Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2024 – 01:42 AM EST

PDB ID	:	4HUQ
Title	:	Crystal Structure of a transporter
Authors	:	Zhang, P.; Xu, K.; Zhang, M.; Zhao, Q.; Yu, F.
Deposited on	:	2012-11-03
Resolution	:	3.00 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 (i) 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 (1)) were used in the production of this report:

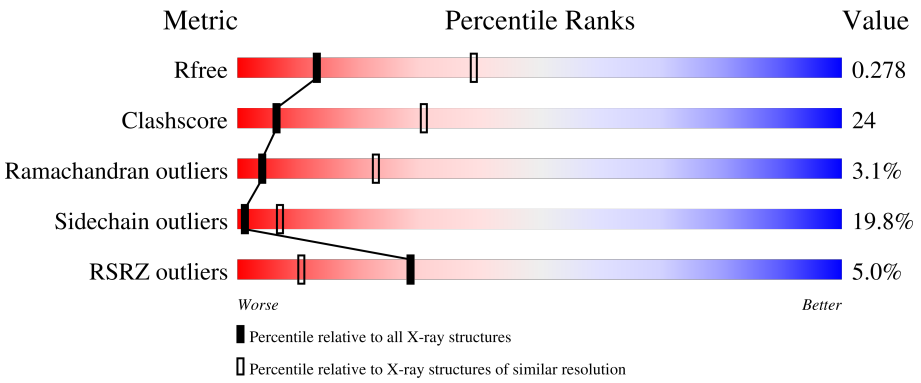
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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	290	2%, 62%, 30%, 6%
2	B	279	4%, 56%, 33%, 9%
3	S	174	5%, 46%, 40%, 8%, 6%
4	T	280	8%, 44%, 31%, 13%, 12%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7601 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 Energy-coupling factor transporter ATP-binding protein EcfA 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	284	2217	1399	389	418	11	0	0	0

- Molecule 2 is a protein called Energy-coupling factor transporter ATP-binding protein EcfA 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	275	2114	1325	365	417	7	0	0	0

- Molecule 3 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	S	164	1293	876	202	208	7	0	0	0

- Molecule 4 is a protein called Energy-coupling factor transporter transmembrane protein EcfT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	T	245	1951	1293	321	325	12	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	-13	MET	-	expression tag	UNP Q03PY7
T	-12	GLY	-	expression tag	UNP Q03PY7
T	-11	SER	-	expression tag	UNP Q03PY7
T	-10	SER	-	expression tag	UNP Q03PY7
T	-9	HIS	-	expression tag	UNP Q03PY7

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-8	HIS	-	expression tag	UNP Q03PY7
T	-7	HIS	-	expression tag	UNP Q03PY7
T	-6	HIS	-	expression tag	UNP Q03PY7
T	-5	HIS	-	expression tag	UNP Q03PY7
T	-4	HIS	-	expression tag	UNP Q03PY7
T	-3	SER	-	expression tag	UNP Q03PY7
T	-2	GLN	-	expression tag	UNP Q03PY7
T	-1	ASP	-	expression tag	UNP Q03PY7
T	0	PRO	-	expression tag	UNP Q03PY7

- Molecule 5 is water.

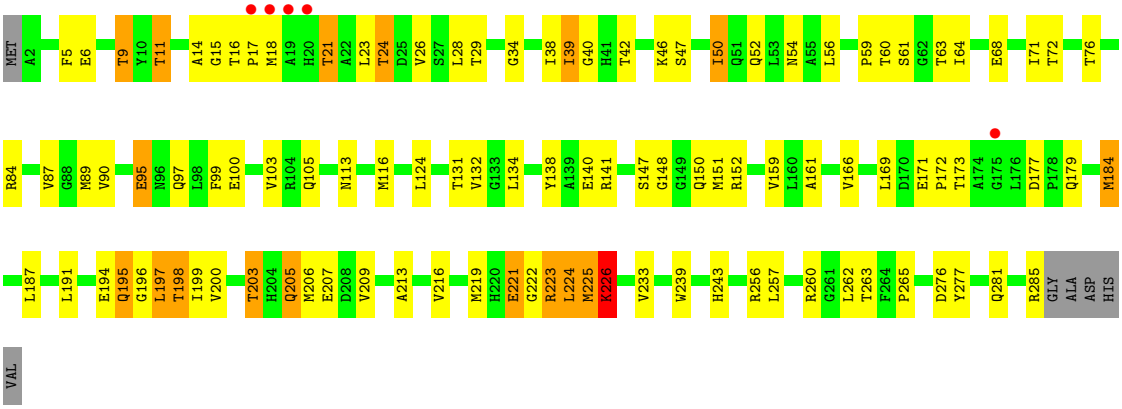
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	10	10	10	0	0
			Total	O		
5	B	6	6	6	0	0
			Total	O		
5	S	9	9	9	0	0
			Total	O		
5	T	1	1	1	0	0

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.

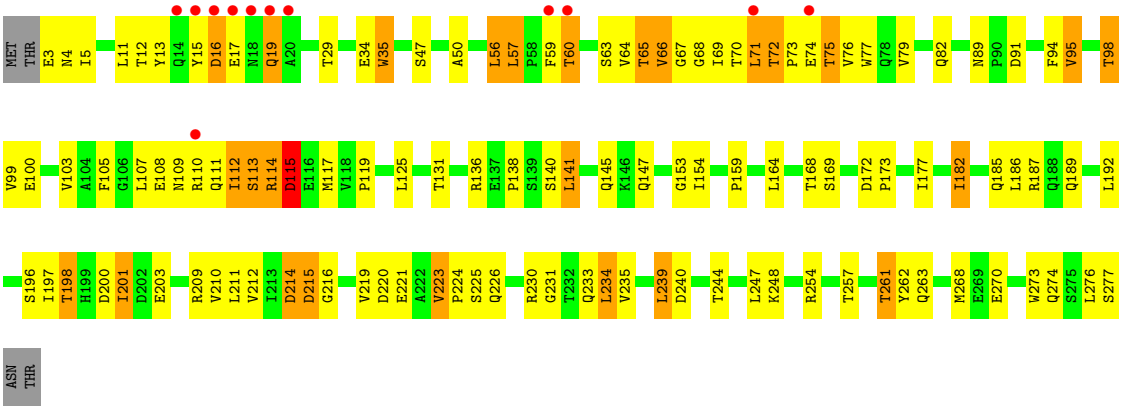
• Molecule 1: Energy-coupling factor transporter ATP-binding protein EcfA 1

