Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 09:10 AM EDT

PDB ID	:	1OYP
Title	:	Crystal Structure of the phosphorolytic exoribonuclease RNase PH from Bacillus subtilis
Authors	:	Harlow, L.S.; Kadziola, A.; Jensen, K.F.; Larsen, S.
Deposited on	:	2003-04-07
Resolution	:	2.76 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

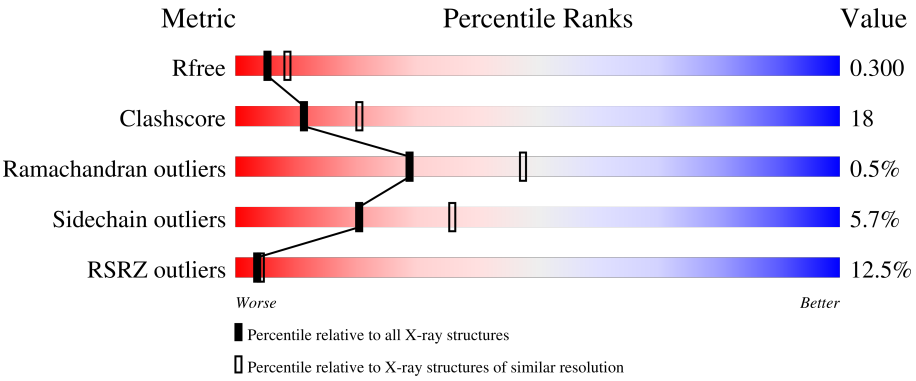
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	245	10% 60% 30% • 8%
1	B	245	13% 60% 31% • 8%
1	C	245	13% 61% 29% • 8%
1	D	245	13% 58% 32% • 8%
1	E	245	13% 59% 31% • 8%

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Mol	Chain	Length	Quality of chain
1	F	245	8% 61% 29% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	E	310	-	-	-	X

2 Entry composition (i)

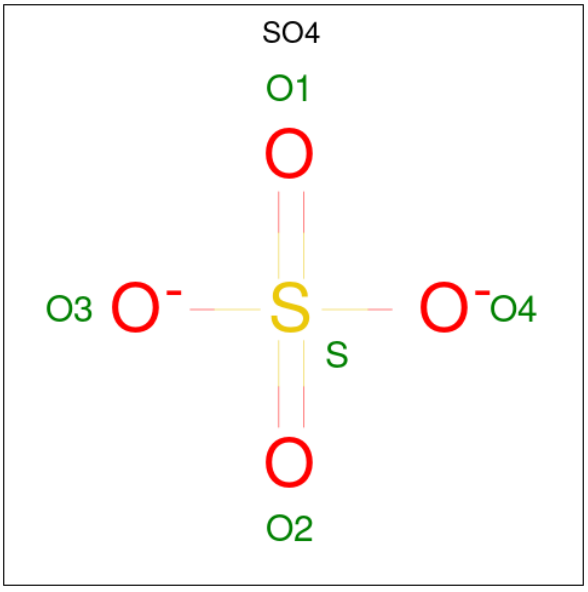
There are 2 unique types of molecules in this entry. The entry contains 10368 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ribonuclease PH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1718	1074	296	340	8			
1	B	226	Total	C	N	O	S	0	0	0
			1718	1074	296	340	8			
1	C	226	Total	C	N	O	S	0	0	0
			1718	1074	296	340	8			
1	D	226	Total	C	N	O	S	0	0	0
			1718	1074	296	340	8			
1	E	226	Total	C	N	O	S	0	0	0
			1718	1074	296	340	8			
1	F	226	Total	C	N	O	S	0	0	0
			1718	1074	296	340	8			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



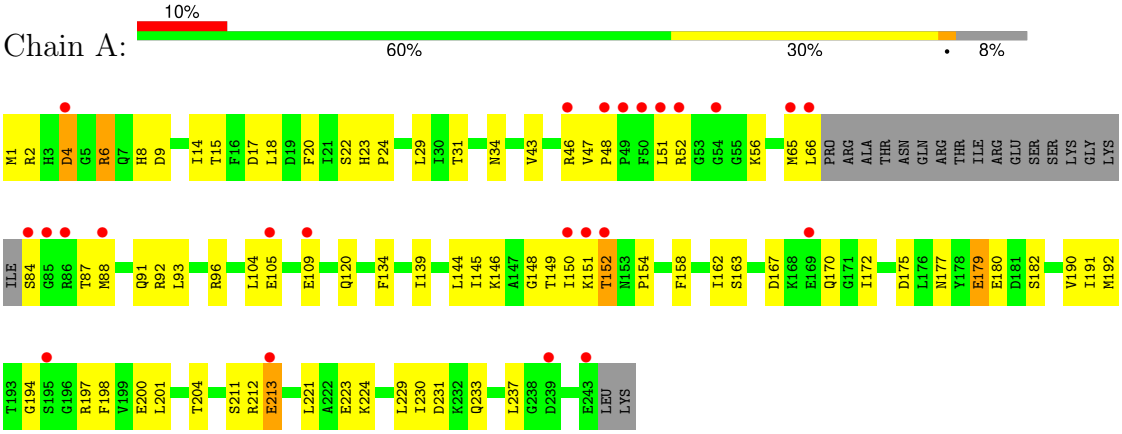
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total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

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

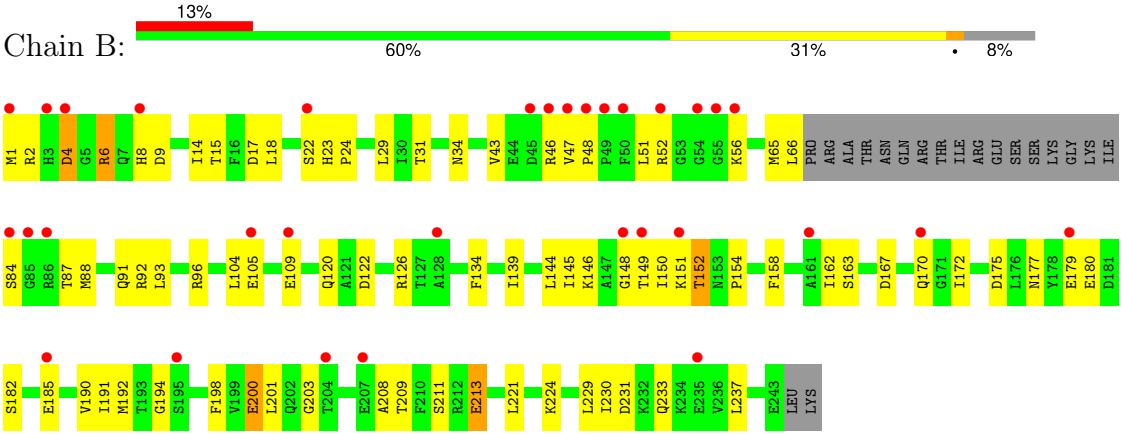
• Molecule 1: Ribonuclease PH

Chain A:



