Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 08:05 am BST

PDB ID	:	2VDU
Title	:	Structure of trm8-trm82, THE YEAST TRNA m7G methylation complex
Authors	:	Leulliot, N.; Chaillet, M.; Durand, D.; Ulryck, N.; Blondeau, K.; Van Tilbeurgh, H.
Deposited on	:	2007-10-11
Resolution	:	2.40 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 following versions of software and data (see references ①) were used in the production of this report:

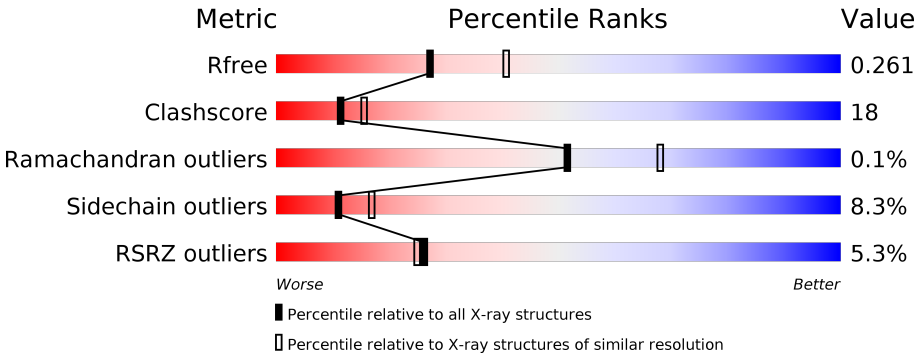
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 >=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	B	450	9% 56% 24% • 17%
1	D	450	3% 58% 22% • 16%
2	E	254	% 50% 25% • 21%
2	F	254	2% 51% 23% 5% 21%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9571 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.

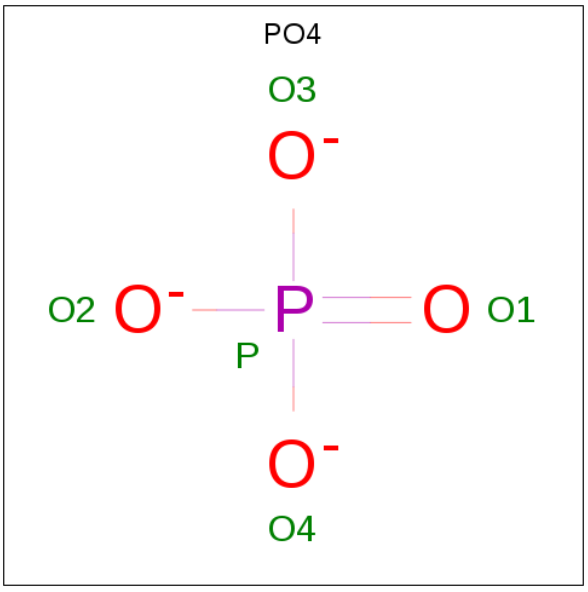
- Molecule 1 is a protein called TRNA (GUANINE-N(7)-)-METHYLTRANSFERASE-ASSOCIATED WD REPEAT PROTEIN TRM82.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	374	Total	C	N	O	S	0	0	0
			3013	1939	493	572	9			
1	D	376	Total	C	N	O	S	0	0	0
			3027	1949	495	574	9			

- Molecule 2 is a protein called TRNA (GUANINE-N(7)-)-METHYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	201	Total	C	N	O	S	0	0	0
			1631	1052	268	299	12			
2	F	201	Total	C	N	O	S	0	0	0
			1631	1052	268	299	12			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total O P 5 4 1	0	0
3	F	1	Total O P 5 4 1	0	0

- Molecule 4 is water.

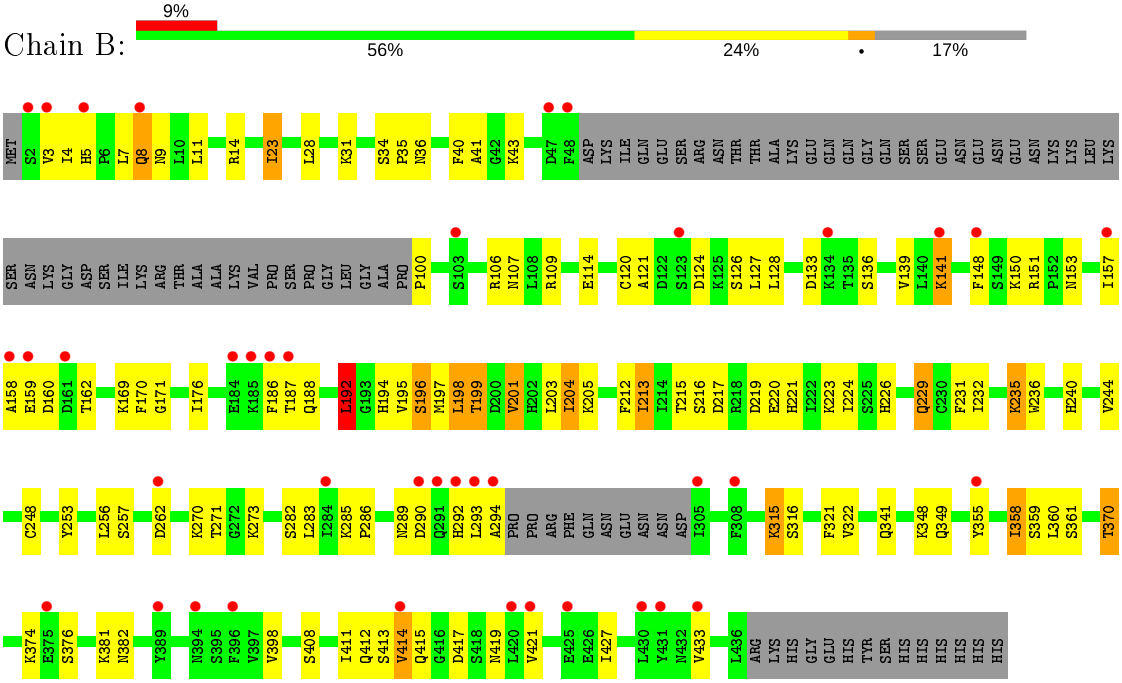
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	61	Total O 61 61	0	0
4	D	102	Total O 102 102	0	0
4	E	45	Total O 45 45	0	0
4	F	51	Total O 51 51	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

