



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 04:06 PM GMT

PDB ID : 2DR3
Title : Crystal Structure of RecA superfamily ATPase PH0284 from *Pyrococcus horikoshii* OT3
Authors : Bagautdinov, B.; Kunishima, N.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2006-06-06
Resolution : 2.00 Å(reported)

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

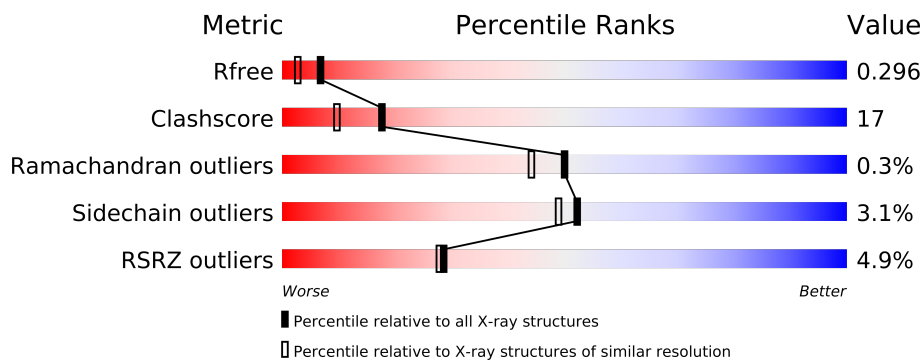
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	247	
1	B	247	
1	C	247	
1	D	247	
1	E	247	
1	F	247	

2 Entry composition i

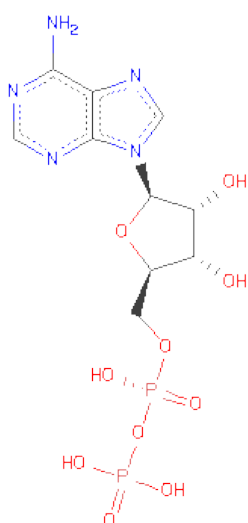
There are 3 unique types of molecules in this entry. The entry contains 12543 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called UPF0273 protein PH0284.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1826	1167	323	328	8			
1	B	240	Total	C	N	O	S	0	0	0
			1875	1195	334	338	8			
1	C	233	Total	C	N	O	S	0	0	0
			1835	1171	324	332	8			
1	D	242	Total	C	N	O	S	0	0	0
			1896	1208	338	342	8			
1	E	236	Total	C	N	O	S	0	0	0
			1853	1184	328	333	8			
1	F	236	Total	C	N	O	S	0	0	0
			1854	1184	329	333	8			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is water.

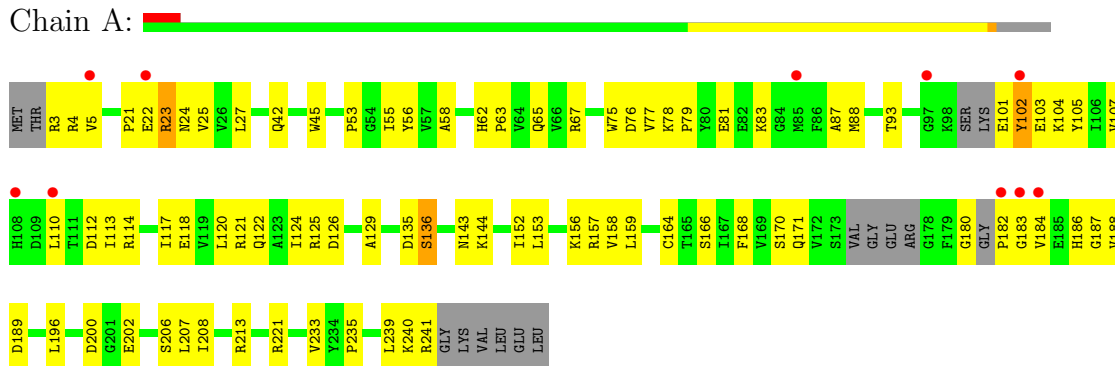
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	190	Total	O	0	0
			190	190		
3	B	220	Total	O	0	0
			220	220		
3	C	213	Total	O	0	0
			213	213		
3	D	228	Total	O	0	0
			228	228		
3	E	196	Total	O	0	0
			196	196		
3	F	195	Total	O	0	0
			195	195		

3 Residue-property plots

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

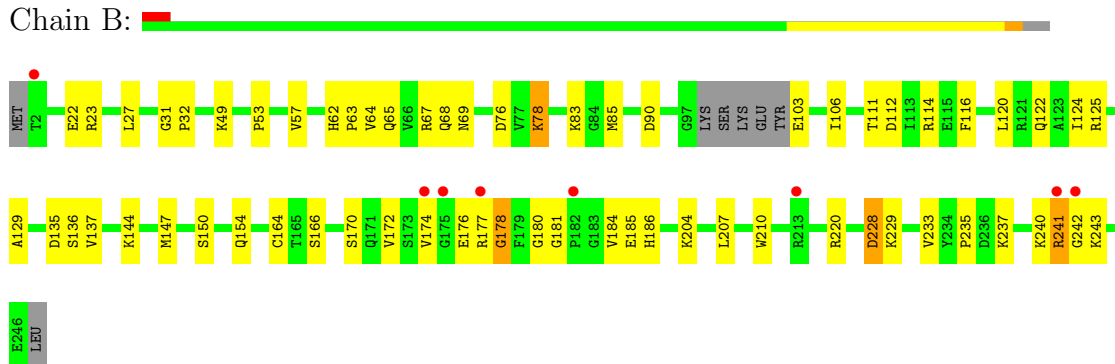
- Molecule 1: UPF0273 protein PH0284

Chain A:



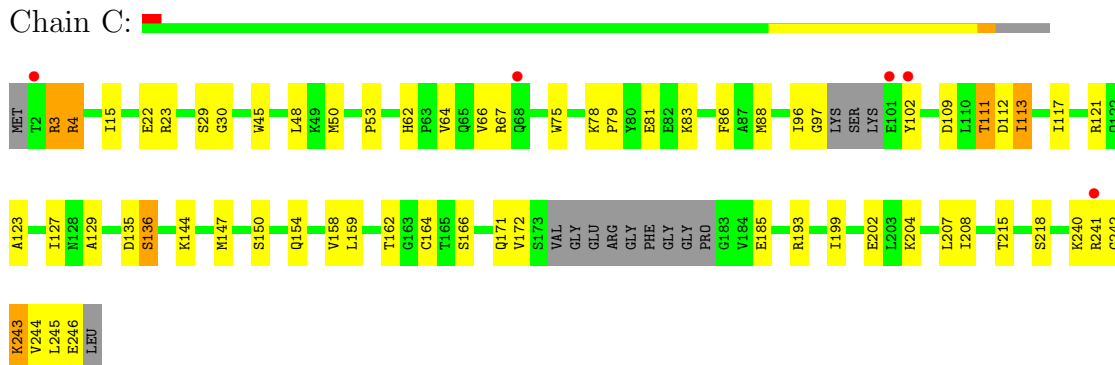
- Molecule 1: UPF0273 protein PH0284

Chain B:



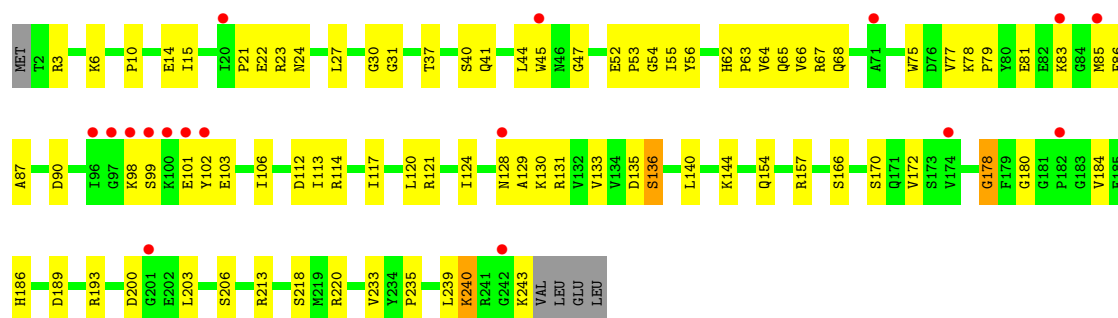
- Molecule 1: UPF0273 protein PH0284

Chain C:



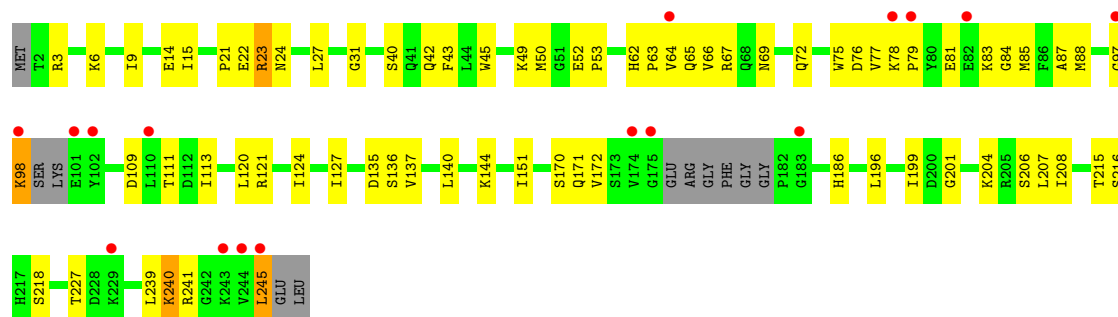
• Molecule 1: UPF0273 protein PH0284

Chain D: 



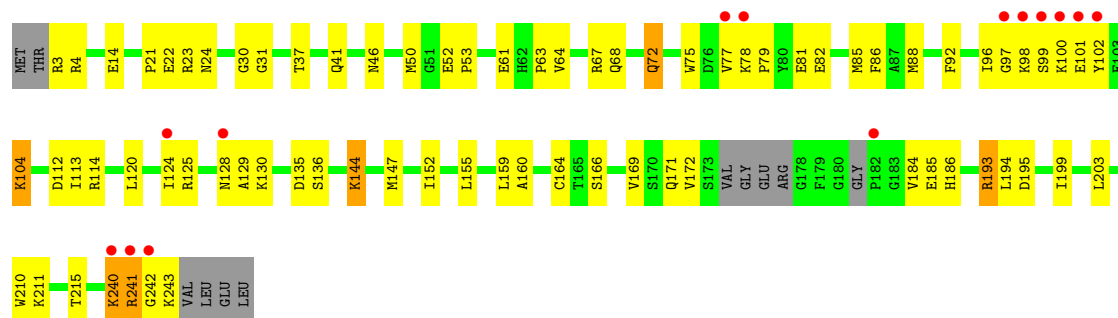
• Molecule 1: UPF0273 protein PH0284

Chain E: 



• Molecule 1: UPF0273 protein PH0284

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	96.06Å 96.06Å 298.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.38 – 2.00 47.42 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.5 (38.38-2.00) 91.5 (47.42-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.40 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.251 , 0.295 0.252 , 0.296	Depositor DCC
R_{free} test set	5013 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.1	EDS
Estimated twinning fraction	0.007 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 99706 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12543	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP

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	0.40	0/1859	0.68	0/2502
1	B	0.41	0/1909	0.76	3/2573 (0.1%)
1	C	0.41	0/1867	0.70	0/2516
1	D	0.48	0/1932	0.72	1/2603 (0.0%)
1	E	0.42	0/1886	0.69	0/2541
1	F	0.48	1/1888 (0.1%)	0.71	1/2540 (0.0%)
All	All	0.43	1/11341 (0.0%)	0.71	5/15275 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	75	TRP	NE1-CE2	8.57	1.48	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	125	ARG	NE-CZ-NH1	-12.66	113.97	120.30
1	B	125	ARG	NE-CZ-NH2	11.05	125.83	120.30
1	D	178	GLY	O-C-N	-5.98	113.13	122.70
1	B	178	GLY	O-C-N	-5.66	113.65	122.70
1	F	185	GLU	O-C-N	-5.10	114.55	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	178	GLY	Mainchain

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1826	0	1867	80	0
1	B	1875	0	1923	52	0
1	C	1835	0	1881	64	0
1	D	1896	0	1944	71	0
1	E	1853	0	1908	66	0
1	F	1854	0	1902	77	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
2	E	27	0	12	0	0
2	F	27	0	12	0	0
3	A	190	0	0	5	0
3	B	220	0	0	11	0
3	C	213	0	0	6	0
3	D	228	0	0	10	0
3	E	196	0	0	11	0
3	F	195	0	0	9	0
All	All	12543	0	11497	395	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (395) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:154:GLN:HA	1:D:157:ARG:HH12	1.08	1.11
1:C:240:LYS:HD3	1:C:245:LEU:HD12	1.31	1.07