Chain A: 2% 62% 30% 6%



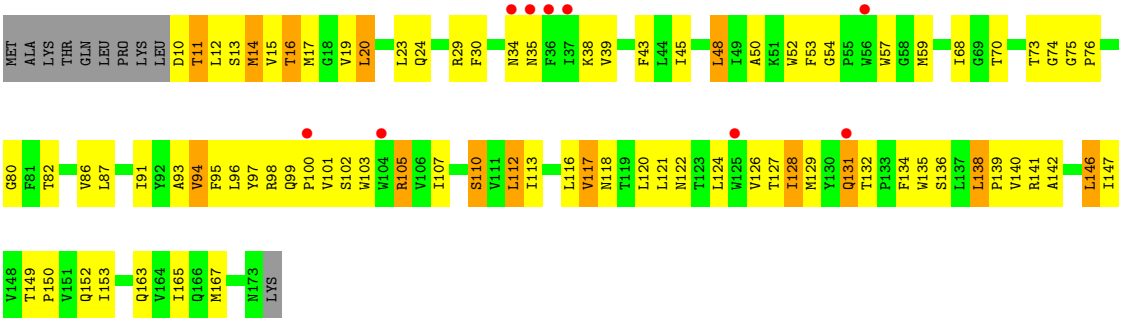
• Molecule 2: Energy-coupling factor transporter ATP-binding protein EcfA 2

Chain B: 4% 56% 33% 9%



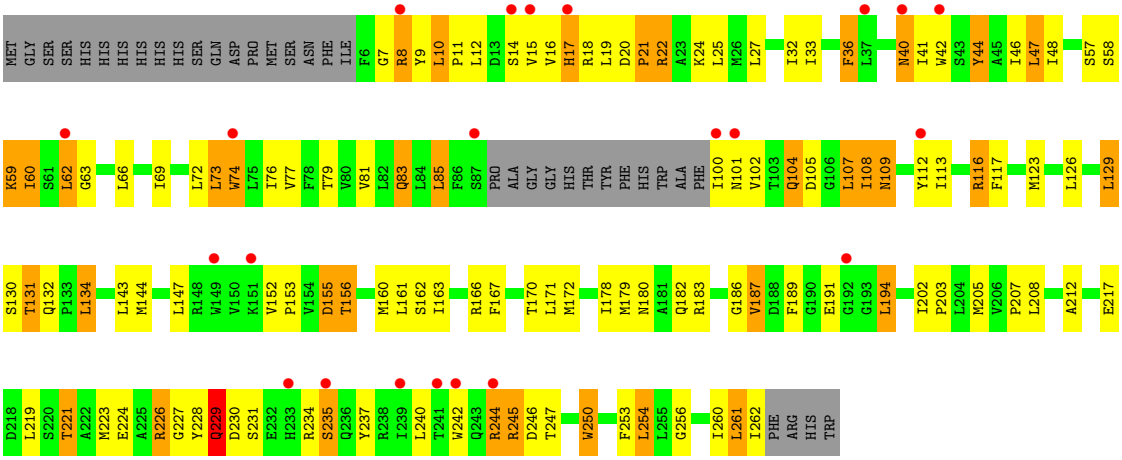
• Molecule 3: Uncharacterized protein

Chain S: 5% 46% 40% 8% 6%



• Molecule 4: Energy-coupling factor transporter transmembrane protein EcfT

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.61Å 149.00Å 170.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.91 – 3.00 41.05 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (38.91-3.00) 90.9 (41.05-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.7.2_869	Depositor
R, R_{free}	0.215 , 0.264 0.244 , 0.278	Depositor DCC
R_{free} test set	2090 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	92.6	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 94.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7601	wwPDB-VP
Average B, all atoms (Å^2)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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 (i)

5.1 Standard geometry (i)

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	0.49	0/2262	0.71	2/3071 (0.1%)
2	B	0.47	0/2148	0.74	6/2922 (0.2%)
3	S	0.43	0/1326	0.57	0/1816
4	T	0.41	0/1993	0.59	0/2703
All	All	0.45	0/7729	0.67	8/10512 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	115	ASP	O-C-N	8.21	135.83	122.70
2	B	111	GLN	O-C-N	8.15	135.75	122.70
2	B	115	ASP	CA-C-N	-6.35	103.24	117.20
2	B	111	GLN	C-N-CA	-6.19	106.23	121.70
2	B	111	GLN	CA-C-N	-6.13	103.72	117.20
1	A	15	GLY	O-C-N	-5.63	113.69	122.70
1	A	15	GLY	C-N-CA	5.51	135.47	121.70
2	B	115	ASP	C-N-CA	-5.10	108.96	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2217	0	2195	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2114	0	2104	123	0
3	S	1293	0	1383	80	0
4	T	1951	0	2061	141	0
5	A	10	0	0	0	0
5	B	6	0	0	0	0
5	S	9	0	0	0	0
5	T	1	0	0	0	0
All	All	7601	0	7743	366	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 24.