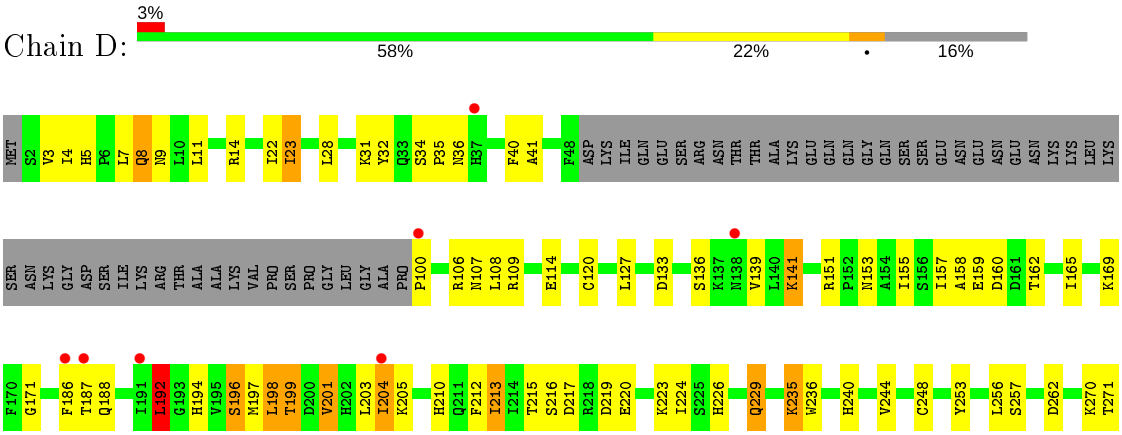
• Molecule 1: TRNA (GUANINE-N(7)-)-METHYLTRANSFERASE-ASSOCIATED WD REPEAT PROTEIN TRM82

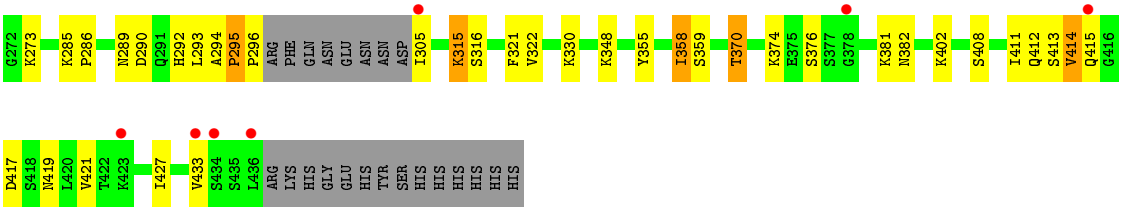
Chain B:



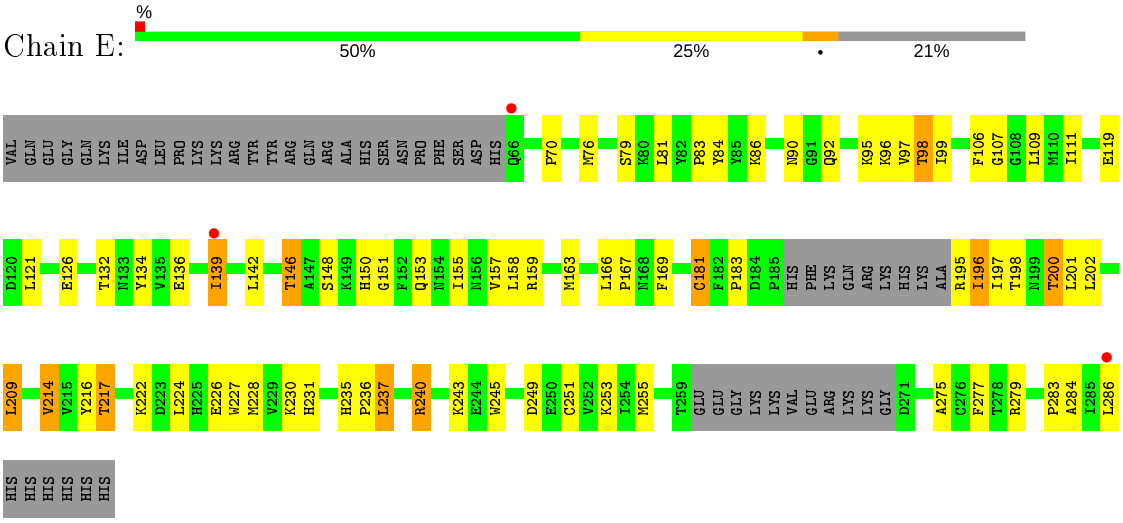
• Molecule 1: TRNA (GUANINE-N(7)-)-METHYLTRANSFERASE-ASSOCIATED WD REPEAT PROTEIN TRM82

Chain D:

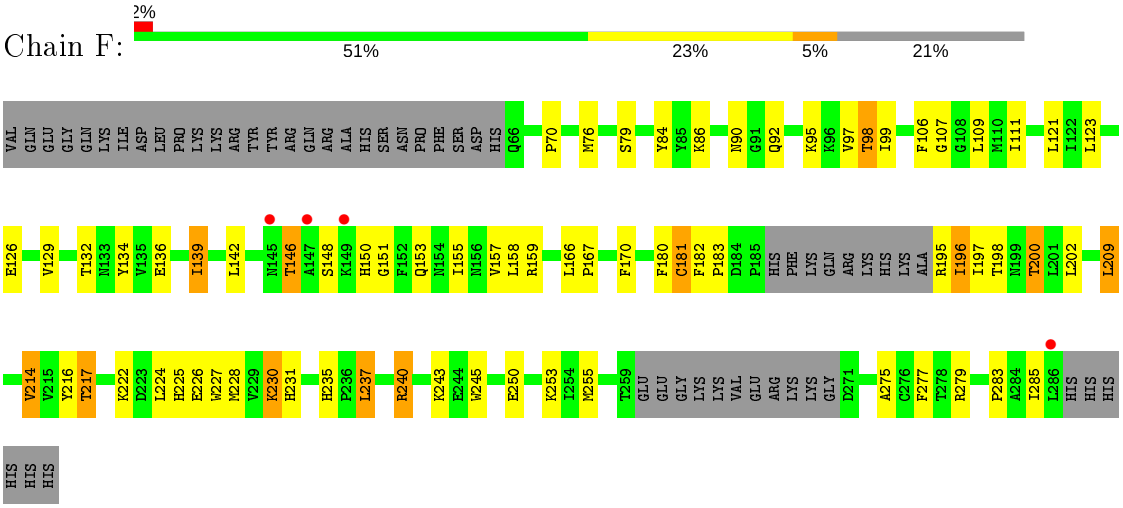




• Molecule 2: TRNA (GUANINE-N(7)-)-METHYLTRANSFERASE



• Molecule 2: TRNA (GUANINE-N(7)-)-METHYLTRANSFERASE



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.38Å 107.68Å 127.75Å 90.00° 91.53° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 63.85 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-2.40) 99.9 (63.85-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 2.40Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.228 , 0.276 0.213 , 0.261	Depositor DCC
R_{free} test set	2776 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	48.6	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9571	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 3.93% 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: PO4

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	B	0.38	0/3079	0.57	2/4161 (0.0%)
1	D	0.40	0/3095	0.58	1/4185 (0.0%)
2	E	0.40	0/1669	0.56	0/2256
2	F	0.41	0/1669	0.56	0/2256
All	All	0.40	0/9512	0.57	3/12858 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	192	LEU	CA-CB-CG	5.96	129.00	115.30
1	B	192	LEU	CA-CB-CG	5.81	128.66	115.30
1	B	294	ALA	N-CA-C	-5.02	97.44	111.00