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:104:LYS:HD2	1:F:104:LYS:H	1.21	1.03
1:D:124:ILE:HG23	1:D:129:ALA:HB3	1.49	0.94
1:C:243:LYS:HE3	1:C:243:LYS:HA	1.50	0.93
1:D:53:PRO:HG2	1:D:128:ASN:HB2	1.51	0.92
1:F:199:ILE:HG21	1:F:242:GLY:HA2	1.49	0.91
1:C:240:LYS:CD	1:C:245:LEU:HD12	2.03	0.86
1:D:101:GLU:HG3	1:D:102:TYR:H	1.40	0.85
1:D:117:ILE:O	1:D:121:ARG:HG3	1.74	0.85
1:A:63:PRO:HB3	1:A:88:MET:HG2	1.57	0.83
1:C:193:ARG:HD3	3:C:3863:HOH:O	1.77	0.83
1:D:154:GLN:HA	1:D:157:ARG:NH1	1.93	0.83
1:C:113:ILE:HD13	1:C:113:ILE:H	1.42	0.82
3:E:3891:HOH:O	1:F:211:LYS:HD2	1.81	0.81
1:C:78:LYS:HB3	1:C:79:PRO:HD3	1.63	0.80
1:C:3:ARG:H	1:C:3:ARG:HE	1.28	0.80
1:A:53:PRO:HB2	1:A:129:ALA:HA	1.64	0.79
1:D:53:PRO:HG2	1:D:128:ASN:O	1.81	0.79
1:E:45:TRP:HE1	1:E:49:LYS:HE3	1.48	0.78
1:A:102:TYR:O	1:A:103:GLU:HG2	1.84	0.77
1:A:143:ASN:O	1:A:144:LYS:HD2	1.85	0.77
1:E:204:LYS:HE2	3:E:3852:HOH:O	1.83	0.76
1:C:4:ARG:HH21	1:C:215:THR:HB	1.50	0.75
1:A:104:LYS:HG2	1:A:105:TYR:CZ	2.20	0.75
1:D:53:PRO:CG	1:D:128:ASN:HB2	2.16	0.75
1:B:178:GLY:HA3	3:B:3815:HOH:O	1.87	0.75
1:A:117:ILE:HD11	1:A:158:VAL:HG11	1.69	0.74
1:F:78:LYS:HB3	1:F:79:PRO:HD3	1.68	0.74
1:E:241:ARG:HB2	3:E:4001:HOH:O	1.87	0.73
1:B:64:VAL:HG12	1:B:68:GLN:HE21	1.53	0.73
1:A:65:GLN:HG3	3:A:3831:HOH:O	1.86	0.72
1:C:53:PRO:HG2	1:C:129:ALA:HA	1.71	0.72
1:E:3:ARG:HE	1:E:22:GLU:CD	1.92	0.72
1:C:113:ILE:HD13	1:C:113:ILE:N	2.05	0.72
1:E:66:VAL:HB	1:E:88:MET:HE3	1.70	0.72
1:C:113:ILE:H	1:C:113:ILE:CD1	2.02	0.72
1:C:241:ARG:HH11	1:C:241:ARG:HG2	1.55	0.71
1:D:79:PRO:HG2	3:D:3957:HOH:O	1.89	0.71
1:C:199:ILE:HG21	1:C:242:GLY:HA3	1.73	0.71
1:A:180:GLY:O	1:A:182:PRO:HD2	1.91	0.70
1:C:66:VAL:HB	1:C:88:MET:HE3	1.73	0.70
1:A:117:ILE:CD1	1:A:158:VAL:HG11	2.21	0.70
1:B:49:LYS:NZ	3:B:4013:HOH:O	2.24	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:220:ARG:HG3	1:B:220:ARG:HH11	1.57	0.69
1:E:45:TRP:NE1	1:E:49:LYS:HE3	2.08	0.69
1:E:87:ALA:HB2	1:E:127:ILE:HD12	1.75	0.69
1:A:3:ARG:CZ	1:A:22:GLU:HG3	2.24	0.68
1:B:242:GLY:HA3	3:B:3964:HOH:O	1.93	0.68
1:D:47:GLY:O	1:D:52:GLU:HB2	1.94	0.68
1:C:144:LYS:HD2	1:C:147:MET:HG3	1.76	0.67
1:C:245:LEU:O	1:C:246:GLU:HB2	1.95	0.67
1:B:114:ARG:HB3	3:B:4000:HOH:O	1.92	0.67
1:E:53:PRO:HB2	1:E:127:ILE:HG22	1.78	0.66
1:C:30:GLY:C	1:C:172:VAL:HG22	2.15	0.66
1:E:15:ILE:HG23	1:E:218:SER:HB3	1.77	0.66
1:D:113:ILE:N	1:D:113:ILE:HD12	2.11	0.66
1:E:206:SER:HB3	1:E:239:LEU:HD12	1.78	0.66
1:F:128:ASN:HB2	3:F:3945:HOH:O	1.96	0.66
1:D:78:LYS:HB2	1:D:79:PRO:HD3	1.76	0.66
1:A:221:ARG:NE	1:A:241:ARG:HD2	2.11	0.66
1:B:112:ASP:HB2	3:B:4000:HOH:O	1.96	0.66
1:E:109:ASP:OD1	1:E:111:THR:HB	1.96	0.65
1:E:186:HIS:ND1	3:E:3839:HOH:O	2.28	0.65
1:A:21:PRO:O	1:A:24:ASN:HB2	1.96	0.65
1:D:101:GLU:HG3	1:D:102:TYR:N	2.11	0.65
1:D:243:LYS:HG3	3:D:4008:HOH:O	1.96	0.65
1:D:157:ARG:HB3	1:D:157:ARG:CZ	2.27	0.64
1:D:157:ARG:NH1	1:D:157:ARG:HB3	2.12	0.64
1:D:120:LEU:O	1:D:124:ILE:HG13	1.97	0.64
1:C:193:ARG:NH1	3:C:3863:HOH:O	2.30	0.64
1:F:96:ILE:HG13	1:F:97:GLY:N	2.13	0.64
1:A:78:LYS:HB3	1:A:79:PRO:HD3	1.81	0.63
1:E:63:PRO:O	1:E:67:ARG:HG3	1.98	0.63
1:D:23:ARG:HD3	3:D:3949:HOH:O	1.98	0.63
1:A:104:LYS:HG2	1:A:105:TYR:CE2	2.33	0.63
1:B:144:LYS:HE3	1:B:147:MET:HG3	1.82	0.62
1:B:76:ASP:OD2	1:B:78:LYS:HE3	2.00	0.62
1:F:96:ILE:HG13	1:F:97:GLY:H	1.65	0.61
1:F:104:LYS:HD2	1:F:104:LYS:N	2.05	0.61
1:A:102:TYR:CG	1:A:103:GLU:N	2.69	0.61
1:B:240:LYS:O	1:B:241:ARG:HG2	2.01	0.61
1:C:29:SER:O	1:C:193:ARG:HD2	2.00	0.60
1:F:240:LYS:NZ	3:F:3895:HOH:O	2.32	0.60
1:A:118:GLU:O	1:A:122:GLN:HG2	2.01	0.60
1:C:81:GLU:HG3	1:C:86:PHE:HD2	1.67	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:3:ARG:NH1	1:C:23:ARG:HH22	1.99	0.60
1:A:114:ARG:HG3	1:A:114:ARG:HH11	1.65	0.60
1:F:104:LYS:CD	1:F:104:LYS:H	2.02	0.60
1:E:27:LEU:HD11	1:E:170:SER:HB2	1.83	0.60
1:D:15:ILE:HG23	1:D:218:SER:HB3	1.83	0.60
1:A:206:SER:HB3	1:A:239:LEU:HD23	1.83	0.60
1:F:136:SER:HB2	1:F:169:VAL:O	2.02	0.60
1:F:98:LYS:HG2	1:F:100:LYS:H	1.66	0.60
1:C:4:ARG:HG2	1:C:4:ARG:HH11	1.67	0.59
1:A:3:ARG:NE	1:A:22:GLU:HG3	2.17	0.59
1:F:23:ARG:HD2	1:F:160:ALA:O	2.02	0.59
1:B:64:VAL:HG12	1:B:68:GLN:NE2	2.17	0.59
1:E:22:GLU:HG2	1:E:23:ARG:HG2	1.84	0.59
1:C:241:ARG:CG	1:C:241:ARG:HH11	2.14	0.59
1:C:111:THR:HG22	1:C:112:ASP:OD2	2.01	0.59
1:E:3:ARG:NE	1:E:22:GLU:OE2	2.35	0.59
1:A:159:LEU:HD13	1:A:166:SER:OG	2.03	0.59
1:C:199:ILE:HD13	1:C:242:GLY:HA2	1.85	0.58
1:D:113:ILE:HG22	1:D:113:ILE:O	2.03	0.58
1:B:62:HIS:HB3	1:B:65:GLN:OE1	2.02	0.58
1:D:233:VAL:O	1:D:235:PRO:HD3	2.03	0.58
1:B:176:GLU:HG2	1:B:178:GLY:H	1.69	0.58
1:F:72:GLN:H	1:F:72:GLN:HE21	1.52	0.58
1:A:25:VAL:HG11	1:A:168:PHE:CE2	2.39	0.58
1:C:204:LYS:HE2	3:C:3902:HOH:O	2.02	0.58
1:F:152:ILE:HG13	1:F:184:VAL:HG13	1.85	0.58
1:E:127:ILE:O	1:E:127:ILE:HG22	2.03	0.58
1:E:78:LYS:HB2	1:E:79:PRO:HD3	1.85	0.58
1:A:55:ILE:HG12	1:A:87:ALA:HB3	1.85	0.57
1:F:112:ASP:HA	3:F:3949:HOH:O	2.04	0.57
1:D:3:ARG:NE	1:D:22:GLU:OE2	2.37	0.57
1:D:77:VAL:O	1:D:81:GLU:HG3	2.03	0.57
1:C:3:ARG:NE	1:C:3:ARG:H	2.00	0.57
1:A:200:ASP:HB3	3:B:3962:HOH:O	2.05	0.57
1:B:184:VAL:HG13	1:B:185:GLU:N	2.20	0.57
1:B:69:ASN:HB3	3:B:3905:HOH:O	2.05	0.57
1:F:64:VAL:HG13	3:F:3964:HOH:O	2.04	0.56
1:E:171:GLN:HB3	1:F:186:HIS:CE1	2.40	0.56
1:C:23:ARG:HA	1:C:164:CYS:O	2.06	0.56
1:C:4:ARG:HH21	1:C:215:THR:CB	2.18	0.56
1:B:150:SER:O	1:B:154:GLN:HG3	2.05	0.56
1:C:102:TYR:HA	3:C:3921:HOH:O	2.06	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:128:ASN:HA	3:F:3952:HOH:O	2.06	0.56
1:E:227:THR:HB	3:E:3986:HOH:O	2.05	0.56
1:A:62:HIS:HD2	1:A:93:THR:CG2	2.18	0.56
1:A:157:ARG:HE	1:F:96:ILE:CD1	2.19	0.56
1:F:68:GLN:NE2	3:F:3982:HOH:O	2.36	0.56
1:A:77:VAL:O	1:A:81:GLU:HG3	2.06	0.56