All (366) 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)
2:B:113:SER:HB2	2:B:114:ARG:CD	1.41	1.50
4:T:15:VAL:CG2	4:T:59:LYS:HD2	1.50	1.38
2:B:113:SER:C	2:B:114:ARG:HD2	1.50	1.30
2:B:72:THR:HG22	2:B:75:THR:OG1	1.34	1.23
4:T:16:VAL:CG2	4:T:59:LYS:HB2	1.70	1.19
3:S:12:LEU:O	3:S:16:THR:HG22	1.44	1.18
2:B:114:ARG:HD2	2:B:114:ARG:N	1.54	1.13
2:B:74:GLU:O	2:B:75:THR:HG23	1.47	1.12
2:B:113:SER:HB2	2:B:114:ARG:HD3	1.29	1.10
4:T:16:VAL:HG22	4:T:59:LYS:HB2	1.33	1.10
2:B:113:SER:CB	2:B:114:ARG:CD	2.30	1.09
4:T:10:LEU:HG	4:T:132:GLN:HG2	1.37	1.07
4:T:15:VAL:CG2	4:T:59:LYS:CD	2.31	1.06
2:B:113:SER:HB2	2:B:114:ARG:NE	1.70	1.05
4:T:100:ILE:O	4:T:100:ILE:HG22	1.58	1.04
3:S:14:MET:HE3	3:S:14:MET:O	1.59	1.02
4:T:15:VAL:HG23	4:T:59:LYS:HD2	1.03	1.02
4:T:16:VAL:CG2	4:T:59:LYS:CB	2.38	1.01
4:T:10:LEU:HD13	4:T:10:LEU:O	1.62	0.99
4:T:16:VAL:HG13	4:T:58:SER:HA	1.45	0.97
2:B:72:THR:HG23	2:B:73:PRO:O	1.64	0.97
2:B:110:ARG:HB3	2:B:112:ILE:HD11	1.48	0.96
2:B:113:SER:HB2	2:B:114:ARG:HD2	1.48	0.96
4:T:15:VAL:HG21	4:T:59:LYS:CD	1.95	0.95
2:B:113:SER:CB	2:B:114:ARG:NE	2.30	0.95
2:B:112:ILE:HD13	2:B:112:ILE:H	1.32	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:TRP:CH2	4:T:228:TYR:O	2.21	0.94
3:S:103:TRP:O	3:S:107:ILE:HG13	1.68	0.93
4:T:17:HIS:H	4:T:17:HIS:CD2	1.80	0.93
3:S:97:TYR:CE2	3:S:98:ARG:HG3	2.04	0.93
4:T:11:PRO:HD2	4:T:129:LEU:O	1.68	0.92
2:B:71:LEU:HD13	2:B:71:LEU:C	1.91	0.92
2:B:112:ILE:N	2:B:112:ILE:CD1	2.30	0.92
4:T:9:TYR:O	4:T:11:PRO:HD3	1.69	0.91
4:T:10:LEU:O	4:T:10:LEU:CD1	2.18	0.91
2:B:59:PHE:CZ	2:B:71:LEU:HD12	2.07	0.90
3:S:16:THR:O	3:S:20:LEU:HD12	1.70	0.90
4:T:16:VAL:HG23	4:T:59:LYS:HB2	1.52	0.89
2:B:114:ARG:CD	2:B:114:ARG:N	2.37	0.88
4:T:16:VAL:HG12	4:T:17:HIS:O	1.73	0.88
3:S:99:GLN:HG2	3:S:100:PRO:HD2	1.57	0.86
4:T:10:LEU:HD23	4:T:131:THR:N	1.90	0.86
3:S:127:THR:O	3:S:129:MET:N	2.08	0.85
4:T:16:VAL:CG1	4:T:58:SER:HA	2.06	0.85
4:T:16:VAL:HG21	4:T:58:SER:O	1.75	0.85
4:T:16:VAL:HG23	4:T:59:LYS:CB	2.05	0.84
2:B:112:ILE:H	2:B:112:ILE:CD1	1.89	0.83
4:T:107:LEU:O	4:T:107:LEU:HD23	1.79	0.82
1:A:100:GLU:HG2	1:A:105:GLN:HB3	1.61	0.82
2:B:153:GLY:HA3	4:T:226:ARG:HH21	1.44	0.82
2:B:71:LEU:HD13	2:B:71:LEU:O	1.79	0.81
4:T:9:TYR:O	4:T:11:PRO:CD	2.30	0.80
2:B:59:PHE:HZ	2:B:71:LEU:HD12	1.46	0.80
4:T:107:LEU:O	4:T:107:LEU:CD2	2.30	0.79
2:B:113:SER:CB	2:B:114:ARG:HD2	2.06	0.79
3:S:97:TYR:CE2	3:S:98:ARG:CG	2.66	0.79
2:B:59:PHE:CZ	2:B:71:LEU:CD1	2.66	0.79
1:A:219:MET:SD	1:A:224:LEU:HB2	2.22	0.79
2:B:114:ARG:N	2:B:114:ARG:HH11	1.81	0.78
2:B:198:THR:HG22	2:B:200:ASP:H	1.48	0.78
2:B:72:THR:CG2	2:B:73:PRO:O	2.30	0.78
2:B:113:SER:CA	2:B:114:ARG:HD2	2.13	0.78
2:B:74:GLU:O	2:B:75:THR:CG2	2.30	0.78
4:T:10:LEU:CG	4:T:132:GLN:HG2	2.14	0.78
2:B:112:ILE:N	2:B:112:ILE:HD12	1.97	0.78
4:T:10:LEU:HD13	4:T:10:LEU:C	2.03	0.78
3:S:14:MET:HE2	3:S:15:VAL:HA	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:100:ILE:O	4:T:100:ILE:CG2	2.30	0.77
1:A:34:GLY:H	1:A:198:THR:HB	1.51	0.76
2:B:113:SER:C	2:B:114:ARG:CD	2.45	0.76
2:B:114:ARG:HH11	2:B:114:ARG:H	1.34	0.76
2:B:110:ARG:C	2:B:112:ILE:HD13	2.06	0.75
3:S:102:SER:HB2	3:S:105:ARG:HB2	1.68	0.75
2:B:13:TYR:HD2	2:B:19:GLN:HG2	1.51	0.75
2:B:110:ARG:CB	2:B:112:ILE:HD11	2.15	0.75
2:B:110:ARG:CB	2:B:112:ILE:CD1	2.63	0.75
3:S:19:VAL:HG22	4:T:167:PHE:CD2	2.22	0.74
3:S:102:SER:HB2	3:S:105:ARG:HD2	1.70	0.74
4:T:10:LEU:HD23	4:T:131:THR:CA	2.18	0.74
4:T:15:VAL:HG21	4:T:59:LYS:HD3	1.70	0.74
1:A:23:LEU:HD22	1:A:26:VAL:HG21	1.70	0.74
4:T:105:ASP:O	4:T:108:ILE:HB	1.88	0.74
2:B:77:TRP:CZ3	4:T:228:TYR:O	2.41	0.74
4:T:22:ARG:HA	4:T:25:LEU:HD23	1.70	0.74
2:B:230:ARG:HB3	2:B:234:LEU:HD13	1.68	0.73
3:S:14:MET:O	3:S:14:MET:CE	2.34	0.73
4:T:10:LEU:HD23	4:T:131:THR:C	2.09	0.73
2:B:72:THR:HG22	2:B:75:THR:HG1	1.53	0.72
3:S:97:TYR:CD2	3:S:98:ARG:HG3	2.24	0.72
2:B:114:ARG:H	2:B:114:ARG:NH1	1.86	0.72
2:B:110:ARG:HB3	2:B:112:ILE:CD1	2.20	0.71
4:T:10:LEU:HG	4:T:132:GLN:CG	2.16	0.71