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	B	3013	0	2985	101	0
1	D	3027	0	2999	100	0
2	E	1631	0	1614	66	0
2	F	1631	0	1614	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	5	0	0	0	0
3	F	5	0	0	1	0
4	B	61	0	0	8	0
4	D	102	0	0	7	0
4	E	45	0	0	4	0
4	F	51	0	0	7	0
All	All	9571	0	9212	328	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 (328) 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:D:23:ILE:HD11	1:D:28:LEU:HG	1.30	1.13
1:B:23:ILE:HD11	1:B:28:LEU:HG	1.34	1.02
2:F:79:SER:HB2	2:F:86:LYS:HE2	1.53	0.91
2:E:79:SER:HB2	2:E:86:LYS:HE2	1.52	0.91
2:F:198:THR:HG22	2:F:200:THR:H	1.37	0.90
1:B:289:ASN:H	1:B:292:HIS:HD2	1.20	0.88
2:E:198:THR:HG22	2:E:200:THR:H	1.35	0.88
1:D:289:ASN:H	1:D:292:HIS:HD2	1.21	0.87
1:D:133:ASP:HB2	1:D:141:LYS:HE3	1.58	0.86
1:B:158:ALA:HA	1:B:203:LEU:HD13	1.56	0.85
1:D:158:ALA:HA	1:D:203:LEU:HD13	1.56	0.85
1:D:271:THR:HG22	1:D:273:LYS:H	1.41	0.85
1:B:133:ASP:HB2	1:B:141:LYS:HE3	1.58	0.85
1:D:159:GLU:HG3	4:D:2018:HOH:O	1.77	0.85
1:B:271:THR:HG22	1:B:273:LYS:H	1.43	0.81
1:B:199:THR:HG21	1:B:244:VAL:O	1.79	0.80
2:E:183:PRO:HG2	2:E:224:LEU:HD21	1.63	0.79
1:D:199:THR:HG21	1:D:244:VAL:O	1.82	0.79
2:E:148:SER:HB2	2:E:150:HIS:CE1	2.19	0.78
2:F:148:SER:HB2	2:F:150:HIS:CE1	2.18	0.78
1:B:315:LYS:HD2	1:B:316:SER:O	1.84	0.78
2:F:183:PRO:HG2	2:F:224:LEU:HD21	1.66	0.76
1:D:210:HIS:HE1	4:D:2029:HOH:O	1.68	0.76
1:D:151:ARG:HH12	1:D:153:ASN:HD22	1.34	0.75
2:F:90:ASN:HB3	2:F:92:GLN:HG2	1.67	0.75
1:D:315:LYS:HD2	1:D:316:SER:O	1.87	0.75
2:E:90:ASN:HB3	2:E:92:GLN:HG2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LEU:O	1:B:370:THR:HG21	1.87	0.73
1:B:151:ARG:HH12	1:B:153:ASN:HD22	1.34	0.73
1:B:271:THR:HG22	1:B:273:LYS:N	2.05	0.72
1:D:7:LEU:O	1:D:370:THR:HG21	1.90	0.72
1:D:229:GLN:H	1:D:229:GLN:NE2	1.87	0.72
1:D:271:THR:HG22	1:D:273:LYS:N	2.05	0.71
1:D:240:HIS:HE1	1:D:257:SER:OG	1.72	0.71
1:B:289:ASN:H	1:B:292:HIS:CD2	2.07	0.70
1:B:224:ILE:HD12	1:B:235:LYS:HD3	1.73	0.69
1:B:8:GLN:N	1:B:8:GLN:HE21	1.91	0.69
4:D:2025:HOH:O	2:F:200:THR:HG23	1.91	0.69
1:B:229:GLN:H	1:B:229:GLN:NE2	1.90	0.68
1:D:40:PHE:CD1	1:D:413:SER:HB2	2.29	0.68
2:F:90:ASN:HB3	2:F:92:GLN:CG	2.23	0.68
2:E:146:THR:HG21	2:E:151:GLY:HA3	1.76	0.68
1:B:40:PHE:CD1	1:B:413:SER:HB2	2.28	0.68
2:F:95:LYS:HG2	2:F:121:LEU:HG	1.75	0.68
2:E:90:ASN:HB3	2:E:92:GLN:CG	2.24	0.67
1:B:240:HIS:HE1	1:B:257:SER:OG	1.76	0.67
2:E:95:LYS:HG2	2:E:121:LEU:HG	1.77	0.67
1:D:289:ASN:H	1:D:292:HIS:CD2	2.08	0.67
1:D:34:SER:CB	1:D:35:PRO:HA	2.25	0.66
2:E:109:LEU:HD22	2:E:181:CYS:SG	2.36	0.66
2:E:217:THR:HB	2:E:275:ALA:O	1.95	0.66
1:B:201:VAL:HG13	1:B:215:THR:HG22	1.78	0.66
1:D:224:ILE:HD12	1:D:235:LYS:HD3	1.78	0.66
2:F:146:THR:HG21	2:F:151:GLY:HA3	1.76	0.65
1:B:321:PHE:HE1	1:B:348:LYS:HG3	1.60	0.65
2:F:109:LEU:HD22	2:F:181:CYS:SG	2.37	0.65
2:F:240:ARG:HD3	4:F:2043:HOH:O	1.98	0.64
1:B:321:PHE:CE1	1:B:348:LYS:HG3	2.33	0.63
2:E:181:CYS:HB2	4:E:2043:HOH:O	1.98	0.63
1:D:34:SER:HB3	1:D:35:PRO:HA	1.81	0.62
1:D:271:THR:HG21	4:D:2057:HOH:O	1.98	0.62
2:E:136:GLU:O	2:E:139:ILE:HD13	2.00	0.62
1:D:201:VAL:HG13	1:D:215:THR:HG22	1.82	0.62
1:D:226:HIS:HD2	4:D:2030:HOH:O	1.83	0.62
1:D:359:SER:OG	1:D:370:THR:HB	2.01	0.61
2:F:227:TRP:CE2	2:F:231:HIS:HE1	2.18	0.61
2:F:214:VAL:HG22	2:F:216:TYR:CE1	2.34	0.61
2:F:230:LYS:HE2	4:F:2036:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:70:PRO:HG3	2:F:76:MET:SD	2.41	0.61
2:E:84:TYR:CB	2:E:153:GLN:HG3	2.31	0.61
2:E:79:SER:CB	2:E:86:LYS:HE2	2.30	0.61
2:F:98:THR:HB	4:F:2010:HOH:O	1.99	0.61
2:F:136:GLU:O	2:F:139:ILE:HD13	2.01	0.61
2:F:227:TRP:CE2	2:F:231:HIS:CE1	2.88	0.61
1:D:295:PRO:HB3	1:D:296:PRO:HD2	1.83	0.60
1:D:8:GLN:HE21	1:D:8:GLN:N	1.98	0.60
2:E:227:TRP:CE2	2:E:231:HIS:CE1	2.89	0.60
2:E:227:TRP:CE2	2:E:231:HIS:HE1	2.19	0.60
1:B:5:HIS:HB3	1:B:23:ILE:HG22	1.83	0.60
2:F:230:LYS:HG2	4:F:2036:HOH:O	2.01	0.60
2:E:196:ILE:HD12	2:E:197:ILE:HD13	1.83	0.59
2:E:70:PRO:HG3	2:E:76:MET:SD	2.41	0.59
1:D:23:ILE:HD11	1:D:28:LEU:CG	2.20	0.59
1:D:23:ILE:CD1	1:D:28:LEU:HG	2.21	0.59
1:D:295:PRO:O	1:D:296:PRO:C	2.41	0.59
2:F:217:THR:HB	2:F:275:ALA:O	2.01	0.59
2:F:84:TYR:CB	2:F:153:GLN:HG3	2.32	0.59
2:F:84:TYR:HB2	2:F:153:GLN:CG	2.33	0.59
1:D:321:PHE:HE1	1:D:348:LYS:HG3	1.68	0.59
2:E:84:TYR:HB2	2:E:153:GLN:CG	2.33	0.58
2:F:196:ILE:HD12	2:F:197:ILE:HD13	1.84	0.58
2:F:79:SER:CB	2:F:86:LYS:HE2	2.31	0.58
1:D:321:PHE:CE1	1:D:348:LYS:HG3	2.38	0.58
2:E:214:VAL:HG22	2:E:216:TYR:CE1	2.37	0.58
1:D:196:SER:HB2	1:D:219:ASP:OD1	2.04	0.58
2:F:227:TRP:CZ2	2:F:231:HIS:CE1	2.92	0.58
1:D:106:ARG:HG2	1:D:120:CYS:HB2	1.86	0.58
1:D:159:GLU:HG2	1:D:205:LYS:NZ	2.18	0.58
1:B:158:ALA:HA	1:B:203:LEU:CD1	2.32	0.58
1:D:5:HIS:HB3	1:D:23:ILE:HG22	1.86	0.58
1:D:7:LEU:O	1:D:370:THR:CG2	2.50	0.58
1:D:14:ARG:HG2	1:D:114:GLU:OE2	2.04	0.58
1:B:7:LEU:O	1:B:370:THR:CG2	2.52	0.57
2:E:227:TRP:CZ2	2:E:231:HIS:CE1	2.92	0.57
2:F:227:TRP:CD2	2:F:231:HIS:HE1	2.22	0.57
2:E:283:PRO:HG3	2:F:245:TRP:CD1	2.39	0.57
1:D:4:ILE:HG12	1:D:421:VAL:HG22	1.86	0.57