1:A:3:ARG:CG	1:A:22:GLU:HG3	2.36	0.55
1:F:98:LYS:NZ	1:F:98:LYS:HB3	2.21	0.55
1:B:62:HIS:CE1	1:B:64:VAL:HG23	2.41	0.55
1:F:79:PRO:O	1:F:82:GLU:HG2	2.07	0.55
1:F:77:VAL:O	1:F:81:GLU:HG3	2.07	0.55
1:E:62:HIS:CE1	1:E:64:VAL:HG23	2.42	0.55
1:D:47:GLY:O	1:D:52:GLU:N	2.36	0.55
1:F:68:GLN:O	1:F:72:GLN:NE2	2.40	0.55
1:E:21:PRO:O	1:E:24:ASN:HB2	2.07	0.54
1:F:144:LYS:CE	1:F:147:MET:HG3	2.37	0.54
1:E:22:GLU:O	1:E:23:ARG:HB2	2.07	0.54
1:F:144:LYS:HE3	1:F:147:MET:HG3	1.90	0.54
1:D:14:GLU:N	1:D:14:GLU:OE1	2.40	0.54
1:D:117:ILE:HG22	1:D:121:ARG:HD2	1.90	0.54
1:F:63:PRO:O	1:F:67:ARG:HG3	2.08	0.54
1:F:243:LYS:HD3	1:F:243:LYS:C	2.27	0.54
1:D:45:TRP:CE3	1:D:75:TRP:HB3	2.42	0.54
1:C:158:VAL:O	1:C:162:THR:HG23	2.07	0.54
1:B:229:LYS:HB2	3:B:4006:HOH:O	2.07	0.54
1:F:112:ASP:OD2	1:F:114:ARG:HB2	2.08	0.53
1:F:37:THR:O	1:F:41:GLN:HG3	2.08	0.53
1:C:15:ILE:HG23	1:C:218:SER:HB3	1.90	0.53
1:A:3:ARG:HG3	1:A:22:GLU:HG3	1.89	0.53
1:C:62:HIS:CE1	1:C:64:VAL:HG23	2.43	0.53
1:C:96:ILE:HG13	1:C:97:GLY:N	2.24	0.53
1:E:69:ASN:HB3	3:E:3864:HOH:O	2.08	0.53
1:E:97:GLY:O	1:E:98:LYS:HB2	2.08	0.53
1:D:240:LYS:NZ	3:D:3844:HOH:O	2.41	0.53
1:B:83:LYS:HD3	1:B:85:MET:HE2	1.90	0.53
1:F:125:ARG:HG2	1:F:125:ARG:HH11	1.74	0.53
1:F:113:ILE:HD11	1:F:155:LEU:HD21	1.91	0.53
1:D:37:THR:O	1:D:41:GLN:HG3	2.09	0.53
1:D:63:PRO:O	1:D:67:ARG:HG3	2.09	0.53
1:A:113:ILE:O	1:A:117:ILE:HG22	2.09	0.52
1:E:113:ILE:HD13	1:E:151:ILE:HG23	1.91	0.52
1:D:128:ASN:O	1:D:130:LYS:HG2	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:79:PRO:O	1:E:83:LYS:HE2	2.08	0.52
1:D:64:VAL:HG12	1:D:68:GLN:HE21	1.73	0.52
1:A:22:GLU:O	1:A:23:ARG:HB2	2.08	0.52
1:D:113:ILE:N	1:D:113:ILE:CD1	2.73	0.52
1:E:98:LYS:HD2	1:E:98:LYS:N	2.24	0.52
1:A:171:GLN:HB3	1:B:186:HIS:CE1	2.44	0.52
1:B:32:PRO:HD2	1:B:174:VAL:CG2	2.39	0.52
1:B:220:ARG:HG3	1:B:220:ARG:NH1	2.24	0.51
1:B:23:ARG:HA	1:B:164:CYS:O	2.10	0.51
1:D:53:PRO:HG2	1:D:128:ASN:CB	2.33	0.51
1:A:114:ARG:O	1:A:118:GLU:HG3	2.10	0.51
1:B:32:PRO:HG3	1:C:185:GLU:OE1	2.10	0.51
1:C:79:PRO:O	1:C:83:LYS:HG3	2.11	0.51
1:D:40:SER:HB3	1:D:133:VAL:HG11	1.92	0.51
1:C:22:GLU:O	1:C:23:ARG:HB2	2.11	0.51
1:A:143:ASN:C	1:A:144:LYS:HD2	2.32	0.51
1:B:27:LEU:HD11	1:B:170:SER:HB2	1.93	0.51
1:A:45:TRP:CE3	1:A:75:TRP:HB3	2.46	0.50
1:B:111:THR:HG22	1:B:112:ASP:OD2	2.12	0.50
1:A:117:ILE:CD1	1:A:158:VAL:HG21	2.41	0.50
1:C:171:GLN:HB3	1:D:186:HIS:CE1	2.47	0.50
1:F:193:ARG:HD2	1:F:195:ASP:CG	2.32	0.50
1:E:76:ASP:OD2	1:E:79:PRO:HD3	2.12	0.50
1:D:62:HIS:CE1	1:D:64:VAL:HG23	2.46	0.49
1:D:114:ARG:HB2	3:D:3965:HOH:O	2.13	0.49
1:B:181:GLY:O	1:B:184:VAL:HG12	2.13	0.49
1:F:193:ARG:HD2	1:F:195:ASP:OD1	2.12	0.49
1:A:117:ILE:HD11	1:A:158:VAL:CG1	2.41	0.49
1:D:140:LEU:O	1:D:144:LYS:HE2	2.13	0.49
1:C:66:VAL:HB	1:C:88:MET:CE	2.42	0.49
1:F:46:ASN:O	1:F:50:MET:HG2	2.12	0.49
1:B:32:PRO:HD2	1:B:174:VAL:HG23	1.94	0.49
1:F:3:ARG:HG3	1:F:3:ARG:HH11	1.77	0.49
1:A:114:ARG:HG3	1:A:114:ARG:NH1	2.28	0.48
1:B:240:LYS:NZ	3:B:4012:HOH:O	2.46	0.48
1:D:157:ARG:NH1	1:D:157:ARG:CB	2.74	0.48
1:F:23:ARG:HA	1:F:164:CYS:O	2.14	0.48
1:B:207:LEU:HD23	1:B:207:LEU:C	2.33	0.48
1:D:22:GLU:O	1:D:23:ARG:HB2	2.14	0.48
1:B:184:VAL:HG13	1:B:185:GLU:H	1.76	0.48
1:F:21:PRO:O	1:F:24:ASN:HB2	2.13	0.48
1:A:152:ILE:HG13	1:A:184:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:245:LEU:HG	1:E:245:LEU:H	1.47	0.48
1:B:243:LYS:HG2	3:B:3985:HOH:O	2.11	0.48
1:E:201:GLY:HA3	1:F:240:LYS:HA	1.95	0.48
1:A:117:ILE:O	1:A:121:ARG:HG3	2.12	0.48
1:E:62:HIS:HB3	1:E:65:GLN:OE1	2.13	0.48
3:A:3848:HOH:O	1:F:98:LYS:HD3	2.13	0.48
1:A:76:ASP:OD1	1:A:79:PRO:HD3	2.14	0.48
1:A:107:VAL:HG11	1:A:110:LEU:CD2	2.44	0.48
1:C:45:TRP:CE3	1:C:75:TRP:HB3	2.48	0.48
1:E:84:GLY:O	1:E:127:ILE:HG23	2.13	0.47
1:A:240:LYS:HB3	3:A:3934:HOH:O	2.14	0.47
1:A:182:PRO:C	1:A:184:VAL:H	2.17	0.47
1:E:87:ALA:HB2	1:E:127:ILE:CD1	2.41	0.47
1:A:189:ASP:O	1:A:213:ARG:HG2	2.14	0.47
1:E:9:ILE:HG23	1:E:42:GLN:NE2	2.30	0.47
1:F:193:ARG:HD3	1:F:194:LEU:N	2.29	0.47
1:E:76:ASP:O	1:E:79:PRO:HD2	2.15	0.47
1:A:101:GLU:HA	3:A:3805:HOH:O	2.14	0.47
1:B:22:GLU:HG2	1:B:23:ARG:HG3	1.97	0.47
1:D:44:LEU:CD1	1:D:56:TYR:HB2	2.44	0.47
1:F:199:ILE:HD13	1:F:242:GLY:H	1.79	0.47
1:E:45:TRP:CE3	1:E:75:TRP:HB3	2.49	0.47
1:C:4:ARG:HG2	1:C:4:ARG:NH1	2.30	0.47
1:E:111:THR:HG22	3:E:3963:HOH:O	2.14	0.47
1:F:98:LYS:HG2	1:F:99:SER:N	2.30	0.47
1:F:72:GLN:N	1:F:72:GLN:HE21	2.13	0.47
1:D:98:LYS:HG2	3:D:4017:HOH:O	2.15	0.47
1:A:153:LEU:O	1:A:156:LYS:HB3	2.14	0.47
1:F:4:ARG:HH12	1:F:215:THR:HG21	1.78	0.47
1:B:32:PRO:CD	1:B:174:VAL:HG23	2.45	0.47
1:B:135:ASP:HA	1:B:136:SER:HA	1.54	0.47
1:C:3:ARG:CZ	1:C:23:ARG:HH12	2.27	0.47
1:E:199:ILE:HB	1:E:204:LYS:NZ	2.29	0.47
1:C:241:ARG:CG	1:C:241:ARG:NH1	2.71	0.47
1:A:120:LEU:O	1:A:124:ILE:HG13	2.15	0.47
1:D:54:GLY:HA2	1:D:131:ARG:O	2.15	0.47
1:A:107:VAL:HG11	1:A:110:LEU:HD23	1.96	0.47
1:D:90:ASP:HB3	1:D:106:ILE:HG12	1.97	0.46
1:E:127:ILE:O	1:E:127:ILE:CG2	2.63	0.46
1:A:233:VAL:O	1:A:235:PRO:HD3	2.14	0.46
1:D:53:PRO:HG2	1:D:128:ASN:C	2.35	0.46
1:D:135:ASP:HA	1:D:136:SER:HA	1.43	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:159:LEU:HD13	1:F:166:SER:OG	2.15	0.46
1:E:201:GLY:CA	1:F:240:LYS:HA	2.45	0.46
1:D:6:LYS:O	1:D:131:ARG:NH2	2.47	0.46
1:C:4:ARG:NH2	1:C:215:THR:CB	2.78	0.46
1:F:124:ILE:HG23	1:F:129:ALA:HB3	1.97	0.46
1:D:27:LEU:HD11	1:D:170:SER:HB2	1.97	0.46
1:E:144:LYS:NZ	3:E:3941:HOH:O	2.48	0.46
1:F:101:GLU:CG	1:F:102:TYR:N	2.79	0.46
1:A:3:ARG:NE	1:A:22:GLU:OE2	2.49	0.46
1:C:135:ASP:HA	1:C:136:SER:HA	1.64	0.46
1:D:101:GLU:CG	1:D:102:TYR:H	2.19	0.45
1:E:207:LEU:C	1:E:207:LEU:HD23	2.36	0.45
1:E:31:GLY:HA2	1:E:172:VAL:O	2.16	0.45
1:E:196:LEU:HD23	1:F:210:TRP:NE1	2.31	0.45
1:D:65:GLN:HG3	3:D:3817:HOH:O	2.15	0.45