2:B:105:PHE:HB3	4:T:226:ARG:HH12	1.56	0.70
4:T:7:GLY:O	4:T:8:ARG:C	2.30	0.70
3:S:13:SER:HB3	3:S:53:PHE:HE1	1.57	0.70
4:T:107:LEU:CD2	4:T:107:LEU:C	2.60	0.70
2:B:95:VAL:HG13	4:T:219:LEU:HD11	1.74	0.69
1:A:260:ARG:NH2	2:B:270:GLU:OE1	2.25	0.69
4:T:16:VAL:CG2	4:T:58:SER:C	2.60	0.69
1:A:225:MET:O	1:A:226:LYS:HB3	1.90	0.69
3:S:11:THR:O	3:S:15:VAL:HG23	1.91	0.69
2:B:50:ALA:HB2	2:B:197:ILE:HG13	1.74	0.69
2:B:182:ILE:HA	2:B:185:GLN:HG2	1.73	0.69
2:B:110:ARG:C	2:B:112:ILE:CD1	2.62	0.68
1:A:87:VAL:HG22	1:A:166:VAL:HB	1.74	0.68
1:A:169:LEU:HB3	1:A:172:PRO:HG3	1.74	0.68
2:B:110:ARG:O	2:B:112:ILE:CD1	2.42	0.68
4:T:16:VAL:HG21	4:T:58:SER:C	2.13	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:THR:HB	1:A:205:GLN:H	1.57	0.67
2:B:113:SER:HB3	2:B:114:ARG:NE	2.10	0.66
1:A:9:THR:HB	1:A:24:THR:HA	1.76	0.66
2:B:35:TRP:HZ3	2:B:196:SER:HG	1.44	0.66
3:S:20:LEU:HD21	3:S:48:LEU:HD13	1.78	0.66
1:A:16:THR:O	1:A:18:MET:N	2.28	0.66
2:B:230:ARG:HG2	2:B:233:GLN:HB3	1.77	0.65
2:B:220:ASP:OD2	2:B:230:ARG:NH2	2.29	0.65
4:T:9:TYR:O	4:T:11:PRO:N	2.30	0.65
3:S:68:ILE:HG12	4:T:161:LEU:HD11	1.78	0.65
2:B:71:LEU:C	2:B:71:LEU:CD1	2.64	0.65
3:S:10:ASP:OD2	3:S:11:THR:N	2.30	0.64
2:B:153:GLY:HA3	4:T:226:ARG:NH2	2.13	0.64
2:B:34:GLU:OE1	2:B:209:ARG:NH1	2.31	0.64
4:T:83:GLN:NE2	4:T:109:ASN:OD1	2.31	0.64
2:B:112:ILE:O	2:B:117:MET:HE3	1.99	0.63
4:T:17:HIS:CD2	4:T:17:HIS:N	2.61	0.63
2:B:72:THR:O	2:B:76:VAL:HG12	1.99	0.63
4:T:22:ARG:HB2	4:T:143:LEU:HD21	1.80	0.63
3:S:97:TYR:CD2	3:S:98:ARG:CG	2.82	0.62
4:T:156:THR:N	4:T:231:SER:OG	2.32	0.62
3:S:14:MET:CE	3:S:14:MET:C	2.67	0.62
3:S:126:VAL:HG11	3:S:134:PHE:HB2	1.82	0.62
3:S:132:THR:HB	4:T:79:THR:HG22	1.82	0.62
1:A:225:MET:O	1:A:226:LYS:CB	2.46	0.62
2:B:108:GLU:HA	2:B:117:MET:HE1	1.82	0.62
3:S:10:ASP:OD2	3:S:10:ASP:C	2.36	0.62
1:A:148:GLY:HA2	1:A:151:MET:HE2	1.83	0.61
1:A:138:TYR:HA	1:A:141:ARG:HG3	1.81	0.61
2:B:110:ARG:CB	2:B:112:ILE:HD13	2.29	0.61
4:T:24:LYS:NZ	4:T:130:SER:O	2.34	0.61
4:T:134:LEU:HD23	4:T:134:LEU:H	1.65	0.61
2:B:114:ARG:HH11	2:B:114:ARG:CA	2.14	0.60
4:T:7:GLY:O	4:T:9:TYR:CG	2.54	0.60
3:S:116:LEU:HD12	3:S:120:LEU:HB2	1.83	0.60
3:S:142:ALA:O	3:S:146:LEU:HB2	2.00	0.60
4:T:16:VAL:HG23	4:T:59:LYS:HB3	1.82	0.60
4:T:217:GLU:O	4:T:221:THR:HG22	2.02	0.60
1:A:221:GLU:O	1:A:223:ARG:N	2.35	0.59
3:S:103:TRP:O	3:S:107:ILE:CG1	2.45	0.59
2:B:113:SER:HB3	4:T:235:SER:OG	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:THR:HG22	1:A:72:THR:HG22	1.84	0.59
3:S:20:LEU:CD2	3:S:48:LEU:HD13	2.33	0.59
4:T:7:GLY:O	4:T:9:TYR:CD2	2.55	0.59
4:T:102:VAL:O	4:T:102:VAL:CG2	2.50	0.59
1:A:54:ASN:O	1:A:84:ARG:NH1	2.36	0.59
3:S:54:GLY:O	3:S:97:TYR:CE1	2.55	0.59
2:B:136:ARG:NH2	2:B:140:SER:O	2.36	0.58
1:A:50:ILE:HD11	1:A:200:VAL:HG11	1.86	0.58
4:T:178:ILE:O	4:T:182:GLN:HG2	2.03	0.58
1:A:95:GLU:OE1	1:A:152:ARG:NE	2.32	0.58
1:A:113:ASN:HB3	4:T:186:GLY:HA3	1.85	0.58
3:S:128:ILE:HB	4:T:36:PHE:CD1	2.38	0.58
4:T:107:LEU:O	4:T:107:LEU:HD22	2.04	0.58
2:B:115:ASP:OD1	2:B:115:ASP:N	2.35	0.57
4:T:202:ILE:HB	4:T:203:PRO:HD3	1.86	0.57
2:B:71:LEU:HD22	2:B:72:THR:N	2.19	0.57
2:B:72:THR:HG23	2:B:73:PRO:N	2.20	0.57
4:T:228:TYR:C	4:T:229:GLN:HG2	2.24	0.57
2:B:103:VAL:HG21	2:B:125:LEU:HD21	1.86	0.56
2:B:112:ILE:O	4:T:235:SER:HB2	2.05	0.56
2:B:115:ASP:O	2:B:119:PRO:HD2	2.05	0.56
2:B:231:GLY:O	2:B:234:LEU:HB2	2.06	0.56
3:S:14:MET:HE2	3:S:15:VAL:CA	2.35	0.56
4:T:15:VAL:HB	4:T:59:LYS:NZ	2.21	0.56
4:T:179:MET:HE3	4:T:183:ARG:HH22	1.70	0.56
3:S:24:GLN:HG3	3:S:45:ILE:HB	1.86	0.56
2:B:110:ARG:HB2	2:B:112:ILE:CD1	2.36	0.56
2:B:276:LEU:O	2:B:277:SER:C	2.43	0.56
4:T:17:HIS:H	4:T:17:HIS:HD2	1.43	0.56
2:B:154:ILE:O	2:B:159:PRO:HD3	2.06	0.55
1:A:34:GLY:N	1:A:198:THR:HB	2.21	0.55
1:A:221:GLU:C	1:A:223:ARG:H	2.09	0.55
4:T:107:LEU:C	4:T:107:LEU:HD22	2.26	0.55
2:B:59:PHE:HZ	2:B:71:LEU:CD1	2.12	0.55
3:S:14:MET:HE3	3:S:14:MET:C	2.21	0.55
1:A:138:TYR:OH	1:A:150:GLN:NE2	2.40	0.54
4:T:16:VAL:HG22	4:T:58:SER:C	2.28	0.54