1:B:23:ILE:CD1	1:B:28:LEU:HG	2.23	0.57
1:B:4:ILE:HG12	1:B:421:VAL:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:84:TYR:HB2	2:F:153:GLN:HG3	1.86	0.57
1:B:106:ARG:HG2	1:B:120:CYS:HB2	1.85	0.57
1:B:285:LYS:HB3	1:B:286:PRO:HD3	1.87	0.57
1:B:14:ARG:HG2	1:B:114:GLU:OE2	2.05	0.56
2:E:84:TYR:HB2	2:E:153:GLN:HG3	1.87	0.56
1:B:34:SER:CB	1:B:35:PRO:HA	2.34	0.56
2:F:198:THR:HG22	2:F:200:THR:N	2.15	0.56
1:B:159:GLU:HG2	1:B:205:LYS:NZ	2.21	0.56
2:E:198:THR:HG22	2:E:200:THR:N	2.13	0.56
1:D:285:LYS:HB3	1:D:286:PRO:HD3	1.86	0.56
2:E:227:TRP:CD2	2:E:231:HIS:HE1	2.23	0.56
1:B:381:LYS:HG2	1:B:382:ASN:H	1.70	0.56
1:D:216:SER:HB2	1:D:244:VAL:HG22	1.88	0.56
1:B:23:ILE:HD11	1:B:28:LEU:CG	2.24	0.56
2:E:196:ILE:CD1	2:E:197:ILE:HD13	2.36	0.56
2:E:132:THR:O	2:E:136:GLU:HG3	2.07	0.55
1:D:34:SER:HA	1:D:36:ASN:H	1.71	0.55
1:B:151:ARG:NH1	1:B:153:ASN:HD22	2.03	0.55
1:B:196:SER:HB2	1:B:219:ASP:OD1	2.06	0.55
2:E:227:TRP:CZ2	2:E:231:HIS:HE1	2.25	0.55
1:D:158:ALA:HA	1:D:203:LEU:CD1	2.32	0.54
1:B:8:GLN:HE22	1:B:23:ILE:HA	1.72	0.54
1:D:151:ARG:HH12	1:D:153:ASN:ND2	2.02	0.54
2:E:97:VAL:HA	2:E:121:LEU:HB2	1.90	0.54
2:F:227:TRP:CZ2	2:F:231:HIS:HE1	2.25	0.54
2:F:196:ILE:CD1	2:F:197:ILE:HD13	2.38	0.54
1:B:199:THR:HG22	1:B:216:SER:OG	2.08	0.54
1:B:34:SER:HA	1:B:36:ASN:H	1.72	0.54
2:F:107:GLY:O	2:F:111:ILE:HG12	2.08	0.54
1:B:151:ARG:HH12	1:B:153:ASN:ND2	2.04	0.54
1:D:296:PRO:HB2	4:D:2067:HOH:O	2.08	0.53
1:D:305:ILE:N	1:D:305:ILE:HD12	2.23	0.53
1:D:194:HIS:NE2	1:D:223:LYS:HE2	2.23	0.53
2:F:132:THR:O	2:F:136:GLU:HG3	2.09	0.53
1:D:151:ARG:NH1	1:D:153:ASN:HD22	2.05	0.53
1:B:41:ALA:HB1	1:B:139:VAL:HG23	1.89	0.53
1:B:359:SER:OG	1:B:370:THR:HB	2.08	0.53
1:D:256:LEU:CD2	1:D:322:VAL:HG21	2.39	0.52
2:E:111:ILE:HD12	2:E:142:LEU:CD1	2.39	0.52
2:E:84:TYR:CB	2:E:153:GLN:CG	2.87	0.52
2:F:97:VAL:HA	2:F:121:LEU:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:381:LYS:HG2	1:D:382:ASN:H	1.75	0.52
1:B:256:LEU:CD2	1:B:322:VAL:HG21	2.40	0.52
1:D:8:GLN:HE22	1:D:23:ILE:HA	1.74	0.52
1:D:199:THR:HG22	1:D:216:SER:OG	2.10	0.52
2:E:222:LYS:HE2	2:E:226:GLU:OE1	2.10	0.52
2:F:240:ARG:HG3	2:F:277:PHE:CZ	2.45	0.52
2:E:227:TRP:CH2	2:E:231:HIS:HE1	2.27	0.51
2:F:111:ILE:HD12	2:F:142:LEU:CD1	2.40	0.51
2:F:227:TRP:CE3	2:F:231:HIS:HE1	2.28	0.51
1:D:355:TYR:OH	1:D:376:SER:HB3	2.10	0.51
1:B:341:GLN:HG2	4:B:2045:HOH:O	2.08	0.51
2:E:227:TRP:CZ3	2:E:231:HIS:HE1	2.29	0.51
2:F:227:TRP:CH2	2:F:231:HIS:HE1	2.28	0.51
2:E:227:TRP:CE3	2:E:231:HIS:HE1	2.29	0.51
1:B:204:ILE:HG22	1:B:212:PHE:HB2	1.93	0.51
1:B:355:TYR:OH	1:B:376:SER:HB3	2.10	0.50
1:B:4:ILE:HG23	1:B:414:VAL:HG11	1.94	0.50
2:F:106:PHE:HD2	2:F:134:TYR:CD2	2.30	0.50
1:B:194:HIS:NE2	1:B:223:LYS:HE2	2.27	0.50
1:D:41:ALA:HB1	1:D:139:VAL:HG23	1.93	0.50
2:E:157:VAL:HG22	2:E:158:LEU:N	2.27	0.50
2:E:107:GLY:O	2:E:111:ILE:HG12	2.12	0.50
2:F:150:HIS:CE1	4:F:2017:HOH:O	2.65	0.50
2:F:227:TRP:CZ3	2:F:231:HIS:HE1	2.30	0.50
2:F:84:TYR:CB	2:F:153:GLN:CG	2.90	0.49
1:B:195:VAL:HG12	1:B:195:VAL:O	2.12	0.49
1:D:295:PRO:CB	1:D:296:PRO:HD2	2.42	0.49
2:E:209:LEU:HD13	2:E:279:ARG:HB2	1.93	0.49
1:D:223:LYS:HD3	1:D:236:TRP:CH2	2.47	0.49
2:F:222:LYS:HE2	2:F:226:GLU:OE1	2.12	0.49
1:B:133:ASP:HB3	1:B:136:SER:HB3	1.94	0.49
1:B:197:MET:HE3	4:B:2018:HOH:O	2.12	0.49
1:B:34:SER:HB3	1:B:35:PRO:HA	1.95	0.48
2:F:209:LEU:HD13	2:F:279:ARG:HB2	1.94	0.48
1:B:192:LEU:HD11	1:B:213:ILE:HD13	1.94	0.48
2:E:106:PHE:HD2	2:E:134:TYR:CD2	2.31	0.48
1:B:374:LYS:HG2	1:B:427:ILE:HD12	1.95	0.48
1:D:408:SER:O	1:D:412:GLN:HG2	2.13	0.48
2:E:163:MET:HE3	2:E:201:LEU:HD11	1.95	0.48
1:D:374:LYS:HG2	1:D:427:ILE:HD12	1.95	0.48
1:D:294:ALA:HB1	1:D:295:PRO:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:HIS:HD2	4:B:2020:HOH:O	1.96	0.48
1:B:240:HIS:CD2	1:B:244:VAL:HG22	2.49	0.48
1:B:290:ASP:HB2	1:B:293:LEU:HD12	1.94	0.48
2:E:181:CYS:CB	4:E:2043:HOH:O	2.58	0.47
2:F:227:TRP:CH2	2:F:231:HIS:CE1	3.03	0.47
2:E:286:LEU:HB3	2:F:250:GLU:HG2	1.95	0.47
1:B:411:ILE:O	1:B:415:GLN:HG3	2.15	0.47
2:E:227:TRP:CD2	2:E:231:HIS:CE1	3.02	0.47
2:E:183:PRO:HG3	2:E:228:MET:CE	2.44	0.47
1:D:133:ASP:HB3	1:D:136:SER:HB3	1.96	0.47
1:D:186:PHE:CZ	1:D:188:GLN:CG	2.98	0.47
2:F:150:HIS:HE1	4:F:2017:HOH:O	1.98	0.47
1:B:8:GLN:H	1:B:8:GLN:HE21	1.62	0.47
1:D:34:SER:HA	1:D:36:ASN:N	2.30	0.47
2:E:227:TRP:CH2	2:E:231:HIS:CE1	3.02	0.47
1:B:157:ILE:HD12	4:B:2008:HOH:O	2.15	0.47
1:D:133:ASP:OD1	1:D:136:SER:HB2	2.14	0.47
2:F:126:GLU:O	2:F:159:ARG:HA	2.15	0.47
2:F:198:THR:O	2:F:202:LEU:HG	2.15	0.47
1:D:290:ASP:HB2	1:D:293:LEU:HD12	1.97	0.46
2:E:84:TYR:HB3	2:E:153:GLN:HG3	1.97	0.46
1:B:398:VAL:HG23	4:B:2056:HOH:O	2.14	0.46
1:D:159:GLU:HG2	1:D:205:LYS:HZ3	1.80	0.46
1:B:109:ARG:CG	1:B:157:ILE:HD11	2.46	0.46
1:D:411:ILE:O	1:D:415:GLN:HG3	2.15	0.46
2:F:227:TRP:CD2	2:F:231:HIS:CE1	3.02	0.46
1:B:408:SER:O	1:B:412:GLN:HG2	2.15	0.46
1:B:159:GLU:HG2	1:B:205:LYS:HZ2	1.80	0.46
1:D:271:THR:CG2	1:D:273:LYS:CB	2.94	0.46
1:B:31:LYS:HG3	1:B:41:ALA:HB2	1.98	0.46