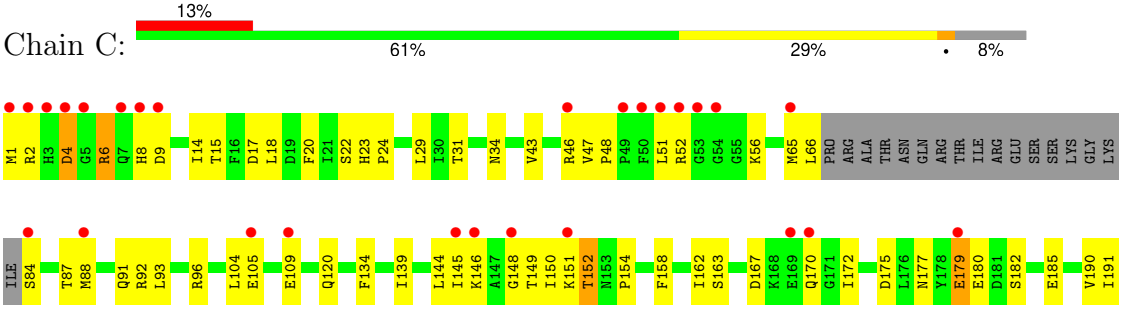
• Molecule 1: Ribonuclease PH

Chain B:



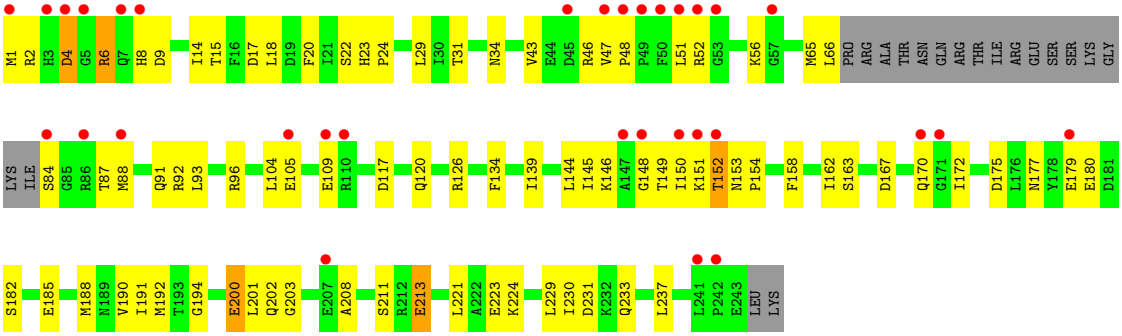
• Molecule 1: Ribonuclease PH

Chain C:



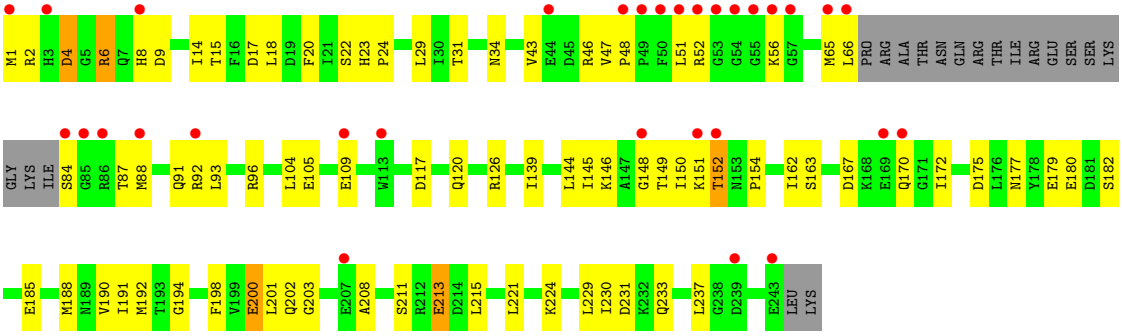
• Molecule 1: Ribonuclease PH

Chain D:



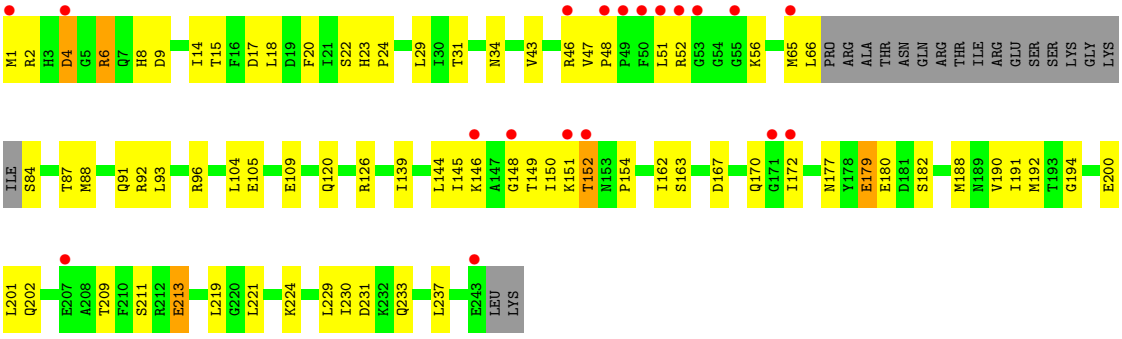
• Molecule 1: Ribonuclease PH

Chain E:



• Molecule 1: Ribonuclease PH

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	51.31Å 163.56Å 166.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 2.76 29.86 – 2.76	Depositor EDS
% Data completeness (in resolution range)	97.6 (29.88-2.76) 98.3 (29.86-2.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.99 (at 2.76Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.285 , 0.305 0.281 , 0.300	Depositor DCC
R_{free} test set	1841 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	39.8	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 33.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.021 for -h,l,k	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	10368	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.24	0/1738	0.50	0/2343
1	B	0.24	0/1738	0.50	0/2343
1	C	0.24	0/1738	0.50	0/2343
1	D	0.24	0/1738	0.50	0/2343
1	E	0.24	0/1738	0.50	0/2343
1	F	0.24	0/1738	0.50	0/2343
All	All	0.24	0/10428	0.50	0/14058