4:T:156:THR:HG22	4:T:231:SER:HB3	1.90	0.54
3:S:102:SER:CB	3:S:105:ARG:HD2	2.37	0.54
1:A:11:THR:HB	1:A:21:THR:HG22	1.88	0.54
3:S:19:VAL:HG22	4:T:167:PHE:CE2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:THR:HG23	1:A:60:THR:HG21	1.89	0.53
4:T:102:VAL:O	4:T:102:VAL:HG22	2.07	0.53
1:A:90:VAL:HG22	1:A:159:VAL:HG21	1.91	0.53
1:A:216:VAL:HB	1:A:233:VAL:HG21	1.90	0.53
3:S:19:VAL:CG2	4:T:167:PHE:CE2	2.92	0.52
3:S:113:ILE:O	3:S:117:VAL:N	2.42	0.52
2:B:34:GLU:CD	2:B:209:ARG:HH11	2.13	0.52
3:S:97:TYR:HE2	3:S:98:ARG:HG3	1.67	0.52
4:T:155:ASP:C	4:T:231:SER:OG	2.48	0.52
4:T:10:LEU:CD1	4:T:132:GLN:HG2	2.38	0.52
4:T:16:VAL:HG22	4:T:59:LYS:CB	2.17	0.52
2:B:64:VAL:O	2:B:71:LEU:HB3	2.10	0.52
4:T:16:VAL:HG22	4:T:59:LYS:N	2.26	0.51
2:B:110:ARG:O	2:B:112:ILE:HD12	2.08	0.51
2:B:115:ASP:O	2:B:119:PRO:CD	2.58	0.51
1:A:147:SER:HB3	1:A:150:GLN:HG3	1.91	0.51
2:B:114:ARG:N	2:B:114:ARG:NH1	2.51	0.51
2:B:220:ASP:OD1	2:B:221:GLU:N	2.43	0.51
1:A:113:ASN:CB	4:T:186:GLY:HA3	2.41	0.50
3:S:97:TYR:CE2	3:S:98:ARG:HG2	2.46	0.50
1:A:11:THR:HA	1:A:21:THR:HA	1.93	0.50
2:B:112:ILE:O	4:T:235:SER:CB	2.59	0.50
2:B:5:ILE:HG12	2:B:29:THR:HG22	1.94	0.50
3:S:128:ILE:O	4:T:116:ARG:NH2	2.45	0.50
4:T:10:LEU:O	4:T:10:LEU:HD12	2.09	0.50
4:T:224:GLU:O	4:T:226:ARG:O	2.30	0.50
3:S:10:ASP:O	3:S:11:THR:CB	2.60	0.50
4:T:72:LEU:O	4:T:76:ILE:HG13	2.11	0.50
2:B:110:ARG:HB2	2:B:112:ILE:HD13	1.93	0.50
1:A:5:PHE:HB2	1:A:28:LEU:HG	1.94	0.50
1:A:134:LEU:HD22	1:A:138:TYR:CE2	2.47	0.50
2:B:214:ASP:O	2:B:216:GLY:N	2.45	0.50
2:B:112:ILE:O	2:B:117:MET:CE	2.59	0.49
4:T:156:THR:HG22	4:T:231:SER:CB	2.42	0.49
2:B:67:GLY:O	2:B:69:ILE:N	2.37	0.49
2:B:98:THR:OG1	2:B:99:VAL:N	2.44	0.49
1:A:194:GLU:O	1:A:196:GLY:N	2.37	0.49
3:S:43:PHE:CZ	3:S:152:GLN:HG2	2.48	0.49
3:S:11:THR:HG22	3:S:12:LEU:N	2.27	0.49
4:T:16:VAL:CG2	4:T:59:LYS:HB3	2.34	0.49
1:A:173:THR:HG22	1:A:184:MET:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:223:MET:O	4:T:226:ARG:O	2.30	0.49
2:B:76:VAL:CG2	2:B:77:TRP:N	2.76	0.48
4:T:144:MET:O	4:T:147:LEU:HB2	2.14	0.48
2:B:277:SER:O	2:B:277:SER:OG	2.30	0.48
1:A:209:VAL:O	1:A:213:ALA:HB3	2.13	0.48
3:S:14:MET:HG2	4:T:160:MET:HE2	1.95	0.48
4:T:178:ILE:HD13	4:T:207:PRO:HB2	1.95	0.48
2:B:173:PRO:O	2:B:177:ILE:HG12	2.14	0.48
2:B:223:VAL:HG12	2:B:224:PRO:HD2	1.96	0.48
3:S:13:SER:HA	3:S:16:THR:CG2	2.43	0.48
1:A:257:LEU:HB3	1:A:262:LEU:HD12	1.95	0.48
4:T:58:SER:O	4:T:60:ILE:N	2.47	0.48
2:B:35:TRP:HZ3	2:B:196:SER:OG	1.97	0.47
4:T:109:ASN:O	4:T:112:TYR:HB3	2.14	0.47
1:A:40:GLY:O	1:A:46:LYS:NZ	2.37	0.47
2:B:100:GLU:HB3	4:T:237:TYR:HE2	1.79	0.47
1:A:276:ASP:OD1	2:B:254:ARG:HD3	2.13	0.47
2:B:5:ILE:HB	2:B:65:THR:HG23	1.96	0.47
3:S:131:GLN:HG2	4:T:113:ILE:HD13	1.95	0.47
4:T:194:LEU:HD23	4:T:194:LEU:HA	1.72	0.47
3:S:10:ASP:O	3:S:11:THR:OG1	2.30	0.47
4:T:179:MET:HG2	4:T:189:PHE:CE2	2.50	0.47
3:S:50:ALA:O	3:S:97:TYR:HD1	1.98	0.47
1:A:177:ASP:OD1	1:A:177:ASP:N	2.43	0.47
2:B:105:PHE:HD2	4:T:226:ARG:HH11	1.63	0.47
4:T:156:THR:HA	4:T:231:SER:OG	2.15	0.46
4:T:101:ASN:O	4:T:101:ASN:OD1	2.34	0.46
3:S:75:GLY:HA2	3:S:76:PRO:HD3	1.73	0.46
4:T:104:GLN:H	4:T:104:GLN:HG2	1.39	0.46
3:S:17:MET:CE	4:T:160:MET:SD	3.04	0.46
4:T:156:THR:CA	4:T:231:SER:OG	2.63	0.46
2:B:141:LEU:HB2	2:B:145:GLN:OE1	2.15	0.46
2:B:198:THR:HG21	2:B:203:GLU:HB3	1.97	0.46
2:B:201:ILE:HD13	2:B:201:ILE:HA	1.77	0.46
4:T:156:THR:O	4:T:160:MET:HG3	2.16	0.46
2:B:71:LEU:O	2:B:71:LEU:CD1	2.57	0.46
2:B:211:LEU:HD12	2:B:221:GLU:HG3	1.97	0.46
3:S:59:MET:HG2	3:S:86:VAL:HG13	1.98	0.46
3:S:93:ALA:O	3:S:97:TYR:CB	2.63	0.46
1:A:52:GLN:HG3	1:A:64:ILE:CD1	2.46	0.46
4:T:63:GLY:HA2	4:T:66:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:73:LEU:HD12	4:T:77:VAL:HG23	1.97	0.45
3:S:131:GLN:HG2	4:T:113:ILE:CD1	2.46	0.45
3:S:52:TRP:CZ2	3:S:165:ILE:HG23	2.52	0.45
3:S:112:LEU:HD13	3:S:112:LEU:HA	1.72	0.45
3:S:121:LEU:HD23	3:S:124:LEU:HD12	1.99	0.45
3:S:94:VAL:HG12	3:S:95:PHE:N	2.32	0.45
2:B:74:GLU:O	2:B:75:THR:CB	2.65	0.45