1:D:204:ILE:HG22	1:D:212:PHE:HB2	1.96	0.46
2:E:126:GLU:O	2:E:159:ARG:HA	2.16	0.46
2:E:235:HIS:CE1	2:E:237:LEU:HB2	2.51	0.45
1:D:229:GLN:H	1:D:229:GLN:HE21	1.64	0.45
1:D:358:ILE:HG22	1:D:370:THR:HG22	1.98	0.45
1:B:171:GLY:C	1:B:198:LEU:HD22	2.37	0.45
2:E:240:ARG:HG3	2:E:277:PHE:CZ	2.51	0.45
1:B:34:SER:HA	1:B:36:ASN:N	2.31	0.45
1:B:8:GLN:NE2	1:B:23:ILE:HA	2.31	0.45
2:F:157:VAL:HG22	2:F:158:LEU:N	2.32	0.45
1:B:186:PHE:CZ	1:B:188:GLN:CG	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:THR:CG2	1:B:273:LYS:CB	2.94	0.45
1:D:8:GLN:NE2	1:D:23:ILE:HA	2.31	0.45
1:B:150:LYS:HD2	1:B:170:PHE:CD1	2.51	0.45
1:D:186:PHE:CZ	1:D:188:GLN:HG3	2.51	0.45
2:E:198:THR:O	2:E:202:LEU:HG	2.17	0.45
2:F:98:THR:HG22	2:F:99:ILE:HG13	1.98	0.45
1:D:109:ARG:CG	1:D:157:ILE:HD11	2.47	0.45
2:E:148:SER:CB	2:E:150:HIS:CE1	2.96	0.45
2:E:284:ALA:O	2:F:250:GLU:N	2.49	0.44
1:B:358:ILE:HD12	1:B:358:ILE:HA	1.68	0.44
1:D:271:THR:HG21	1:D:273:LYS:HB3	2.00	0.44
1:B:171:GLY:HA2	1:B:198:LEU:HD22	1.98	0.44
1:D:192:LEU:HD11	1:D:213:ILE:HD13	1.98	0.44
2:E:98:THR:HG22	2:E:99:ILE:HG13	1.99	0.44
1:B:360:LEU:HD12	1:B:361:SER:N	2.32	0.44
1:D:358:ILE:HD12	1:D:358:ILE:HA	1.73	0.44
2:E:166:LEU:N	2:E:167:PRO:CD	2.81	0.44
1:B:133:ASP:OD1	1:B:136:SER:HB2	2.17	0.44
2:F:235:HIS:CE1	2:F:237:LEU:HB2	2.53	0.44
2:E:237:LEU:HA	2:E:237:LEU:HD12	1.82	0.43
1:B:186:PHE:CZ	1:B:188:GLN:HG3	2.52	0.43
1:B:253:TYR:CZ	1:B:270:LYS:HD2	2.53	0.43
1:D:330:LYS:HG3	4:D:2081:HOH:O	2.18	0.43
1:B:139:VAL:O	1:B:141:LYS:HE2	2.19	0.43
1:D:253:TYR:CZ	1:D:270:LYS:HD2	2.53	0.43
1:D:417:ASP:OD2	1:D:419:ASN:HB3	2.18	0.43
2:E:236:PRO:HA	4:E:2037:HOH:O	2.18	0.43
1:B:381:LYS:HB3	1:B:381:LYS:HE3	1.76	0.43
2:F:183:PRO:HG3	2:F:228:MET:CE	2.48	0.43
2:F:214:VAL:HG22	2:F:216:TYR:CZ	2.53	0.43
1:B:40:PHE:CE1	1:B:413:SER:HB2	2.54	0.43
2:F:84:TYR:HB3	2:F:153:GLN:HG3	2.00	0.43
1:D:196:SER:OG	1:D:217:ASP:HB2	2.19	0.43
1:D:381:LYS:HB3	1:D:381:LYS:HE3	1.75	0.43
2:F:166:LEU:N	2:F:167:PRO:CD	2.82	0.43
2:E:245:TRP:CD1	2:F:283:PRO:HG3	2.54	0.43
1:B:271:THR:CG2	1:B:273:LYS:HB2	2.48	0.43
1:B:223:LYS:HD3	1:B:236:TRP:CH2	2.54	0.42
1:B:271:THR:HG21	1:B:273:LYS:HB3	2.01	0.42
1:B:28:LEU:HD21	1:B:43:LYS:HD3	2.00	0.42
1:D:271:THR:CG2	1:D:273:LYS:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:374:LYS:HB2	1:D:374:LYS:HE3	1.86	0.42
1:D:40:PHE:CE1	1:D:413:SER:HB2	2.53	0.42
1:B:160:ASP:CG	1:B:162:THR:HG22	2.39	0.42
1:B:196:SER:OG	1:B:217:ASP:HB2	2.20	0.42
1:B:360:LEU:HD12	1:B:361:SER:H	1.84	0.42
2:E:235:HIS:HA	2:E:236:PRO:HD3	1.91	0.42
1:B:315:LYS:NZ	1:B:315:LYS:HB3	2.34	0.42
1:D:34:SER:HB3	1:D:35:PRO:CA	2.48	0.42
1:B:417:ASP:OD2	1:B:419:ASN:HB3	2.19	0.42
1:D:160:ASP:CG	1:D:162:THR:HG22	2.40	0.42
1:D:169:LYS:O	1:D:197:MET:HG3	2.19	0.42
1:D:171:GLY:C	1:D:198:LEU:HD22	2.40	0.42
2:E:249:ASP:OD1	2:E:251:CYS:HB2	2.19	0.42
1:D:139:VAL:O	1:D:141:LYS:HE2	2.20	0.42
1:D:294:ALA:HA	1:D:295:PRO:HD3	1.56	0.42
1:B:285:LYS:CB	4:B:2037:HOH:O	2.67	0.42
1:B:374:LYS:HE3	1:B:374:LYS:HB2	1.85	0.42
1:D:31:LYS:HG3	1:D:41:ALA:HB2	2.01	0.42
1:B:221:HIS:HA	4:B:2022:HOH:O	2.18	0.42
1:D:22:ILE:HD11	1:D:108:LEU:HG	2.02	0.42
1:D:235:LYS:HG2	1:D:236:TRP:N	2.35	0.42
1:B:204:ILE:HD13	1:B:204:ILE:HA	1.92	0.41
1:D:240:HIS:CE1	1:D:257:SER:OG	2.63	0.41
2:F:182:PHE:HA	4:F:2030:HOH:O	2.20	0.41
2:E:70:PRO:HD3	2:E:169:PHE:CE1	2.55	0.41
1:B:195:VAL:CG1	1:B:195:VAL:O	2.69	0.41
1:B:348:LYS:O	1:B:349:GLN:HB2	2.20	0.41
1:B:121:ALA:HB2	1:B:128:LEU:HD11	2.03	0.41
1:D:106:ARG:HG3	1:D:107:ASN:ND2	2.35	0.41
2:F:180:PHE:CD2	2:F:196:ILE:HD13	2.55	0.41
2:E:158:LEU:HD12	2:E:158:LEU:O	2.20	0.41
2:E:81:LEU:C	2:E:83:PRO:HD3	2.40	0.41
1:D:229:GLN:HG2	2:F:285:ILE:HD11	2.01	0.41
1:D:32:TYR:CZ	1:D:402:LYS:HE3	2.55	0.41
2:F:148:SER:CB	2:F:150:HIS:CE1	2.96	0.41
2:F:225:HIS:NE2	3:F:1287:PO4:O1	2.51	0.41
1:B:231:PHE:CD1	1:B:232:ILE:HG13	2.55	0.41
1:B:124:ASP:HB3	1:B:126:SER:OG	2.21	0.41
1:B:169:LYS:O	1:B:197:MET:HG3	2.21	0.41
2:E:119:GLU:HB3	4:E:2010:HOH:O	2.20	0.41
1:B:148:PHE:HZ	1:B:176:ILE:HG13	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:123:LEU:HD23	2:F:170:PHE:HZ	1.86	0.41
1:B:282:SER:C	4:B:2037:HOH:O	2.58	0.40
1:D:155:ILE:HA	1:D:165:ILE:O	2.21	0.40
1:D:4:ILE:HG23	1:D:414:VAL:HG11	2.03	0.40
2:F:166:LEU:HD23	2:F:166:LEU:HA	1.88	0.40
1:B:235:LYS:HG2	1:B:236:TRP:N	2.36	0.40
1:B:283:LEU:O	1:B:286:PRO:HD2	2.22	0.40
2:E:119:GLU:O	2:E:119:GLU:HG2	2.22	0.40
2:E:96:LYS:HD3	2:E:96:LYS:HA	1.84	0.40
1:B:106:ARG:HG3	1:B:107:ASN:ND2	2.36	0.40
1:D:109:ARG:HG3	1:D:157:ILE:HD11	2.04	0.40
1:D:198:LEU:HA	1:D:198:LEU:HD12	1.88	0.40
1:D:271:THR:HG21	1:D:273:LYS:CB	2.52	0.40
2:E:196:ILE:HG13	2:E:196:ILE:H	1.69	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	B	368/450 (82%)	344 (94%)	24 (6%)	0	100	100
1	D	370/450 (82%)	348 (94%)	21 (6%)	1 (0%)	41	55
2	E	195/254 (77%)	190 (97%)	5 (3%)	0	100	100
2	F	195/254 (77%)	189 (97%)	6 (3%)	0	100	100
All	All	1128/1408 (80%)	1071 (95%)	56 (5%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	295	PRO