1:D:21:PRO:O	1:D:24:ASN:HB2	2.17	0.45
1:C:123:ALA:O	1:C:127:ILE:HG12	2.17	0.45
1:E:121:ARG:HG2	1:E:121:ARG:HH11	1.81	0.45
1:F:135:ASP:HA	1:F:136:SER:HA	1.56	0.45
1:C:109:ASP:OD2	1:C:111:THR:HB	2.16	0.45
1:A:27:LEU:HD11	1:A:170:SER:HB2	1.99	0.45
1:F:104:LYS:NZ	3:F:3905:HOH:O	2.50	0.45
1:F:52:GLU:HG2	1:F:130:LYS:NZ	2.31	0.45
1:E:66:VAL:HB	1:E:88:MET:CE	2.43	0.45
1:B:144:LYS:CE	1:B:147:MET:HG3	2.46	0.45
1:F:113:ILE:HG13	1:F:113:ILE:O	2.17	0.45
1:D:124:ILE:HG23	1:D:129:ALA:CB	2.35	0.45
1:F:243:LYS:HA	3:F:3915:HOH:O	2.16	0.45
1:D:83:LYS:HE3	1:D:85:MET:SD	2.56	0.45
1:B:64:VAL:O	1:B:68:GLN:HG3	2.17	0.44
1:D:6:LYS:HE2	3:D:3945:HOH:O	2.17	0.44
1:F:86:PHE:HE2	1:F:88:MET:HG2	1.81	0.44
1:A:202:GLU:HB2	1:B:220:ARG:HD3	1.99	0.44
1:A:186:HIS:CE1	1:F:171:GLN:HB3	2.52	0.44
1:A:62:HIS:HD2	1:A:93:THR:HG23	1.82	0.44
1:F:30:GLY:HA2	1:F:193:ARG:HE	1.83	0.44
1:F:120:LEU:O	1:F:124:ILE:HG13	2.17	0.44
1:C:243:LYS:HE3	1:C:243:LYS:CA	2.33	0.44
1:C:4:ARG:NH2	1:C:215:THR:OG1	2.51	0.44
1:C:241:ARG:NH1	1:C:241:ARG:HG2	2.28	0.44
1:E:6:LYS:HD3	1:E:50:MET:HE1	1.98	0.44
1:A:3:ARG:HH11	1:A:3:ARG:HG2	1.82	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:240:LYS:HE3	1:E:240:LYS:HB3	1.66	0.44
1:D:203:LEU:HG	1:E:208:ILE:HD11	2.00	0.44
1:B:103:GLU:HB3	1:B:106:ILE:CG1	2.48	0.44
1:D:101:GLU:OE1	1:D:101:GLU:HA	2.17	0.44
1:C:199:ILE:HG21	1:C:242:GLY:CA	2.46	0.44
1:A:206:SER:HB3	1:A:239:LEU:CD2	2.46	0.44
1:D:189:ASP:HA	1:D:213:ARG:HH11	1.83	0.44
1:F:22:GLU:HG2	1:F:23:ARG:HG3	1.99	0.44
1:C:159:LEU:HD13	1:C:166:SER:OG	2.17	0.44
1:D:10:PRO:HA	3:D:3850:HOH:O	2.18	0.43
1:D:23:ARG:HG3	1:D:23:ARG:HH11	1.83	0.43
1:F:4:ARG:HH12	1:F:215:THR:CB	2.30	0.43
1:F:78:LYS:N	1:F:79:PRO:CD	2.81	0.43
1:E:140:LEU:O	1:E:144:LYS:HE3	2.18	0.43
1:C:67:ARG:HG3	1:C:88:MET:HE2	2.01	0.43
1:D:52:GLU:HA	1:D:53:PRO:HD3	1.76	0.43
1:A:207:LEU:HD23	1:A:208:ILE:N	2.34	0.43
1:B:120:LEU:O	1:B:124:ILE:HG13	2.18	0.43
1:A:117:ILE:O	1:A:117:ILE:HD12	2.18	0.43
1:D:62:HIS:O	1:D:66:VAL:HG23	2.19	0.43
1:A:135:ASP:HA	1:A:136:SER:HA	1.45	0.43
1:D:55:ILE:HG12	1:D:87:ALA:HB3	1.99	0.43
1:A:117:ILE:HD13	1:A:158:VAL:HG21	2.00	0.43
1:C:30:GLY:O	1:C:172:VAL:HG22	2.17	0.43
1:C:48:LEU:C	1:C:50:MET:H	2.22	0.43
1:F:100:LYS:O	1:F:101:GLU:HB2	2.19	0.43
1:B:53:PRO:HB2	1:B:129:ALA:HA	1.99	0.43
1:F:199:ILE:CG2	1:F:242:GLY:HA2	2.35	0.43
1:B:237:LYS:HE3	3:B:4011:HOH:O	2.17	0.43
1:E:120:LEU:O	1:E:124:ILE:HG13	2.19	0.42
1:E:40:SER:O	1:E:43:PHE:HB3	2.18	0.42
1:F:22:GLU:O	1:F:23:ARG:HB2	2.19	0.42
1:F:68:GLN:HA	1:F:68:GLN:HE21	1.84	0.42
1:A:23:ARG:HA	1:A:164:CYS:O	2.19	0.42
1:F:3:ARG:HD3	3:F:3980:HOH:O	2.20	0.42
1:F:241:ARG:HD3	1:F:241:ARG:HA	1.47	0.42
1:E:121:ARG:NH1	1:E:121:ARG:HG2	2.34	0.42
1:E:135:ASP:HA	1:E:136:SER:HA	1.46	0.42
1:C:202:GLU:HB2	1:D:220:ARG:NE	2.35	0.42
1:C:117:ILE:HD12	3:C:3927:HOH:O	2.19	0.42
1:C:3:ARG:NH1	1:C:23:ARG:NH2	2.67	0.42
1:F:78:LYS:N	1:F:79:PRO:HD2	2.35	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:150:SER:O	1:C:154:GLN:HG3	2.19	0.42
1:D:99:SER:HB2	3:D:4023:HOH:O	2.18	0.42
1:A:78:LYS:HA	1:A:81:GLU:OE1	2.20	0.42
1:A:27:LEU:HB2	1:A:188:VAL:HG11	2.01	0.42
1:B:90:ASP:HB2	1:B:103:GLU:HG2	2.02	0.42
1:D:206:SER:HB3	1:D:239:LEU:HD23	2.01	0.42
1:C:48:LEU:HD11	1:C:86:PHE:CD1	2.56	0.41
1:B:103:GLU:HB3	1:B:106:ILE:HG12	2.01	0.41
1:A:183:GLY:O	1:A:187:GLY:N	2.51	0.41
1:F:53:PRO:HA	1:F:85:MET:O	2.20	0.41
1:C:207:LEU:HD23	1:C:208:ILE:N	2.35	0.41
1:E:52:GLU:HA	1:E:53:PRO:HD2	1.94	0.41
1:E:77:VAL:O	1:E:81:GLU:HG3	2.20	0.41
1:B:67:ARG:HD3	1:B:78:LYS:HD2	2.02	0.41
1:E:85:MET:HE3	3:E:3893:HOH:O	2.20	0.41
1:A:23:ARG:HH11	1:A:23:ARG:HG2	1.85	0.41
1:B:63:PRO:O	1:B:67:ARG:HG3	2.20	0.41
1:D:64:VAL:HG12	1:D:68:GLN:NE2	2.35	0.41
1:E:45:TRP:HE1	1:E:49:LYS:CE	2.27	0.41
1:A:3:ARG:O	1:A:4:ARG:HD3	2.19	0.41
1:A:125:ARG:NH1	3:A:3957:HOH:O	2.48	0.41
1:F:78:LYS:HB3	1:F:79:PRO:CD	2.44	0.41
1:A:3:ARG:HG3	1:A:22:GLU:CG	2.51	0.41
1:E:62:HIS:ND1	1:E:63:PRO:HD2	2.35	0.41
1:D:31:GLY:HA2	1:D:172:VAL:O	2.20	0.41
1:C:78:LYS:HB3	1:C:79:PRO:CD	2.44	0.41
1:A:112:ASP:OD1	1:A:114:ARG:HB2	2.20	0.41
1:E:67:ARG:NH1	1:E:81:GLU:OE2	2.53	0.41
1:A:208:ILE:HD11	1:F:203:LEU:HG	2.03	0.41
1:A:56:TYR:HE1	1:A:58:ALA:HB2	1.86	0.41
1:B:228:ASP:OD1	1:B:228:ASP:N	2.53	0.41
1:F:199:ILE:HD13	1:F:242:GLY:N	2.36	0.41
1:A:63:PRO:O	1:A:67:ARG:HG3	2.21	0.41
1:E:67:ARG:HD2	3:E:3894:HOH:O	2.21	0.41
1:D:81:GLU:HG2	1:D:86:PHE:HD2	1.86	0.41
1:E:69:ASN:O	1:E:72:GLN:HB3	2.21	0.41
1:E:215:THR:OG1	1:E:216:SER:N	2.53	0.41
1:A:196:LEU:HD23	1:B:210:TRP:NE1	2.36	0.41
1:F:31:GLY:HA2	1:F:172:VAL:O	2.21	0.41
1:A:5:VAL:CG2	1:A:22:GLU:OE1	2.69	0.41
1:E:83:LYS:NZ	3:E:3974:HOH:O	2.50	0.41
1:F:125:ARG:HG2	1:F:125:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:57:VAL:HG11	1:B:116:PHE:CZ	2.56	0.41
1:C:243:LYS:CE	1:C:244:VAL:H	2.35	0.40
1:A:42:GLN:HG3	1:A:75:TRP:CZ2	2.56	0.40
1:A:56:TYR:CE1	1:A:58:ALA:HB2	2.56	0.40
1:A:157:ARG:NH2	1:F:92:PHE:HE2	2.20	0.40
1:D:30:GLY:C	1:D:172:VAL:HG22	2.41	0.40
1:B:31:GLY:HA2	1:B:172:VAL:O	2.20	0.40
1:A:23:ARG:HD2	1:A:23:ARG:N	2.36	0.40
1:A:207:LEU:HD23	1:A:207:LEU:C	2.41	0.40
1:C:121:ARG:HD2	3:C:3854:HOH:O	2.21	0.40
1:B:233:VAL:O	1:B:235:PRO:HD3	2.22	0.40
1:B:204:LYS:NZ	1:B:242:GLY:HA2	2.36	0.40
1:E:14:GLU:OE2	1:E:14:GLU:N	2.52	0.40
1:D:124:ILE:CG2	1:D:129:ALA:HB3	2.36	0.40
1:A:114:ARG:O	1:A:117:ILE:CG2	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	224/247 (91%)	217 (97%)	7 (3%)	0	100	100
1	B	236/247 (96%)	228 (97%)	7 (3%)	1 (0%)	43	36
1	C	227/247 (92%)	217 (96%)	10 (4%)	0	100	100
1	D	240/247 (97%)	228 (95%)	9 (4%)	3 (1%)	18	8
1	E	230/247 (93%)	221 (96%)	9 (4%)	0	100	100
1	F	230/247 (93%)	215 (94%)	15 (6%)	0	100	100
All	All	1387/1482 (94%)	1326 (96%)	57 (4%)	4 (0%)	50	44