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1718	0	1730	77	0
1	B	1718	0	1730	63	0
1	C	1718	0	1730	58	0
1	D	1718	0	1730	61	0
1	E	1718	0	1730	60	0
1	F	1718	0	1730	63	0
2	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	0	1	0
2	C	10	0	0	0	0
2	D	10	0	0	1	0
2	E	10	0	0	1	0
2	F	10	0	0	1	0
All	All	10368	0	10380	369	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (369) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:LEU:HD12	1:B:203:GLY:H	1.36	0.88
1:A:47:VAL:HG11	1:A:51:LEU:HB2	1.66	0.76
1:F:47:VAL:HG11	1:F:51:LEU:HB2	1.67	0.76
1:C:47:VAL:HG11	1:C:51:LEU:HB2	1.67	0.76
1:D:1:MET:HG3	1:D:2:ARG:H	1.51	0.76
1:E:47:VAL:HG11	1:E:51:LEU:HB2	1.68	0.76
1:D:47:VAL:HG11	1:D:51:LEU:HB2	1.67	0.74
1:A:56:LYS:HB3	1:A:105:GLU:HG2	1.69	0.74
1:B:47:VAL:HG11	1:B:51:LEU:HB2	1.68	0.74
1:D:56:LYS:HB3	1:D:105:GLU:HG2	1.69	0.74
1:E:56:LYS:HB3	1:E:105:GLU:HG2	1.69	0.74
1:E:23:HIS:HB3	1:E:24:PRO:HD3	1.71	0.73
1:F:23:HIS:HB3	1:F:24:PRO:HD3	1.70	0.73
1:B:23:HIS:HB3	1:B:24:PRO:HD3	1.71	0.73
1:C:56:LYS:HB3	1:C:105:GLU:HG2	1.71	0.73
1:B:56:LYS:HB3	1:B:105:GLU:HG2	1.70	0.72
1:D:23:HIS:HB3	1:D:24:PRO:HD3	1.70	0.72
1:F:56:LYS:HB3	1:F:105:GLU:HG2	1.71	0.72
1:A:20:PHE:CE1	1:A:29:LEU:HD22	2.24	0.72
1:D:211:SER:OG	1:D:213:GLU:HG2	1.90	0.71
1:A:201:LEU:CD1	1:B:203:GLY:H	2.03	0.71
1:A:23:HIS:HB3	1:A:24:PRO:HD3	1.70	0.71
1:C:211:SER:OG	1:C:213:GLU:HG2	1.90	0.71
1:E:211:SER:OG	1:E:213:GLU:HG2	1.91	0.70
1:B:1:MET:HG3	1:B:2:ARG:H	1.56	0.70
1:C:23:HIS:HB3	1:C:24:PRO:HD3	1.71	0.70
1:F:1:MET:HG3	1:F:2:ARG:H	1.57	0.70
1:F:211:SER:OG	1:F:213:GLU:HG2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:ASN:O	1:F:120:GLN:HG2	1.93	0.69
1:C:1:MET:HG3	1:C:2:ARG:H	1.59	0.68
1:B:211:SER:OG	1:B:213:GLU:HG2	1.92	0.68
1:D:34:ASN:O	1:D:120:GLN:HG2	1.93	0.68
1:E:203:GLY:H	1:F:201:LEU:HD12	1.57	0.68
1:F:144:LEU:O	1:F:149:THR:HG22	1.93	0.68
1:E:46:ARG:HH12	1:E:52:ARG:HD3	1.58	0.68
1:E:144:LEU:O	1:E:149:THR:HG22	1.93	0.68
1:B:144:LEU:O	1:B:149:THR:HG22	1.94	0.68
1:D:144:LEU:O	1:D:149:THR:HG22	1.93	0.68
1:A:34:ASN:O	1:A:120:GLN:HG2	1.94	0.67
1:B:167:ASP:HB3	1:B:170:GLN:HB2	1.77	0.67
1:F:167:ASP:HB3	1:F:170:GLN:HB2	1.76	0.67
1:A:1:MET:HG3	1:A:2:ARG:H	1.59	0.67
1:E:167:ASP:HB3	1:E:170:GLN:HB2	1.78	0.66
1:C:167:ASP:HB3	1:C:170:GLN:HB2	1.78	0.66
1:D:46:ARG:HH12	1:D:52:ARG:HD3	1.61	0.66
1:E:34:ASN:O	1:E:120:GLN:HG2	1.95	0.66
1:A:144:LEU:O	1:A:149:THR:HG22	1.95	0.66
1:C:145:ILE:HG13	1:C:150:ILE:HD11	1.77	0.66
1:F:145:ILE:HG13	1:F:150:ILE:HD11	1.78	0.66
1:A:211:SER:OG	1:A:213:GLU:HG2	1.96	0.66
1:C:144:LEU:O	1:C:149:THR:HG22	1.95	0.65
1:B:145:ILE:HG13	1:B:150:ILE:HD11	1.78	0.65
1:E:1:MET:HG3	1:E:2:ARG:H	1.60	0.65
1:A:167:ASP:HB3	1:A:170:GLN:HB2	1.78	0.65
1:A:2:ARG:NH2	1:A:6:ARG:NH2	2.45	0.65
1:C:34:ASN:O	1:C:120:GLN:HG2	1.97	0.65
1:D:167:ASP:HB3	1:D:170:GLN:HB2	1.80	0.65
1:B:46:ARG:HH12	1:B:52:ARG:HD3	1.62	0.64
1:F:46:ARG:HH12	1:F:52:ARG:HD3	1.63	0.64
1:E:145:ILE:HG13	1:E:150:ILE:HD11	1.78	0.64
1:A:145:ILE:HG13	1:A:150:ILE:HD11	1.80	0.64
1:E:65:MET:HG3	1:E:66:LEU:H	1.63	0.64
1:A:46:ARG:HH12	1:A:52:ARG:HD3	1.63	0.63
1:C:46:ARG:HH12	1:C:52:ARG:HD3	1.63	0.63
1:C:2:ARG:HB2	1:C:6:ARG:O	1.99	0.63
1:D:145:ILE:HG13	1:D:150:ILE:HD11	1.80	0.63
1:A:2:ARG:HH22	1:A:6:ARG:NH2	1.97	0.63
1:F:177:ASN:OD1	1:F:180:GLU:HG3	1.99	0.63
1:B:2:ARG:HB2	1:B:6:ARG:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:MET:HG3	1:B:66:LEU:H	1.65	0.62
1:F:65:MET:HG3	1:F:66:LEU:H	1.64	0.61
1:A:2:ARG:HB2	1:A:6:ARG:O	1.99	0.61
1:C:65:MET:HG3	1:C:66:LEU:H	1.65	0.60
1:F:172:ILE:HG22	1:F:221:LEU:HD12	1.84	0.60
1:A:65:MET:HG3	1:A:66:LEU:H	1.65	0.60
1:F:201:LEU:HD12	1:F:201:LEU:O	2.01	0.60
1:D:201:LEU:O	1:D:201:LEU:HD12	2.03	0.59
1:A:17:ASP:HB2	1:A:29:LEU:HB3	1.84	0.59
1:A:201:LEU:HD12	1:A:201:LEU:O	2.02	0.59
1:C:9:ASP:OD1	1:C:224:LYS:HE3	2.02	0.59
1:D:2:ARG:HB2	1:D:6:ARG:O	2.02	0.59
1:E:2:ARG:HB2	1:E:6:ARG:O	2.03	0.59
1:E:201:LEU:HD12	1:E:201:LEU:O	2.02	0.59
1:C:201:LEU:HD12	1:C:201:LEU:O	2.02	0.59
1:D:65:MET:HG3	1:D:66:LEU:H	1.66	0.59
1:F:177:ASN:CG	1:F:180:GLU:HG3	2.23	0.58
1:B:201:LEU:HD12	1:B:201:LEU:O	2.03	0.58