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	B	344/411 (84%)	318 (92%)	26 (8%)	13 20
1	D	346/411 (84%)	320 (92%)	26 (8%)	13 21
2	E	180/228 (79%)	163 (91%)	17 (9%)	8 13
2	F	180/228 (79%)	162 (90%)	18 (10%)	7 11
All	All	1050/1278 (82%)	963 (92%)	87 (8%)	11 17

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3	VAL
1	B	8	GLN
1	B	9	ASN
1	B	11	LEU
1	B	23	ILE
1	B	100	PRO
1	B	127	LEU
1	B	141	LYS
1	B	187	THR
1	B	192	LEU
1	B	196	SER
1	B	198	LEU
1	B	199	THR
1	B	201	VAL
1	B	204	ILE
1	B	213	ILE
1	B	220	GLU
1	B	229	GLN
1	B	235	LYS
1	B	248	CYS
1	B	262	ASP
1	B	315	LYS
1	B	358	ILE
1	B	370	THR

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Mol	Chain	Res	Type
1	B	414	VAL
1	B	433	VAL
1	D	3	VAL
1	D	8	GLN
1	D	9	ASN
1	D	11	LEU
1	D	23	ILE
1	D	100	PRO
1	D	127	LEU
1	D	141	LYS
1	D	187	THR
1	D	192	LEU
1	D	196	SER
1	D	198	LEU
1	D	199	THR
1	D	201	VAL
1	D	204	ILE
1	D	213	ILE
1	D	220	GLU
1	D	229	GLN
1	D	235	LYS
1	D	248	CYS
1	D	262	ASP
1	D	315	LYS
1	D	358	ILE
1	D	370	THR
1	D	414	VAL
1	D	433	VAL
2	E	98	THR
2	E	139	ILE
2	E	146	THR
2	E	155	ILE
2	E	181	CYS
2	E	195	ARG
2	E	196	ILE
2	E	200	THR
2	E	209	LEU
2	E	214	VAL
2	E	217	THR
2	E	230	LYS
2	E	237	LEU
2	E	240	ARG