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	184	VAL
1	D	103	GLU
1	D	180	GLY
1	B	180	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	197/209 (94%)	192 (98%)	5 (2%)	60	59
1	B	202/209 (97%)	195 (96%)	7 (4%)	48	43
1	C	199/209 (95%)	193 (97%)	6 (3%)	53	50
1	D	204/209 (98%)	198 (97%)	6 (3%)	55	52
1	E	201/209 (96%)	196 (98%)	5 (2%)	60	59
1	F	200/209 (96%)	192 (96%)	8 (4%)	42	36
All	All	1203/1254 (96%)	1166 (97%)	37 (3%)	52	49

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	83	LYS
1	A	102	TYR
1	A	126	ASP
1	A	136	SER
1	B	78	LYS
1	B	122	GLN
1	B	137	VAL
1	B	166	SER
1	B	177	ARG
1	B	228	ASP
1	B	241	ARG
1	C	3	ARG
1	C	4	ARG
1	C	111	THR
1	C	113	ILE

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Mol	Chain	Res	Type
1	C	136	SER
1	C	243	LYS
1	D	112	ASP
1	D	136	SER
1	D	166	SER
1	D	193	ARG
1	D	200	ASP
1	D	240	LYS
1	E	23	ARG
1	E	98	LYS
1	E	137	VAL
1	E	240	LYS
1	E	245	LEU
1	F	14	GLU
1	F	61	GLU
1	F	72	GLN
1	F	104	LYS
1	F	144	LYS
1	F	193	ARG
1	F	240	LYS
1	F	241	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	68	GLN
1	B	72	GLN
1	B	186	HIS
1	C	68	GLN
1	D	46	ASN
1	D	68	GLN
1	D	69	ASN
1	F	68	GLN
1	F	72	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