1:C:17:ASP:HB2	1:C:29:LEU:HB3	1.86	0.58
1:A:172:ILE:HG22	1:A:221:LEU:HD12	1.85	0.58
1:E:46:ARG:NH1	1:E:52:ARG:HD3	2.19	0.57
1:F:17:ASP:HB2	1:F:29:LEU:HB3	1.86	0.57
1:C:51:LEU:CD2	1:C:56:LYS:HG3	2.35	0.57
1:D:51:LEU:CD2	1:D:56:LYS:HG3	2.34	0.57
1:C:172:ILE:HG22	1:C:221:LEU:HD12	1.87	0.57
1:D:172:ILE:HG22	1:D:221:LEU:HD12	1.87	0.57
1:A:51:LEU:CD2	1:A:56:LYS:HG3	2.34	0.56
1:F:144:LEU:HG	1:F:149:THR:HG21	1.87	0.56
1:A:2:ARG:NH1	1:A:6:ARG:NH2	2.53	0.56
1:E:17:ASP:HB2	1:E:29:LEU:HB3	1.87	0.56
1:E:144:LEU:HG	1:E:149:THR:HG21	1.87	0.56
1:E:172:ILE:HG22	1:E:221:LEU:HD12	1.87	0.56
1:D:17:ASP:HB2	1:D:29:LEU:HB3	1.87	0.56
1:D:144:LEU:HG	1:D:149:THR:HG21	1.86	0.56
1:B:51:LEU:CD2	1:B:56:LYS:HG3	2.36	0.56
1:B:144:LEU:HG	1:B:149:THR:HG21	1.88	0.56
1:C:144:LEU:HG	1:C:149:THR:HG21	1.88	0.56
1:E:51:LEU:CD2	1:E:56:LYS:HG3	2.36	0.56
1:F:2:ARG:HB2	1:F:6:ARG:O	2.05	0.56
1:B:17:ASP:HB2	1:B:29:LEU:HB3	1.88	0.56
1:B:34:ASN:O	1:B:120:GLN:HG2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:LEU:CD2	1:F:56:LYS:HG3	2.36	0.56
1:B:172:ILE:HG22	1:B:221:LEU:HD12	1.87	0.55
1:F:18:LEU:HD22	1:F:139:ILE:HD11	1.89	0.55
1:D:20:PHE:CE1	1:D:29:LEU:HD22	2.42	0.55
1:A:46:ARG:NH1	1:A:52:ARG:HD3	2.22	0.55
1:A:144:LEU:HG	1:A:149:THR:HG21	1.88	0.55
1:C:46:ARG:NH1	1:C:52:ARG:HD3	2.22	0.54
1:C:65:MET:CG	1:C:66:LEU:N	2.71	0.54
1:C:201:LEU:HD12	1:D:203:GLY:H	1.73	0.54
1:D:47:VAL:HG13	1:D:48:PRO:HD2	1.89	0.54
1:E:65:MET:CG	1:E:66:LEU:N	2.71	0.54
1:F:20:PHE:CE1	1:F:29:LEU:HD22	2.43	0.54
1:F:65:MET:CG	1:F:66:LEU:N	2.71	0.54
1:A:65:MET:CG	1:A:66:LEU:N	2.71	0.54
1:C:47:VAL:HG13	1:C:48:PRO:HD2	1.90	0.53
1:D:46:ARG:NH1	1:D:52:ARG:HD3	2.22	0.53
1:B:46:ARG:NH1	1:B:52:ARG:HD3	2.22	0.53
1:E:18:LEU:HD22	1:E:139:ILE:HD11	1.90	0.53
1:F:47:VAL:HG13	1:F:48:PRO:HD2	1.90	0.53
1:F:46:ARG:NH1	1:F:52:ARG:HD3	2.24	0.53
1:A:47:VAL:HG13	1:A:48:PRO:HD2	1.89	0.53
1:D:177:ASN:ND2	1:D:180:GLU:HG3	2.24	0.53
1:E:47:VAL:HG13	1:E:48:PRO:HD2	1.91	0.53
1:B:47:VAL:HG13	1:B:48:PRO:HD2	1.90	0.53
1:B:65:MET:CG	1:B:66:LEU:N	2.71	0.53
1:A:151:LYS:O	1:A:152:THR:HB	2.10	0.52
1:C:20:PHE:CE1	1:C:29:LEU:HD22	2.44	0.52
1:A:2:ARG:HH22	1:A:6:ARG:HH21	1.58	0.52
1:B:200:GLU:HG3	1:B:201:LEU:N	2.24	0.52
1:F:43:VAL:HG21	1:F:144:LEU:HD11	1.91	0.52
1:A:18:LEU:HD22	1:A:139:ILE:HD11	1.92	0.52
1:A:197:ARG:NH2	1:B:209:THR:O	2.43	0.52
1:E:152:THR:O	1:E:152:THR:HG23	2.10	0.52
1:A:2:ARG:HH12	1:A:6:ARG:NH2	2.08	0.52
1:C:152:THR:O	1:C:154:PRO:HD3	2.10	0.52
1:D:65:MET:CG	1:D:66:LEU:N	2.72	0.52
1:F:177:ASN:ND2	1:F:180:GLU:HG3	2.25	0.52
1:A:162:ILE:HG13	1:A:163:SER:N	2.25	0.52
1:A:162:ILE:HG13	1:A:163:SER:H	1.75	0.52
1:C:152:THR:O	1:C:152:THR:HG23	2.10	0.52
1:E:20:PHE:CE1	1:E:29:LEU:HD22	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:47:VAL:HG21	1:E:109:GLU:HG3	1.92	0.52
1:E:151:LYS:O	1:E:152:THR:HB	2.10	0.52
1:F:152:THR:O	1:F:154:PRO:HD3	2.10	0.52
1:A:152:THR:HG23	1:A:152:THR:O	2.10	0.51
1:B:18:LEU:HD22	1:B:139:ILE:HD11	1.91	0.51
1:D:43:VAL:HG21	1:D:144:LEU:HD11	1.93	0.51
1:E:162:ILE:HG13	1:E:163:SER:N	2.26	0.51
1:F:162:ILE:HG13	1:F:163:SER:N	2.25	0.51
1:C:18:LEU:HD22	1:C:139:ILE:HD11	1.91	0.51
1:D:151:LYS:O	1:D:152:THR:HB	2.11	0.51
1:A:2:ARG:CZ	1:A:6:ARG:NH2	2.74	0.51
1:A:200:GLU:HG3	1:A:201:LEU:N	2.25	0.51
1:D:152:THR:HG23	1:D:152:THR:O	2.10	0.51
1:E:152:THR:O	1:E:154:PRO:HD3	2.11	0.51
1:A:56:LYS:HE3	1:A:104:LEU:HB2	1.93	0.51
1:B:152:THR:HG23	1:B:152:THR:O	2.10	0.51
1:E:162:ILE:HG13	1:E:163:SER:H	1.76	0.51
1:B:151:LYS:O	1:B:152:THR:HB	2.11	0.51
1:F:151:LYS:O	1:F:152:THR:HB	2.11	0.51
1:B:152:THR:O	1:B:154:PRO:HD3	2.11	0.51
1:D:92:ARG:O	1:D:96:ARG:HB2	2.12	0.51
1:D:152:THR:O	1:D:154:PRO:HD3	2.10	0.51
1:A:152:THR:O	1:A:154:PRO:HD3	2.11	0.50
1:B:177:ASN:ND2	1:B:180:GLU:HG3	2.25	0.50
1:E:43:VAL:HG21	1:E:144:LEU:HD11	1.92	0.50
1:F:200:GLU:HG3	1:F:201:LEU:N	2.26	0.50
1:B:56:LYS:HE3	1:B:104:LEU:HB2	1.92	0.50
1:D:18:LEU:HD22	1:D:139:ILE:HD11	1.92	0.50
1:A:43:VAL:HG21	1:A:144:LEU:HD11	1.92	0.50
1:E:56:LYS:HE3	1:E:104:LEU:HB2	1.93	0.50
1:A:2:ARG:NH2	1:A:6:ARG:CZ	2.75	0.50
1:C:43:VAL:HG21	1:C:144:LEU:HD11	1.93	0.50
1:B:177:ASN:OD1	1:B:180:GLU:HG3	2.11	0.50