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Mol	Chain	Res	Type
2	E	243	LYS
2	E	253	LYS
2	E	255	MET
2	F	98	THR
2	F	129	VAL
2	F	139	ILE
2	F	146	THR
2	F	155	ILE
2	F	181	CYS
2	F	195	ARG
2	F	196	ILE
2	F	200	THR
2	F	209	LEU
2	F	214	VAL
2	F	217	THR
2	F	230	LYS
2	F	237	LEU
2	F	240	ARG
2	F	243	LYS
2	F	253	LYS
2	F	255	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	8	GLN
1	B	33	GLN
1	B	37	HIS
1	B	153	ASN
1	B	211	GLN
1	B	226	HIS
1	B	229	GLN
1	B	240	HIS
1	B	274	ASN
1	B	292	HIS
1	B	356	ASN
1	D	8	GLN
1	D	33	GLN
1	D	37	HIS
1	D	153	ASN
1	D	210	HIS
1	D	211	GLN

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Mol	Chain	Res	Type
1	D	226	HIS
1	D	229	GLN
1	D	240	HIS
1	D	292	HIS
1	D	356	ASN
2	E	90	ASN
2	E	92	GLN
2	E	133	ASN
2	E	199	ASN
2	E	231	HIS
2	E	257	ASN
2	F	90	ASN
2	F	92	GLN
2	F	133	ASN
2	F	150	HIS
2	F	168	ASN
2	F	199	ASN
2	F	231	HIS
2	F	257	ASN

5.3.3 RNA

There are no RNA molecules 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

2 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	$\#\|Z\| > 2$
3	PO4	F	1287	-	4,4,4	0.79	0	6,6,6	1.00	0
3	PO4	E	1287	-	4,4,4	0.83	0	6,6,6	0.51	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1287	PO4	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	B	374/450 (83%)	0.65	40 (10%) 6 5	11, 34, 73, 100	0
1	D	376/450 (83%)	0.36	14 (3%) 41 41	10, 29, 72, 100	0
2	E	201/254 (79%)	0.08	3 (1%) 73 72	8, 26, 70, 90	0
2	F	201/254 (79%)	0.20	4 (1%) 65 63	8, 25, 70, 90	0
All	All	1152/1408 (81%)	0.38	61 (5%) 26 25	8, 30, 72, 100	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	186	PHE	10.1
1	B	159	GLU	6.5
1	D	187	THR	6.2
1	B	185	LYS	5.4
1	B	2	SER	5.4
1	B	433	VAL	5.4
1	B	305	ILE	5.2
2	E	286	LEU	5.1
2	F	145	ASN	5.0
1	B	294	ALA	4.7
1	B	3	VAL	4.7
1	B	158	ALA	4.4
1	B	291	GLN	3.9
1	B	187	THR	3.8
1	B	48	PHE	3.7
1	B	292	HIS	3.6
1	B	421	VAL	3.5
1	B	396	PHE	3.5
1	D	186	PHE	3.4
1	D	100	PRO	3.4
1	B	141	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	103	SER	3.0
1	B	157	ILE	3.0
1	B	262	ASP	2.9
1	D	434	SER	2.9
1	B	420	LEU	2.8
1	B	389	TYR	2.8
1	D	305	ILE	2.8
1	B	148	PHE	2.8
1	B	431	TYR	2.7
1	B	161	ASP	2.7
1	B	414	VAL	2.6
1	D	37	HIS	2.6
2	E	139	ILE	2.6
1	B	284	ILE	2.6
1	B	47	ASP	2.6
1	B	430	LEU	2.5
1	D	433	VAL	2.5
1	B	293	LEU	2.5
2	F	286	LEU	2.5
1	B	425	GLU	2.5
1	D	415	GLN	2.5
1	B	375	GLU	2.5
1	D	436	LEU	2.4
1	B	123	SER	2.4
2	F	149	LYS	2.3
1	B	5	HIS	2.3
1	B	8	GLN	2.3
1	B	290	ASP	2.3
1	B	308	PHE	2.2
1	D	423	LYS	2.2
2	E	66	GLN	2.2
1	B	355	TYR	2.1
1	B	134	LYS	2.1
1	B	394	ASN	2.1
2	F	147	ALA	2.1
1	D	378	GLY	2.1
1	B	184	GLU	2.1
1	D	191	ILE	2.0
1	D	138	ASN	2.0
1	D	204	ILE	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 carbohydrates 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
3	PO4	E	1287	5/5	0.91	0.19	30,45,76,80	0
3	PO4	F	1287	5/5	0.94	0.15	25,33,81,88	0

6.5 Other polymers (i)

There are no such residues in this entry.