/271 (99%)	0.63	28 (10%) 7 6	31, 55, 98, 114	0
2	B	232/245 (94%)	0.15	11 (4%) 30 27	20, 43, 91, 100	0
2	E	237/245 (96%)	0.35	16 (6%) 17 15	20, 40, 91, 106	0
2	H	234/245 (95%)	0.31	14 (5%) 21 18	25, 50, 80, 104	0
3	C	222/249 (89%)	0.98	37 (16%) 2 2	31, 64, 120, 144	0
3	F	215/249 (86%)	0.72	23 (10%) 6 6	28, 59, 84, 93	0
3	I	206/249 (82%)	1.40	58 (28%) 1 1	39, 85, 120, 131	0
All	All	2128/2295 (92%)	0.60	242 (11%) 6 5	20, 53, 109, 144	0

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	237	TYR	7.8
1	A	271	ILE	6.5
3	C	203	SER	6.4
2	E	2	LEU	6.2
3	C	116	LEU	6.1
3	C	199	PRO	6.0
2	B	238	VAL	5.8
2	E	14	GLY	5.8
2	E	4	VAL	5.3
3	I	145	GLY	5.3
3	F	110	ILE	5.3
3	C	185	SER	5.2
2	H	62	HIS	5.2
2	E	5	GLU	5.1
1	D	270	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
1	D	185	GLY	4.9
3	C	200	SER	4.7
1	G	126	LEU	4.7
1	G	78	THR	4.6
3	F	203	SER	4.6
3	I	8	LYS	4.4
1	D	7	ASN	4.4
2	E	6	ARG	4.4
3	C	135	ARG	4.4
1	D	138	TRP	4.3
1	A	171	TYR	4.2
3	I	106	LEU	4.2
1	A	103	PRO	4.2
1	D	165	LEU	4.2
2	H	64	ARG	4.2
1	G	185	GLY	4.1
1	G	184	VAL	4.1
2	B	14	GLY	4.1
2	E	3	GLN	4.1
1	D	171	TYR	4.1
3	I	27	GLU	4.0
2	H	8	LYS	4.0
1	D	132	GLU	4.0
3	I	151	VAL	4.0
1	D	271	ILE	4.0
3	I	175	TYR	3.9
1	D	172	LYS	3.8
1	A	8	GLN	3.8
1	A	9	ASN	3.8
1	G	127	THR	3.8
3	F	11	LEU	3.8
1	D	101	GLY	3.7
2	B	181	TRP	3.7
3	I	141	LEU	3.7
2	E	181	TRP	3.7
3	I	181	LYS	3.6
2	H	238	VAL	3.6
3	I	45	SER	3.6
2	H	166	ALA	3.6
2	H	180	MET	3.6
2	B	237	TYR	3.6
3	C	227	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
3	C	171	ASN	3.6
1	G	176	ILE	3.6
1	D	184	VAL	3.6
3	F	180	SER	3.6
3	I	153	ASN	3.5
1	G	1	MET	3.5
3	F	25	GLU	3.4
3	C	178	LEU	3.4
2	E	9	LEU	3.4
3	I	84	GLU	3.4
3	I	220	ILE	3.4
2	E	64	ARG	3.4
1	G	76	GLU	3.3
3	F	109	SER	3.3
3	F	220	ILE	3.3
3	C	9	ILE	3.3
1	A	183	VAL	3.3
3	F	174	MET	3.3
2	H	65	HIS	3.3
1	D	78	THR	3.2
3	I	208	ILE	3.2
3	C	117	ARG	3.2
1	G	138	TRP	3.2
3	I	185	SER	3.2
1	G	173	VAL	3.2
3	F	141	LEU	3.2
1	D	164	ALA	3.1
3	I	214	ILE	3.1
1	G	75	TYR	3.1
2	B	180	MET	3.1
1	G	181	ASN	3.1
1	A	78	THR	3.0
3	I	184	CYS	3.0
3	C	202	PHE	3.0
3	I	86	TYR	3.0
3	I	195	TRP	3.0
3	I	39	ILE	3.0
3	C	14	ARG	3.0
3	C	169	GLY	3.0
1	D	76	GLU	3.0
1	A	10	ILE	3.0
2	H	14	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
3	F	197	THR	2.9
1	G	182	GLU	2.9
2	B	7	PRO	2.9
1	G	175	GLN	2.9
3	F	169	GLY	2.9
2	H	87	GLU	2.9
3	C	25	GLU	2.9
1	D	29	GLN	2.9
3	F	117	ARG	2.9
3	I	150	ARG	2.9
1	D	137	VAL	2.9
3	I	85	ILE	2.8
1	A	229	LEU	2.8
1	G	7	ASN	2.8