1:C:200:GLU:HG3	1:C:201:LEU:N	2.25	0.50
1:C:56:LYS:HE3	1:C:104:LEU:HB2	1.94	0.50
1:F:162:ILE:HG13	1:F:163:SER:H	1.76	0.50
1:B:47:VAL:HG21	1:B:109:GLU:HG3	1.94	0.50
1:F:152:THR:O	1:F:152:THR:HG23	2.10	0.50
1:A:47:VAL:HG21	1:A:109:GLU:HG3	1.94	0.49
1:C:151:LYS:O	1:C:152:THR:HB	2.11	0.49
1:A:14:ILE:HD13	1:A:229:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:VAL:HG21	1:B:144:LEU:HD11	1.93	0.49
1:B:92:ARG:O	1:B:96:ARG:HB2	2.13	0.49
1:B:177:ASN:CG	1:B:180:GLU:HG3	2.33	0.49
1:C:162:ILE:HG13	1:C:163:SER:N	2.28	0.49
1:E:65:MET:HG3	1:E:66:LEU:N	2.26	0.49
1:D:56:LYS:HE3	1:D:104:LEU:HB2	1.93	0.49
1:B:9:ASP:OD1	1:B:224:LYS:HE3	2.13	0.49
1:D:200:GLU:HG3	1:D:201:LEU:N	2.26	0.49
1:E:200:GLU:HG3	1:E:201:LEU:N	2.26	0.49
1:E:14:ILE:HD13	1:E:229:LEU:HD21	1.95	0.48
1:A:92:ARG:O	1:A:96:ARG:HB2	2.13	0.48
1:B:65:MET:HG3	1:B:66:LEU:N	2.28	0.48
1:B:190:VAL:HG11	1:B:192:MET:HE2	1.95	0.48
1:D:14:ILE:HD13	1:D:229:LEU:HD21	1.94	0.48
1:A:9:ASP:OD1	1:A:224:LYS:HE3	2.13	0.48
1:D:162:ILE:HG13	1:D:163:SER:N	2.28	0.48
1:D:177:ASN:CG	1:D:180:GLU:HG3	2.34	0.48
1:F:56:LYS:HE3	1:F:104:LEU:HB2	1.94	0.48
1:E:190:VAL:HG11	1:E:192:MET:HE2	1.95	0.48
1:B:4:ASP:HB3	1:B:6:ARG:HG2	1.96	0.48
1:A:2:ARG:CZ	1:A:6:ARG:CZ	2.92	0.47
1:B:162:ILE:HG13	1:B:163:SER:N	2.29	0.47
1:C:47:VAL:HG21	1:C:109:GLU:HG3	1.96	0.47
1:D:177:ASN:OD1	1:D:180:GLU:HG3	2.14	0.47
1:F:65:MET:HG3	1:F:66:LEU:N	2.29	0.47
1:C:190:VAL:HG11	1:C:192:MET:HE2	1.96	0.47
1:D:1:MET:HG3	1:D:2:ARG:N	2.23	0.47
1:D:4:ASP:HB3	1:D:6:ARG:HG2	1.96	0.47
1:D:65:MET:HG3	1:D:66:LEU:N	2.29	0.47
1:F:4:ASP:HB3	1:F:6:ARG:HG2	1.96	0.47
1:F:9:ASP:OD1	1:F:224:LYS:HE3	2.15	0.47
1:F:14:ILE:HD13	1:F:229:LEU:HD21	1.95	0.47
1:C:92:ARG:O	1:C:96:ARG:HB2	2.14	0.47
1:F:47:VAL:HG21	1:F:109:GLU:HG3	1.96	0.47
1:C:162:ILE:HG13	1:C:163:SER:H	1.80	0.47
1:E:92:ARG:O	1:E:96:ARG:HB2	2.13	0.47
1:A:6:ARG:NH2	1:A:175:ASP:O	2.47	0.47
1:D:213:GLU:CD	1:D:213:GLU:H	2.18	0.47
1:B:126:ARG:HG2	2:B:303:SO4:O4	2.15	0.47
1:A:4:ASP:HB3	1:A:6:ARG:HG2	1.97	0.47
1:B:14:ILE:HD13	1:B:229:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:THR:O	1:A:91:GLN:HB2	2.15	0.47
1:D:162:ILE:HG13	1:D:163:SER:H	1.80	0.47
1:E:43:VAL:HG11	1:E:144:LEU:HD21	1.97	0.47
1:D:9:ASP:OD1	1:D:224:LYS:HE3	2.15	0.46
1:D:47:VAL:HG21	1:D:109:GLU:HG3	1.97	0.46
1:E:213:GLU:CD	1:E:213:GLU:H	2.18	0.46
1:F:92:ARG:O	1:F:96:ARG:HB2	2.15	0.46
1:C:14:ILE:HD13	1:C:229:LEU:HD21	1.98	0.46
1:B:6:ARG:NH2	1:B:175:ASP:O	2.49	0.46
1:A:2:ARG:HD2	1:A:180:GLU:OE2	2.16	0.46
1:C:43:VAL:HG11	1:C:144:LEU:HD21	1.98	0.46
1:D:43:VAL:HG11	1:D:144:LEU:HD21	1.97	0.46
1:E:4:ASP:HB3	1:E:6:ARG:HG2	1.97	0.46
1:A:47:VAL:CG1	1:A:51:LEU:HB2	2.43	0.46
1:B:43:VAL:HG11	1:B:144:LEU:HD21	1.97	0.46
1:C:4:ASP:HB3	1:C:6:ARG:HG2	1.97	0.46
1:C:213:GLU:CD	1:C:213:GLU:H	2.19	0.45
1:A:43:VAL:HG11	1:A:144:LEU:HD21	1.99	0.45
1:E:6:ARG:NH2	1:E:175:ASP:O	2.49	0.45
1:F:190:VAL:HG11	1:F:192:MET:HE2	1.97	0.45
1:A:204:THR:HG21	1:B:96:ARG:CD	2.47	0.45
1:C:177:ASN:OD1	1:C:180:GLU:HG3	2.16	0.45
1:F:87:THR:O	1:F:91:GLN:HB2	2.16	0.45
1:C:51:LEU:HD21	1:C:56:LYS:HG3	1.99	0.45
1:E:215:LEU:HD21	1:F:219:LEU:HD11	1.98	0.45
1:A:20:PHE:HZ	1:F:20:PHE:HZ	1.64	0.45
1:A:213:GLU:CD	1:A:213:GLU:H	2.20	0.45
1:D:15:THR:OG1	1:D:31:THR:HB	2.16	0.45
1:D:87:THR:O	1:D:91:GLN:HB2	2.17	0.45
1:F:47:VAL:CG1	1:F:51:LEU:HB2	2.44	0.45
1:A:177:ASN:ND2	1:A:180:GLU:HG3	2.32	0.45
1:B:190:VAL:HG12	1:B:191:ILE:N	2.32	0.45
1:B:213:GLU:CD	1:B:213:GLU:H	2.19	0.45
1:D:117:ASP:OD1	1:E:117:ASP:OD1	2.35	0.45
1:E:9:ASP:OD1	1:E:224:LYS:HE3	2.16	0.45
1:B:162:ILE:HG13	1:B:163:SER:H	1.81	0.44
1:A:2:ARG:NH1	1:A:180:GLU:OE1	2.50	0.44
1:A:2:ARG:HH12	1:A:6:ARG:HH22	1.64	0.44
1:F:43:VAL:HG11	1:F:144:LEU:HD21	1.99	0.44
1:A:51:LEU:HD21	1:A:56:LYS:HG3	1.99	0.44
1:C:15:THR:OG1	1:C:31:THR:HB	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:87:THR:O	1:E:91:GLN:HB2	2.17	0.44
1:B:146:LYS:C	1:B:148:GLY:H	2.21	0.44
1:C:87:THR:O	1:C:91:GLN:HB2	2.17	0.44
1:F:126:ARG:HG2	2:F:311:SO4:O4	2.18	0.44
1:B:1:MET:HG3	1:B:2:ARG:N	2.28	0.43
1:B:87:THR:O	1:B:91:GLN:HB2	2.17	0.43
1:C:194:GLY:HA2	1:C:230:ILE:HD13	2.00	0.43