6 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	ADP	A	3801	-	29,29,29	1.05	2 (6%)	45,45,45	1.90	6 (13%)
2	ADP	B	3802	-	29,29,29	1.11	2 (6%)	45,45,45	1.88	7 (15%)
2	ADP	C	3803	-	29,29,29	1.00	1 (3%)	45,45,45	1.90	7 (15%)
2	ADP	D	3804	-	29,29,29	1.07	2 (6%)	45,45,45	1.93	8 (17%)
2	ADP	E	3805	-	29,29,29	1.08	2 (6%)	45,45,45	1.85	6 (13%)
2	ADP	F	3806	-	29,29,29	1.09	2 (6%)	45,45,45	1.91	8 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	3801	-	-	0/16/32/32	0/1/3/3
2	ADP	B	3802	-	-	0/16/32/32	0/1/3/3
2	ADP	C	3803	-	-	0/16/32/32	0/1/3/3
2	ADP	D	3804	-	-	0/16/32/32	0/1/3/3
2	ADP	E	3805	-	-	0/16/32/32	0/1/3/3
2	ADP	F	3806	-	-	0/16/32/32	0/1/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3803	ADP	C4-N9	-3.33	1.32	1.37
2	E	3805	ADP	C4-N9	-3.14	1.33	1.37
2	A	3801	ADP	C4-N9	-3.04	1.33	1.37
2	B	3802	ADP	C4-N9	-3.02	1.33	1.37
2	B	3802	ADP	O4'-C1'	2.95	1.45	1.41
2	F	3806	ADP	C4-N9	-2.93	1.33	1.37
2	E	3805	ADP	O4'-C1'	2.86	1.45	1.41
2	D	3804	ADP	O4'-C1'	2.79	1.45	1.41
2	F	3806	ADP	O4'-C1'	2.52	1.45	1.41
2	D	3804	ADP	C4-N9	-2.52	1.34	1.37
2	A	3801	ADP	O4'-C1'	2.42	1.45	1.41