4:T:155:ASP:OD1	4:T:155:ASP:N	2.49	0.45
2:B:72:THR:O	2:B:76:VAL:CG1	2.63	0.45
2:B:235:VAL:HA	2:B:239:LEU:O	2.17	0.45
4:T:179:MET:HE3	4:T:183:ARG:NH2	2.30	0.45
1:A:225:MET:H	1:A:225:MET:HG2	1.69	0.45
4:T:253:PHE:HD2	4:T:254:LEU:HD13	1.82	0.45
3:S:53:PHE:C	3:S:97:TYR:HE1	2.21	0.44
1:A:64:ILE:HB	1:A:71:ILE:HB	1.99	0.44
2:B:244:THR:O	2:B:248:LYS:HG3	2.17	0.44
2:B:66:VAL:HG21	2:B:79:VAL:HG13	1.99	0.44
1:A:191:LEU:O	1:A:195:GLN:HB3	2.18	0.44
2:B:100:GLU:HB3	4:T:237:TYR:CE2	2.52	0.44
3:S:73:THR:O	4:T:9:TYR:CE1	2.71	0.44
4:T:46:ILE:H	4:T:46:ILE:HG13	1.50	0.44
2:B:94:PHE:CE2	2:B:138:PRO:HB3	2.53	0.44
2:B:114:ARG:HH11	2:B:114:ARG:HA	1.82	0.44
3:S:93:ALA:O	3:S:97:TYR:HB3	2.18	0.44
4:T:22:ARG:HD2	4:T:240:LEU:HD13	1.99	0.44
3:S:13:SER:HB3	3:S:53:PHE:CE1	2.45	0.44
1:A:277:TYR:O	1:A:281:GLN:HG3	2.18	0.44
2:B:15:TYR:HA	2:B:16:ASP:HA	1.68	0.43
3:S:99:GLN:HG2	3:S:100:PRO:CD	2.39	0.43
4:T:17:HIS:NE2	4:T:57:SER:HB2	2.32	0.43
4:T:44:TYR:O	4:T:48:ILE:HG13	2.18	0.43
3:S:16:THR:C	3:S:20:LEU:HD12	2.36	0.43
3:S:110:SER:OG	3:S:153:ILE:HG12	2.18	0.43
4:T:47:LEU:HD23	4:T:47:LEU:HA	1.82	0.43
1:A:184:MET:O	1:A:187:LEU:HB3	2.18	0.43
3:S:14:MET:HE2	3:S:15:VAL:N	2.33	0.43
4:T:73:LEU:HD13	4:T:73:LEU:HA	1.72	0.43
2:B:56:LEU:H	2:B:56:LEU:HG	1.41	0.43
4:T:15:VAL:HB	4:T:59:LYS:HZ3	1.83	0.43
4:T:18:ARG:C	4:T:19:LEU:HD22	2.38	0.43
1:A:171:GLU:OE2	1:A:203:THR:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:VAL:O	2:B:221:GLU:HA	2.18	0.43
4:T:66:LEU:HA	4:T:69:ILE:HD12	1.99	0.43
2:B:187:ARG:HA	2:B:192:LEU:HD23	2.01	0.43
4:T:21:PRO:O	4:T:24:LYS:N	2.52	0.43
2:B:107:LEU:O	2:B:112:ILE:HB	2.19	0.43
2:B:72:THR:CG2	2:B:75:THR:OG1	2.30	0.43
3:S:138:LEU:HB3	3:S:139:PRO:HD3	1.99	0.43
4:T:261:LEU:HB3	4:T:262:ILE:HD12	2.00	0.43
2:B:109:ASN:CG	4:T:227:GLY:O	2.58	0.42
3:S:131:GLN:HG3	3:S:132:THR:N	2.33	0.42
2:B:212:VAL:HB	2:B:220:ASP:HB3	2.00	0.42
3:S:38:LYS:HB3	3:S:38:LYS:HE2	1.86	0.42
1:A:221:GLU:C	1:A:223:ARG:N	2.71	0.42
3:S:87:LEU:O	3:S:91:ILE:HG13	2.19	0.42
4:T:244:ARG:O	4:T:247:THR:OG1	2.35	0.42
3:S:99:GLN:CG	3:S:100:PRO:HD2	2.39	0.42
4:T:10:LEU:CD2	4:T:131:THR:N	2.72	0.42
4:T:256:GLY:O	4:T:260:ILE:HG12	2.19	0.42
2:B:110:ARG:C	2:B:112:ILE:H	2.20	0.42
2:B:110:ARG:CA	2:B:112:ILE:HD13	2.49	0.42
4:T:19:LEU:HG	4:T:245:ARG:CZ	2.49	0.42
2:B:261:THR:OG1	2:B:262:TYR:N	2.53	0.42
3:S:23:LEU:HD13	4:T:171:LEU:HD13	2.01	0.42
2:B:273:TRP:O	2:B:277:SER:N	2.43	0.42
1:A:39:ILE:HD13	1:A:203:THR:O	2.19	0.42
3:S:19:VAL:CG1	4:T:212:ALA:HB1	2.50	0.42
1:A:5:PHE:HB2	1:A:28:LEU:H	1.85	0.41
1:A:239:TRP:O	1:A:243:HIS:CD2	2.73	0.41
2:B:56:LEU:O	2:B:57:LEU:HB2	2.20	0.41
4:T:81:VAL:O	4:T:85:LEU:HG	2.19	0.41
3:S:19:VAL:CG2	4:T:167:PHE:CD2	2.99	0.41
3:S:120:LEU:HD22	3:S:120:LEU:HA	1.74	0.41
4:T:32:ILE:HG22	4:T:36:PHE:CE1	2.54	0.41
4:T:180:ASN:OD1	4:T:183:ARG:NH1	2.53	0.41
4:T:41:ILE:HD13	4:T:41:ILE:HA	1.84	0.41
4:T:152:VAL:HA	4:T:153:PRO:HD3	1.89	0.41
4:T:40:ASN:HB3	4:T:41:ILE:H	1.61	0.41
3:S:57:TRP:CZ3	4:T:160:MET:HE1	2.56	0.41
3:S:80:GLY:HA3	3:S:124:LEU:HD22	2.01	0.41
4:T:20:ASP:OD2	4:T:246:ASP:N	2.54	0.41
1:A:59:PRO:HG3	1:A:64:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:LEU:HD21	1:A:161:ALA:O	2.20	0.41
4:T:123:MET:O	4:T:126:LEU:HB3	2.20	0.41
4:T:254:LEU:HD12	4:T:254:LEU:HA	1.89	0.41
1:A:195:GLN:HG2	1:A:197:LEU:HD13	2.02	0.41
2:B:60:THR:O	2:B:60:THR:OG1	2.39	0.41
3:S:29:ARG:HB2	3:S:30:PHE:CE2	2.55	0.40
1:A:256:ARG:O	1:A:260:ARG:HG2	2.20	0.40
1:A:23:LEU:HD23	1:A:23:LEU:HA	1.82	0.40
3:S:120:LEU:O	3:S:124:LEU:HG	2.21	0.40
3:S:126:VAL:HG21	3:S:134:PHE:HD1	1.85	0.40
2:B:164:LEU:HD12	2:B:196:SER:HB3	2.03	0.40
3:S:149:THR:HB	3:S:150:PRO:HD3	2.04	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	282/290 (97%)	259 (92%)	15 (5%)	8 (3%)	5 25
2	B	273/279 (98%)	241 (88%)	24 (9%)	8 (3%)	4 24
3	S	162/174 (93%)	143 (88%)	15 (9%)	4 (2%)	5 28
4	T	241/280 (86%)	215 (89%)	16 (7%)	10 (4%)	3 16
All	All	958/1023 (94%)	858 (90%)	70 (7%)	30 (3%)	4 23