1:D:84:SER:HA	1:D:87:THR:HB	2.00	0.43
1:F:1:MET:HG3	1:F:2:ARG:N	2.28	0.43
1:F:213:GLU:CD	1:F:213:GLU:H	2.21	0.43
1:A:204:THR:CG2	1:B:96:ARG:HD2	2.48	0.43
1:F:15:THR:OG1	1:F:31:THR:HB	2.18	0.43
1:E:15:THR:OG1	1:E:31:THR:HB	2.18	0.43
1:F:179:GLU:HG3	1:F:180:GLU:N	2.33	0.43
1:C:6:ARG:NH2	1:C:175:ASP:O	2.50	0.43
1:D:146:LYS:C	1:D:148:GLY:H	2.22	0.43
1:E:146:LYS:C	1:E:148:GLY:H	2.21	0.43
1:D:188:MET:HG3	1:D:202:GLN:C	2.38	0.43
1:A:204:THR:HG23	1:B:200:GLU:OE2	2.17	0.43
1:C:177:ASN:ND2	1:C:180:GLU:HG3	2.33	0.43
1:C:190:VAL:HG12	1:C:191:ILE:N	2.34	0.43
1:D:190:VAL:HG12	1:D:191:ILE:N	2.33	0.43
1:A:2:ARG:CD	1:A:180:GLU:OE2	2.67	0.43
1:A:146:LYS:C	1:A:148:GLY:H	2.21	0.43
1:B:47:VAL:CG1	1:B:51:LEU:HB2	2.44	0.43
1:B:185:GLU:HB2	1:B:208:ALA:HB3	2.01	0.43
1:D:185:GLU:HB2	1:D:208:ALA:HB3	2.01	0.43
1:E:56:LYS:CE	1:E:104:LEU:HD12	2.49	0.43
1:F:194:GLY:HA2	1:F:230:ILE:HD13	2.01	0.43
1:A:149:THR:HG23	1:A:150:ILE:HG23	2.01	0.42
1:A:190:VAL:HG12	1:A:191:ILE:N	2.34	0.42
1:C:84:SER:HA	1:C:87:THR:HB	2.01	0.42
1:D:190:VAL:HG11	1:D:192:MET:HE2	1.99	0.42
1:F:188:MET:HG3	1:F:202:GLN:C	2.40	0.42
1:E:190:VAL:HG12	1:E:191:ILE:N	2.33	0.42
1:A:15:THR:OG1	1:A:31:THR:HB	2.19	0.42
1:A:192:MET:HE3	1:A:223:GLU:HA	2.02	0.42
1:B:134:PHE:CZ	1:B:158:PHE:HA	2.55	0.42
1:D:126:ARG:HG2	2:D:307:SO4:O4	2.19	0.42
1:F:146:LYS:C	1:F:148:GLY:H	2.22	0.42
1:A:1:MET:HG3	1:A:2:ARG:N	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:SER:HA	1:A:87:THR:HB	2.01	0.42
1:A:194:GLY:HA2	1:A:230:ILE:HD13	2.01	0.42
1:C:179:GLU:HG3	1:C:180:GLU:N	2.35	0.42
1:D:6:ARG:NH2	1:D:175:ASP:O	2.52	0.42
1:D:233:GLN:O	1:D:237:LEU:HB2	2.20	0.42
1:F:51:LEU:HD21	1:F:56:LYS:HG3	2.01	0.42
1:A:190:VAL:HG11	1:A:192:MET:HE2	2.02	0.42
1:B:15:THR:OG1	1:B:31:THR:HB	2.20	0.42
1:D:51:LEU:HD21	1:D:56:LYS:HG3	2.00	0.42
1:B:84:SER:HA	1:B:87:THR:HB	2.02	0.42
1:D:153:ASN:HA	1:D:154:PRO:HD3	1.88	0.42
1:D:192:MET:HE3	1:D:223:GLU:HA	2.02	0.42
1:E:51:LEU:HD21	1:E:56:LYS:HG3	2.01	0.42
1:E:126:ARG:HG2	2:E:309:SO4:O4	2.19	0.42
1:E:194:GLY:HA2	1:E:230:ILE:HD13	2.01	0.42
1:B:51:LEU:HD21	1:B:56:LYS:HG3	2.01	0.41
1:B:194:GLY:HA2	1:B:230:ILE:HD13	2.01	0.41
1:C:177:ASN:CG	1:C:180:GLU:HG3	2.40	0.41
1:C:185:GLU:HB2	1:C:208:ALA:HB3	2.02	0.41
1:C:146:LYS:C	1:C:148:GLY:H	2.23	0.41
1:F:172:ILE:HG22	1:F:221:LEU:CD1	2.48	0.41
1:F:233:GLN:O	1:F:237:LEU:HB2	2.21	0.41
1:A:51:LEU:HD22	1:A:56:LYS:O	2.20	0.41
1:B:233:GLN:O	1:B:237:LEU:HB2	2.21	0.41
1:C:192:MET:HE3	1:C:223:GLU:HA	2.02	0.41
1:E:84:SER:HA	1:E:87:THR:HB	2.03	0.41
1:E:185:GLU:HB2	1:E:208:ALA:HB3	2.02	0.41
1:E:149:THR:HG23	1:E:150:ILE:HG23	2.02	0.41
1:E:192:MET:HG2	1:E:198:PHE:HA	2.02	0.41
1:A:233:GLN:O	1:A:237:LEU:HB2	2.21	0.41
1:C:149:THR:HG23	1:C:150:ILE:HG23	2.02	0.41
1:C:233:GLN:O	1:C:237:LEU:HB2	2.21	0.41
1:E:47:VAL:CG1	1:E:51:LEU:HB2	2.45	0.41
1:A:134:PHE:CZ	1:A:158:PHE:HA	2.55	0.41
1:A:177:ASN:OD1	1:A:180:GLU:HG3	2.21	0.41
1:A:192:MET:HG2	1:A:198:PHE:HA	2.02	0.41
1:D:56:LYS:CE	1:D:104:LEU:HD12	2.51	0.41
1:D:194:GLY:HA2	1:D:230:ILE:HD13	2.01	0.41
1:E:188:MET:HG3	1:E:202:GLN:C	2.41	0.41
1:E:198:PHE:O	1:F:209:THR:HB	2.21	0.41
1:F:51:LEU:HD22	1:F:56:LYS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:56:LYS:CE	1:F:104:LEU:HD12	2.50	0.41
1:B:34:ASN:HB2	1:B:122:ASP:OD2	2.21	0.41
1:E:233:GLN:O	1:E:237:LEU:HB2	2.22	0.40
1:A:179:GLU:HG3	1:A:180:GLU:N	2.36	0.40
1:E:177:ASN:ND2	1:E:180:GLU:HG3	2.36	0.40
1:F:190:VAL:HG12	1:F:191:ILE:N	2.36	0.40
1:C:47:VAL:CG1	1:C:51:LEU:HB2	2.44	0.40
1:C:134:PHE:CZ	1:C:158:PHE:HA	2.56	0.40
1:A:212:ARG:HB2	1:B:198:PHE:HE1	1.85	0.40
1:F:14:ILE:HA	1:F:31:THR:O	2.22	0.40
1:C:221:LEU:HD23	1:C:221:LEU:HA	1.88	0.40
1:D:134:PHE:CZ	1:D:158:PHE:HA	2.57	0.40
1:F:84:SER:HA	1:F:87:THR:HB	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	222/245 (91%)	199 (90%)	22 (10%)	1 (0%)	29	47
1	B	222/245 (91%)	200 (90%)	21 (10%)	1 (0%)	29	47
1	C	222/245 (91%)	199 (90%)	22 (10%)	1 (0%)	29	47
1	D	222/245 (91%)	200 (90%)	21 (10%)	1 (0%)	29	47
1	E	222/245 (91%)	199 (90%)	22 (10%)	1 (0%)	29	47
1	F	222/245 (91%)	199 (90%)	22 (10%)	1 (0%)	29	47
All	All	1332/1470 (91%)	1196 (90%)	130 (10%)	6 (0%)	29	47