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3803	ADP	N3-C2-N1	-9.39	120.86	128.71
2	A	3801	ADP	N3-C2-N1	-9.37	120.88	128.71
2	F	3806	ADP	N3-C2-N1	-9.32	120.92	128.71
2	D	3804	ADP	N3-C2-N1	-9.29	120.94	128.71
2	B	3802	ADP	N3-C2-N1	-9.22	121.00	128.71
2	E	3805	ADP	N3-C2-N1	-9.10	121.10	128.71
2	B	3802	ADP	N3-C4-N9	4.72	133.95	125.43
2	D	3804	ADP	N3-C4-N9	4.71	133.94	125.43
2	F	3806	ADP	N3-C4-N9	4.66	133.85	125.43
2	E	3805	ADP	N3-C4-N9	4.54	133.63	125.43
2	C	3803	ADP	N3-C4-N9	4.45	133.47	125.43
2	A	3801	ADP	N3-C4-N9	4.38	133.34	125.43
2	A	3801	ADP	C4'-O4'-C1'	-3.95	105.46	109.75
2	D	3804	ADP	C4'-O4'-C1'	-3.39	106.07	109.75
2	C	3803	ADP	C4'-O4'-C1'	-2.90	106.59	109.75
2	D	3804	ADP	C5-C4-N3	-2.84	119.53	125.70
2	B	3802	ADP	C5-C4-N3	-2.79	119.63	125.70
2	C	3803	ADP	O4'-C1'-N9	-2.76	105.87	108.44
2	F	3806	ADP	C5-C4-N3	-2.76	119.69	125.70
2	F	3806	ADP	C4'-O4'-C1'	-2.75	106.76	109.75
2	E	3805	ADP	C5-C4-N3	-2.75	119.72	125.70
2	C	3803	ADP	C5-C4-N3	-2.67	119.89	125.70
2	A	3801	ADP	C5-C4-N3	-2.65	119.93	125.70
2	B	3802	ADP	C3'-C2'-C1'	2.52	104.86	100.91
2	D	3804	ADP	C2-N3-C4	2.48	121.08	114.01
2	D	3804	ADP	PA-O3A-PB	-2.48	124.41	131.68
2	E	3805	ADP	C4'-O4'-C1'	-2.48	107.06	109.75
2	B	3802	ADP	C4'-O4'-C1'	-2.48	107.06	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	3806	ADP	PA-O3A-PB	-2.44	124.53	131.68
2	E	3805	ADP	C3'-C2'-C1'	2.40	104.67	100.91
2	E	3805	ADP	C2-N3-C4	2.40	120.85	114.01
2	F	3806	ADP	C3'-C2'-C1'	2.38	104.64	100.91
2	C	3803	ADP	C2-N3-C4	2.38	120.78	114.01
2	B	3802	ADP	C2-N3-C4	2.37	120.75	114.01
2	F	3806	ADP	C2-N3-C4	2.34	120.66	114.01
2	A	3801	ADP	C2-N3-C4	2.33	120.65	114.01
2	D	3804	ADP	C3'-C2'-C1'	2.22	104.39	100.91
2	F	3806	ADP	O4'-C1'-N9	-2.20	106.39	108.44
2	B	3802	ADP	PA-O3A-PB	-2.19	125.25	131.68
2	A	3801	ADP	C3'-C2'-C1'	2.16	104.29	100.91
2	C	3803	ADP	C3'-C2'-C1'	2.12	104.22	100.91
2	D	3804	ADP	C4-C5-N7	-2.03	107.78	109.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	232/247 (93%)	0.47	10 (4%) 34 32	27, 50, 77, 97	0
1	B	240/247 (97%)	0.18	8 (3%) 44 44	26, 40, 63, 78	0
1	C	233/247 (94%)	0.21	5 (2%) 60 61	24, 40, 64, 80	0
1	D	242/247 (97%)	0.61	17 (7%) 16 15	27, 49, 74, 93	0
1	E	236/247 (95%)	0.40	16 (6%) 17 16	23, 43, 66, 83	0
1	F	236/247 (95%)	0.44	14 (5%) 22 21	27, 44, 69, 92	0
All	All	1419/1482 (95%)	0.38	70 (4%) 28 28	23, 44, 71, 97	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	174	VAL	8.6
1	C	102	TYR	7.7
1	F	182	PRO	6.7
1	D	128	ASN	6.5
1	D	102	TYR	6.4
1	F	102	TYR	6.2
1	F	99	SER	6.1
1	F	100	LYS	5.7
1	C	241	ARG	5.3
1	A	110	LEU	5.2
1	B	177	ARG	4.5
1	E	82	GLU	4.5
1	A	183	GLY	4.5
1	D	242	GLY	4.5
1	C	2	THR	4.4
1	D	45	TRP	4.3
1	E	98	LYS	4.2
1	A	102	TYR	4.2
1	B	174	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	78	LYS	4.0
1	D	97	GLY	3.9
1	E	97	GLY	3.9
1	E	245	LEU	3.8
1	B	175	GLY	3.8
1	D	182	PRO	3.6
1	F	128	ASN	3.5
1	E	175	GLY	3.4
1	D	99	SER	3.2
1	A	182	PRO	3.2
1	F	242	GLY	3.2
1	E	78	LYS	3.1
1	E	243	LYS	3.1
1	F	101	GLU	3.1
1	C	101	GLU	3.0
1	E	102	TYR	2.9
1	B	182	PRO	2.9
1	B	241	ARG	2.9
1	A	22	GLU	2.8
1	D	101	GLU	2.8
1	D	71	ALA	2.8
1	E	64	VAL	2.8
1	A	97	GLY	2.8
1	E	183	GLY	2.8
1	D	85	MET	2.7
1	E	79	PRO	2.7
1	A	108	HIS	2.7
1	A	85	MET	2.6
1	F	241	ARG	2.6
1	D	174	VAL	2.5
1	E	101	GLU	2.5
1	F	124	ILE	2.4
1	E	244	VAL	2.3
1	B	2	THR	2.3
1	E	110	LEU	2.3
1	F	97	GLY	2.2
1	D	98	LYS	2.2
1	D	100	LYS	2.2
1	E	229	LYS	2.2
1	A	5	VAL	2.2
1	D	201	GLY	2.2
1	B	242	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	98	LYS	2.1
1	D	96	ILE	2.1
1	A	184	VAL	2.1
1	B	213	ARG	2.1
1	D	83	LYS	2.1
1	D	20	ILE	2.0
1	C	68	GLN	2.0
1	F	77	VAL	2.0
1	F	240	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q < 0.9
2	ADP	B	3802	27/27	0.16	1.18	36,55,63,63	0
2	ADP	D	3804	27/27	0.14	0.25	44,50,60,61	0
2	ADP	F	3806	27/27	0.12	-0.20	35,44,48,49	0
2	ADP	E	3805	27/27	0.10	-0.39	31,41,45,45	0
2	ADP	A	3801	27/27	0.10	-0.50	31,36,40,42	0
2	ADP	C	3803	27/27	0.10	-0.81	30,35,40,42	0

6.5 Other polymers ⓘ

There are no such residues in this entry.