1	A	79	PRO	2.8
3	I	53	VAL	2.8
1	G	128	LYS	2.8
2	E	237	TYR	2.7
3	F	221	LYS	2.7
2	B	87	GLU	2.7
3	I	113	GLY	2.7
3	I	36	ILE	2.7
3	C	120	LEU	2.7
1	G	73	LYS	2.7
3	C	7	GLN	2.7
3	I	147	ASP	2.7
1	A	11	ILE	2.6
3	I	60	VAL	2.6
3	F	198	CYS	2.6
3	C	131	GLU	2.6
1	A	172	LYS	2.6
3	I	9	ILE	2.6
1	D	129	LEU	2.6
2	B	92	ALA	2.6
1	D	37	TYR	2.6
1	D	19	ILE	2.6
1	D	130	VAL	2.6
1	G	24	GLU	2.6
3	C	18	VAL	2.6
3	I	171	ASN	2.6
1	G	8	GLN	2.6
3	I	109	SER	2.6

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Mol	Chain	Res	Type	RSRZ
3	I	88	TRP	2.6
2	B	215	PHE	2.6
3	F	12	GLN	2.6
3	I	216	ASN	2.6
3	I	24	ALA	2.5
1	G	259	VAL	2.5
1	D	71	ILE	2.5
3	I	206	ILE	2.5
3	I	105	LEU	2.5
3	I	143	VAL	2.5
3	C	176	GLU	2.5
3	C	177	THR	2.5
3	I	211	ILE	2.5
1	A	39	PRO	2.5
1	A	76	GLU	2.5
3	I	78	GLY	2.5
3	I	12	GLN	2.5
2	H	119	ARG	2.5
3	I	14	ARG	2.5
3	I	197	THR	2.5
1	A	6	SER	2.5
1	A	184	VAL	2.5
1	D	170	VAL	2.5
3	C	186	ILE	2.5
1	D	80	ASN	2.5
1	D	123	ALA	2.4
3	I	19	PRO	2.4
2	E	87	GLU	2.4
3	I	20	GLY	2.4
3	F	206	ILE	2.4
3	I	218	SER	2.4
1	D	166	TYR	2.4
1	G	203	LYS	2.4
1	G	261	LEU	2.4
1	D	168	THR	2.4
2	H	181	TRP	2.4
2	E	11	LEU	2.4
1	D	8	GLN	2.4
3	C	198	CYS	2.4
1	D	194	VAL	2.4
3	F	136	SER	2.3
3	F	55	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
3	I	108	ARG	2.3
3	I	46	THR	2.3
1	A	2	SER	2.3
3	F	152	SER	2.3
3	F	218	SER	2.3
1	D	267	LYS	2.3
3	C	206	ILE	2.3
2	E	62	HIS	2.3
3	I	58	PHE	2.3
1	D	133	PRO	2.3
3	C	115	ASP	2.3
1	D	10	ILE	2.3
2	B	64	ARG	2.2
3	C	224	THR	2.2
1	A	80	ASN	2.2
3	I	111	ASN	2.2
2	E	63	PRO	2.2
3	I	120	LEU	2.2
3	F	153	ASN	2.2
1	A	75	TYR	2.2
3	C	44	TYR	2.2
3	I	25	GLU	2.2
3	C	152	SER	2.2
1	D	45	ASP	2.2
3	C	211	ILE	2.2
1	G	69	LEU	2.2
2	E	66	LEU	2.2
3	I	47	VAL	2.2
2	E	171	ILE	2.2
3	C	175	TYR	2.2
1	D	124	LEU	2.1
3	I	30	ILE	2.1
1	G	140	VAL	2.1
3	C	112	VAL	2.1
3	I	180	SER	2.1
3	F	81	GLU	2.1
2	H	11	LEU	2.1
3	I	43	TYR	2.1
3	I	28	PHE	2.1
3	I	173	SER	2.1
2	B	89	LYS	2.1
1	G	130	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
3	I	132	ASN	2.1
3	C	20	GLY	2.0
1	D	136	SER	2.0
3	I	15	SER	2.0
1	G	13	ILE	2.0
1	G	129	LEU	2.0
3	I	77	ILE	2.0
1	A	120	ASP	2.0
2	H	132	ASP	2.0
3	C	228	LYS	2.0
3	C	207	LEU	2.0
3	F	85	ILE	2.0
1	G	186	LYS	2.0
1	D	20	VAL	2.0
3	C	180	SER	2.0
3	C	170	LYS	2.0
3	C	77	ILE	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
4	SO4	E	246	5/5	0.07	-1.82	45,45,46,46	0
4	SO4	B	246	5/5	0.07	-1.94	45,45,46,46	0
4	SO4	H	246	5/5	0.05	-3.82	49,49,50,50	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.