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	THR
1	B	152	THR
1	C	152	THR
1	D	152	THR
1	E	152	THR
1	F	152	THR

5.3.2 Protein sidechains (i)

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	184/201 (92%)	174 (95%)	10 (5%)	22	38
1	B	184/201 (92%)	173 (94%)	11 (6%)	19	33
1	C	184/201 (92%)	174 (95%)	10 (5%)	22	38
1	D	184/201 (92%)	173 (94%)	11 (6%)	19	33
1	E	184/201 (92%)	173 (94%)	11 (6%)	19	33
1	F	184/201 (92%)	174 (95%)	10 (5%)	22	38
All	All	1104/1206 (92%)	1041 (94%)	63 (6%)	20	36

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

Mol	Chain	Res	Type
1	A	4	ASP
1	A	6	ARG
1	A	8	HIS
1	A	22	SER
1	A	88	MET
1	A	93	LEU
1	A	179	GLU
1	A	182	SER
1	A	213	GLU
1	A	231	ASP
1	B	4	ASP
1	B	6	ARG
1	B	8	HIS

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Mol	Chain	Res	Type
1	B	22	SER
1	B	88	MET
1	B	93	LEU
1	B	179	GLU
1	B	182	SER
1	B	200	GLU
1	B	213	GLU
1	B	231	ASP
1	C	4	ASP
1	C	6	ARG
1	C	8	HIS
1	C	22	SER
1	C	88	MET
1	C	93	LEU
1	C	179	GLU
1	C	182	SER
1	C	213	GLU
1	C	231	ASP
1	D	4	ASP
1	D	6	ARG
1	D	8	HIS
1	D	22	SER
1	D	88	MET
1	D	93	LEU
1	D	179	GLU
1	D	182	SER
1	D	200	GLU
1	D	213	GLU
1	D	231	ASP
1	E	4	ASP
1	E	6	ARG
1	E	8	HIS
1	E	22	SER
1	E	88	MET
1	E	93	LEU
1	E	179	GLU
1	E	182	SER
1	E	200	GLU
1	E	213	GLU
1	E	231	ASP
1	F	4	ASP
1	F	6	ARG

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Mol	Chain	Res	Type
1	F	8	HIS
1	F	22	SER
1	F	88	MET
1	F	93	LEU
1	F	179	GLU
1	F	182	SER
1	F	213	GLU
1	F	231	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	40	ASN
1	A	170	GLN
1	B	7	GLN
1	B	40	ASN
1	B	170	GLN
1	C	7	GLN
1	C	40	ASN
1	C	170	GLN
1	D	7	GLN
1	D	40	ASN
1	D	170	GLN
1	E	7	GLN
1	E	40	ASN
1	E	170	GLN
1	F	7	GLN
1	F	40	ASN
1	F	170	GLN
1	F	189	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	302	-	4,4,4	0.37	0	6,6,6	0.08	0
2	SO4	D	308	-	4,4,4	0.36	0	6,6,6	0.08	0
2	SO4	E	310	-	4,4,4	0.36	0	6,6,6	0.08	0
2	SO4	C	306	-	4,4,4	0.37	0	6,6,6	0.08	0
2	SO4	F	312	-	4,4,4	0.37	0	6,6,6	0.08	0
2	SO4	C	305	-	4,4,4	0.37	0	6,6,6	0.07	0
2	SO4	D	307	-	4,4,4	0.36	0	6,6,6	0.07	0
2	SO4	B	304	-	4,4,4	0.37	0	6,6,6	0.08	0
2	SO4	F	311	-	4,4,4	0.36	0	6,6,6	0.07	0
2	SO4	E	309	-	4,4,4	0.36	0	6,6,6	0.07	0
2	SO4	B	303	-	4,4,4	0.36	0	6,6,6	0.07	0
2	SO4	A	301	-	4,4,4	0.37	0	6,6,6	0.07	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.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	307	SO4	1	0
2	F	311	SO4	1	0
2	E	309	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	303	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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^{th} 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	226/245 (92%)	0.83	24 (10%) 6 6	13, 31, 55, 68	0
1	B	226/245 (92%)	1.01	32 (14%) 2 3	14, 32, 55, 67	0
1	C	226/245 (92%)	0.94	32 (14%) 2 3	14, 31, 56, 68	0
1	D	226/245 (92%)	0.76	32 (14%) 2 3	14, 31, 56, 67	0
1	E	226/245 (92%)	1.03	31 (13%) 3 3	14, 31, 57, 68	0
1	F	226/245 (92%)	0.77	19 (8%) 11 13	13, 31, 55, 68	0
All	All	1356/1470 (92%)	0.89	170 (12%) 3 4	13, 31, 57, 68	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	8.9
1	E	50	PHE	8.8
1	E	3	HIS	8.6
1	F	50	PHE	7.8
1	A	50	PHE	7.6
1	B	48	PRO	7.6
1	C	50	PHE	7.5
1	D	1	MET	7.3
1	D	50	PHE	7.2
1	B	49	PRO	6.6
1	A	49	PRO	6.5
1	B	54	GLY	6.3
1	C	3	HIS	6.2
1	B	50	PHE	6.0
1	E	49	PRO	6.0
1	A	151	LYS	5.9
1	E	1	MET	5.9
1	E	48	PRO	5.9
1	E	54	GLY	5.8