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	265	PRO
2	B	75	THR
2	B	215	ASP

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Mol	Chain	Res	Type
3	S	11	THR
3	S	128	ILE
4	T	8	ARG
4	T	40	ASN
4	T	62	LEU
4	T	74	TRP
1	A	222	GLY
2	B	95	VAL
3	S	35	ASN
4	T	10	LEU
4	T	21	PRO
4	T	59	LYS
4	T	250	TRP
1	A	14	ALA
1	A	17	PRO
1	A	116	MET
2	B	17	GLU
2	B	263	GLN
4	T	187	VAL
4	T	229	GLN
1	A	221	GLU
1	A	226	LYS
2	B	57	LEU
1	A	99	PHE
2	B	89	ASN
3	S	74	GLY
2	B	68	GLY

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	233/237 (98%)	195 (84%)	38 (16%)	2 11
2	B	230/234 (98%)	182 (79%)	48 (21%)	1 5
3	S	143/152 (94%)	116 (81%)	27 (19%)	1 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	T	213/243 (88%)	164 (77%)	49 (23%)	1 4
All	All	819/866 (95%)	657 (80%)	162 (20%)	1 7

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	9	THR
1	A	11	THR
1	A	21	THR
1	A	24	THR
1	A	29	THR
1	A	38	ILE
1	A	39	ILE
1	A	42	THR
1	A	47	SER
1	A	50	ILE
1	A	56	LEU
1	A	61	SER
1	A	68	GLU
1	A	76	THR
1	A	89	MET
1	A	95	GLU
1	A	97	GLN
1	A	103	VAL
1	A	131	THR
1	A	132	VAL
1	A	140	GLU
1	A	179	GLN
1	A	184	MET
1	A	195	GLN
1	A	197	LEU
1	A	198	THR
1	A	199	ILE
1	A	203	THR
1	A	205	GLN
1	A	206	MET
1	A	207	GLU
1	A	223	ARG
1	A	224	LEU
1	A	225	MET
1	A	226	LYS

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Mol	Chain	Res	Type
1	A	263	THR
1	A	285	ARG
2	B	3	GLU
2	B	4	ASN
2	B	11	LEU
2	B	12	THR
2	B	16	ASP
2	B	19	GLN
2	B	35	TRP
2	B	47	SER
2	B	56	LEU
2	B	60	THR
2	B	63	SER
2	B	65	THR
2	B	66	VAL
2	B	70	THR
2	B	71	LEU
2	B	72	THR
2	B	82	GLN
2	B	91	ASP
2	B	98	THR
2	B	112	ILE
2	B	113	SER
2	B	114	ARG
2	B	115	ASP
2	B	131	THR
2	B	141	LEU
2	B	147	GLN
2	B	168	THR
2	B	169	SER
2	B	172	ASP
2	B	182	ILE
2	B	186	LEU
2	B	189	GLN
2	B	198	THR
2	B	201	ILE
2	B	214	ASP
2	B	215	ASP
2	B	219	VAL
2	B	223	VAL
2	B	225	SER
2	B	226	GLN

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Mol	Chain	Res	Type
2	B	234	LEU
2	B	239	LEU
2	B	240	ASP
2	B	247	LEU
2	B	257	THR
2	B	261	THR
2	B	268	MET
2	B	274	GLN
3	S	14	MET
3	S	16	THR
3	S	20	LEU
3	S	34	ASN
3	S	39	VAL
3	S	48	LEU
3	S	70	THR
3	S	82	THR
3	S	94	VAL
3	S	96	LEU
3	S	101	VAL
3	S	105	ARG
3	S	110	SER
3	S	112	LEU
3	S	117	VAL
3	S	118	ASN
3	S	122	ASN
3	S	131	GLN
3	S	135	TRP
3	S	136	SER
3	S	138	LEU
3	S	140	VAL
3	S	141	ARG
3	S	146	LEU
3	S	147	ILE
3	S	163	GLN
3	S	167	MET
4	T	12	LEU
4	T	14	SER
4	T	17	HIS
4	T	22	ARG
4	T	27	LEU
4	T	33	ILE
4	T	36	PHE

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Mol	Chain	Res	Type
4	T	42	TRP
4	T	44	TYR
4	T	47	LEU
4	T	60	ILE
4	T	62	LEU
4	T	73	LEU
4	T	74	TRP
4	T	83	GLN
4	T	85	LEU
4	T	104	GLN
4	T	107	LEU
4	T	108	ILE
4	T	109	ASN
4	T	116	ARG
4	T	117	PHE
4	T	129	LEU
4	T	131	THR
4	T	134	LEU
4	T	155	ASP
4	T	156	THR
4	T	162	SER
4	T	163	ILE
4	T	166	ARG
4	T	170	THR
4	T	172	MET
4	T	187	VAL
4	T	191	GLU
4	T	194	LEU
4	T	205	MET
4	T	208	LEU
4	T	221	THR
4	T	226	ARG
4	T	229	GLN
4	T	230	ASP
4	T	234	ARG
4	T	235	SER
4	T	242	TRP
4	T	244	ARG
4	T	245	ARG
4	T	250	TRP
4	T	254	LEU
4	T	261	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	GLN
3	S	131	GLN
4	T	17	HIS
4	T	83	GLN
4	T	109	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)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	284/290 (97%)	-0.06	5 (1%)	68	40	53, 83, 126, 189	0
2	B	275/279 (98%)	0.09	12 (4%)	34	13	62, 109, 174, 273	0
3	S	164/174 (94%)	0.20	9 (5%)	25	9	25, 123, 192, 292	0
4	T	245/280 (87%)	0.33	22 (8%)	9	3	56, 135, 190, 254	0
All	All	968/1023 (94%)	0.13	48 (4%)	28	10	25, 109, 179, 292	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	18	ASN	5.7
2	B	20	ALA	5.1
4	T	100	ILE	5.0
4	T	242	TRP	4.9
4	T	244	ARG	4.8
2	B	74	GLU	4.5
2	B	16	ASP	4.5
4	T	15	VAL	4.3
1	A	20	HIS	4.3
4	T	101	ASN	4.1
3	S	125	TRP	3.7
2	B	15	TYR	3.5
4	T	87	SER	3.3
2	B	60	THR	3.3
4	T	233	HIS	3.2
2	B	17	GLU	3.1
2	B	19	GLN	2.9
1	A	19	ALA	2.9
4	T	37	LEU	2.8
3	S	37	ILE	2.8
4	T	8	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	14	GLN	2.7
4	T	149	TRP	2.7
3	S	104	TRP	2.6
3	S	131	GLN	2.6
4	T	241	THR	2.6
4	T	14	SER	2.6
4	T	192	GLY	2.6
2	B	71	LEU	2.4
4	T	17	HIS	2.3
4	T	40	ASN	2.3
3	S	35	ASN	2.3
4	T	62	LEU	2.3
4	T	74	TRP	2.3
1	A	17	PRO	2.2
1	A	175	GLY	2.2
4	T	42	TRP	2.2
4	T	151	LYS	2.2
4	T	239	ILE	2.2
3	S	56	TRP	2.1
4	T	235	SER	2.1
3	S	100	PRO	2.1
2	B	110	ARG	2.1
4	T	112	TYR	2.1
3	S	36	PHE	2.1
1	A	18	MET	2.1
3	S	34	ASN	2.0
2	B	59	PHE	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.