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Mol	Chain	Res	Type	RSRZ
1	C	151	LYS	5.6
1	F	49	PRO	5.4
1	B	1	MET	5.4
1	E	170	GLN	5.3
1	C	239	ASP	5.2
1	E	51	LEU	5.1
1	C	146	LYS	5.0
1	D	3	HIS	5.0
1	A	52	ARG	4.8
1	F	51	LEU	4.8
1	C	170	GLN	4.7
1	D	105	GLU	4.5
1	D	49	PRO	4.4
1	A	239	ASP	4.3
1	F	48	PRO	4.1
1	E	169	GLU	4.1
1	E	207	GLU	4.1
1	B	4	ASP	4.1
1	A	88	MET	4.0
1	B	3	HIS	4.0
1	F	152	THR	4.0
1	F	46	ARG	4.0
1	F	151	LYS	4.0
1	E	55	GLY	3.9
1	F	53	GLY	3.9
1	C	2	ARG	3.9
1	A	152	THR	3.9
1	D	151	LYS	3.8
1	A	48	PRO	3.8
1	A	109	GLU	3.8
1	B	55	GLY	3.8
1	D	53	GLY	3.7
1	C	8	HIS	3.7
1	E	66	LEU	3.7
1	F	55	GLY	3.6
1	E	88	MET	3.6
1	E	84	SER	3.6
1	A	169	GLU	3.5
1	F	171	GLY	3.5
1	B	151	LYS	3.4
1	E	52	ARG	3.4
1	A	46	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	243	GLU	3.4
1	D	207	GLU	3.4
1	C	179	GLU	3.3
1	E	56	LYS	3.3
1	E	243	GLU	3.3
1	C	243	GLU	3.2
1	B	8	HIS	3.2
1	C	169	GLU	3.2
1	C	5	GLY	3.2
1	A	51	LEU	3.2
1	E	109	GLU	3.2
1	D	148	GLY	3.2
1	E	151	LYS	3.1
1	E	86	ARG	3.1
1	B	84	SER	3.1
1	B	109	GLU	3.0
1	B	47	VAL	3.0
1	C	105	GLU	3.0
1	A	85	GLY	3.0
1	C	145	ILE	3.0
1	B	148	GLY	2.9
1	B	56	LYS	2.9
1	A	243	GLU	2.9
1	D	57	GLY	2.9
1	F	207	GLU	2.9
1	D	242	PRO	2.9
1	D	5	GLY	2.9
1	B	207	GLU	2.9
1	E	44	GLU	2.9
1	D	171	GLY	2.9
1	C	65	MET	2.9
1	B	46	ARG	2.9
1	B	149	THR	2.9
1	B	105	GLU	2.8
1	B	22	SER	2.8
1	B	235	GLU	2.8
1	E	53	GLY	2.8
1	B	179	GLU	2.8
1	C	7	GLN	2.7
1	D	8	HIS	2.7
1	C	84	SER	2.7
1	D	170	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	207	GLU	2.7
1	A	4	ASP	2.7
1	E	92	ARG	2.7
1	A	105	GLU	2.6
1	C	52	ARG	2.6
1	C	49	PRO	2.6
1	F	65	MET	2.6
1	B	85	GLY	2.6
1	D	84	SER	2.6
1	D	48	PRO	2.5
1	D	88	MET	2.5
1	C	9	ASP	2.5
1	A	195	SER	2.5
1	B	170	GLN	2.5
1	B	185	GLU	2.5
1	D	52	ARG	2.5
1	B	45	ASP	2.5
1	F	1	MET	2.5
1	E	152	THR	2.5
1	A	54	GLY	2.4
1	D	147	ALA	2.4
1	A	86	ARG	2.4
1	C	4	ASP	2.4
1	E	148	GLY	2.4
1	D	4	ASP	2.4
1	D	86	ARG	2.4
1	E	65	MET	2.4
1	C	109	GLU	2.3
1	E	8	HIS	2.3
1	A	213	GLU	2.3
1	F	172	ILE	2.3
1	D	45	ASP	2.3
1	D	179	GLU	2.3
1	D	51	LEU	2.3
1	D	7	GLN	2.3
1	F	4	ASP	2.3
1	A	65	MET	2.2
1	B	161	ALA	2.2
1	C	53	GLY	2.2
1	F	146	LYS	2.2
1	B	86	ARG	2.2
1	E	57	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	85	GLY	2.2
1	C	206	GLU	2.2
1	F	148	GLY	2.2
1	B	52	ARG	2.2
1	B	195	SER	2.2
1	F	52	ARG	2.2
1	C	88	MET	2.2
1	D	152	THR	2.2
1	A	84	SER	2.1
1	D	241	LEU	2.1
1	A	66	LEU	2.1
1	C	51	LEU	2.1
1	C	242	PRO	2.1
1	C	54	GLY	2.1
1	B	204	THR	2.1
1	E	113	TRP	2.1
1	E	239	ASP	2.1
1	D	109	GLU	2.1
1	D	47	VAL	2.1
1	C	148	GLY	2.1
1	C	46	ARG	2.0
1	A	150	ILE	2.0
1	D	150	ILE	2.0
1	B	128	ALA	2.0
1	D	110	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	E	310	5/5	0.49	0.41	85,85,86,87	0
2	SO4	F	312	5/5	0.69	0.31	85,86,86,86	0
2	SO4	B	304	5/5	0.79	0.35	85,85,86,86	0
2	SO4	A	302	5/5	0.85	0.25	83,84,84,84	0
2	SO4	B	303	5/5	0.87	0.24	43,45,45,47	0
2	SO4	C	306	5/5	0.90	0.18	81,81,81,82	0
2	SO4	D	308	5/5	0.90	0.21	82,82,83,84	0
2	SO4	F	311	5/5	0.93	0.18	42,43,44,45	0
2	SO4	E	309	5/5	0.94	0.17	44,45,45,46	0
2	SO4	D	307	5/5	0.95	0.15	45,45,45,46	0
2	SO4	C	305	5/5	0.95	0.17	40,41,43,43	0
2	SO4	A	301	5/5	0.96	0.14	40,40,42,43	0

6.5 Other polymers (i)

There are no such residues in this entry.