



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:31 AM GMT

PDB ID : 2RF4
Title : Crystal structure of the RNA Polymerase I subcomplex A14/43
Authors : Geiger, S.R.; Kuhn, C.D.; Cramer, P.
Deposited on : 2007-09-28
Resolution : 3.10 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>

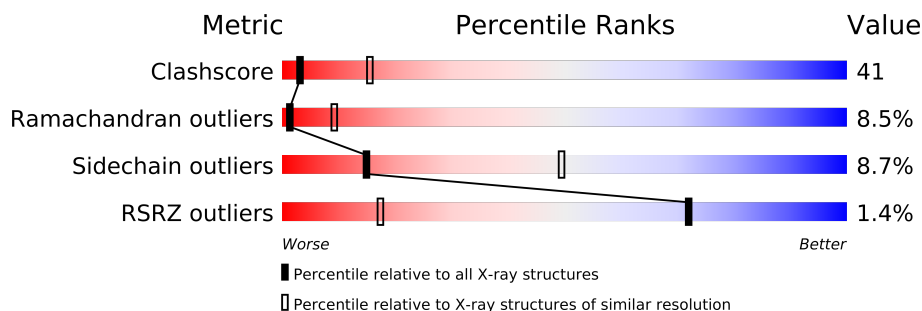
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.10 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))
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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	214	
1	C	214	
1	E	214	
2	B	87	
2	D	87	
2	F	87	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5530 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 DNA-directed RNA polymerase I subunit RPA4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	Se	0	0	0
			1363	877	234	247	2	3			
1	C	172	Total	C	N	O	S	Se	0	0	0
			1346	865	232	244	2	3			
1	E	175	Total	C	N	O	S	Se	0	0	0
			1373	881	239	248	2	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	INITIATING METHIONINE	UNP P46669
C	1	MSE	-	INITIATING METHIONINE	UNP P46669
E	1	MSE	-	INITIATING METHIONINE	UNP P46669

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	61	Total	C	N	O	0	0	0
			488	309	82	97			
2	D	60	Total	C	N	O	0	0	0
			480	303	81	96			
2	F	60	Total	C	N	O	0	0	0
			480	303	81	96			



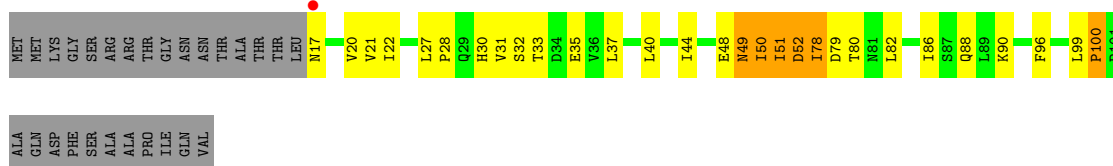
• Molecule 2: DNA-directed RNA polymerase I subunit RPA4

Chain B:



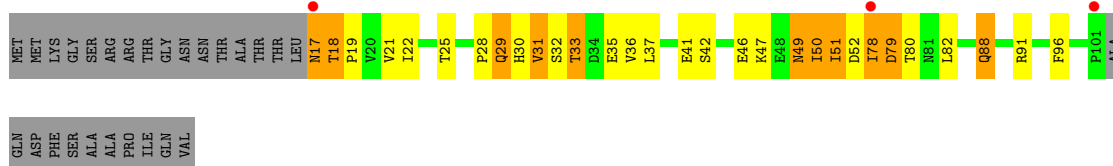
• Molecule 2: DNA-directed RNA polymerase I subunit RPA4

Chain D:



• Molecule 2: DNA-directed RNA polymerase I subunit RPA4

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	229.86Å 63.94Å 65.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.10 29.51 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-3.10) 99.7 (29.51-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.35 (at 3.11Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.252 , 0.285 0.260 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	77.2	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.7	EDS
Estimated twinning fraction	0.064 for -h,l,k	Xtriage
L-test for twinning	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 18175 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5530	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.45	0/1394	0.94	8/1894 (0.4%)
1	C	0.47	0/1375	0.84	4/1867 (0.2%)
1	E	0.47	0/1403	0.83	2/1906 (0.1%)
2	B	0.49	0/496	0.80	1/674 (0.1%)
2	D	0.45	0/488	0.74	0/663
2	F	0.44	0/488	0.73	1/663 (0.2%)
All	All	0.46	0/5644	0.84	16/7667 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	VAL	N-CA-C	-13.74	73.91	111.00
1	A	113	PHE	N-CA-C	7.84	132.18	111.00
1	A	216	HIS	N-CA-C	6.39	128.25	111.00
1	E	216	HIS	N-CA-C	6.31	128.03	111.00
2	F	51	ILE	N-CA-C	-6.15	94.39	111.00
1	A	222	GLY	N-CA-C	5.92	127.89	113.10
1	E	217	TRP	N-CA-C	5.89	126.91	111.00
1	A	114	GLY	N-CA-C	5.75	127.48	113.10
1	C	217	TRP	N-CA-C	5.73	126.48	111.00
1	C	216	HIS	N-CA-C	5.68	126.34	111.00
1	A	217	TRP	N-CA-C	5.62	126.18	111.00
1	C	144	HIS	N-CA-C	5.53	125.92	111.00
1	A	23	GLN	N-CA-C	5.22	125.10	111.00
1	C	125	TRP	N-CA-C	-5.21	96.92	111.00
1	A	125	TRP	N-CA-C	-5.18	97.02	111.00
2	B	51	ILE	N-CA-C	-5.09	97.26	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1363	0	1350	145	0
1	C	1346	0	1340	112	0
1	E	1373	0	1371	115	0
2	B	488	0	491	42	0
2	D	480	0	480	38	0
2	F	480	0	480	44	0
All	All	5530	0	5512	454	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 41.

All (454) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:30:GLU:CG	1:A:31:LYS:H	1.52	1.19
1:A:30:GLU:HG3	1:A:31:LYS:N	1.53	1.17
1:E:47:VAL:HG23	1:E:64:GLN:HE21	1.16	1.07
1:C:157:ILE:HD13	1:C:249:LEU:HD23	1.39	1.01
1:C:66:LEU:HD13	2:D:78:ILE:HD12	1.42	0.97
1:A:89:ILE:O	1:A:89:ILE:HD13	1.66	0.93
2:D:31:VAL:HG22	2:D:35:GLU:HB2	1.49	0.93
1:E:47:VAL:CG2	1:E:64:GLN:HE21	1.84	0.91
1:E:211:ASN:HD21	1:E:214:LEU:HD12	1.35	0.90
1:A:66:LEU:HD13	2:B:78:ILE:HD12	1.52	0.90
1:C:47:VAL:HG23	1:C:64:GLN:HE21	1.37	0.89
1:E:66:LEU:HD13	2:F:78:ILE:HD12	1.52	0.89
1:A:229:LEU:HD12	1:A:249:LEU:HD11	1.53	0.88
1:A:88:LYS:HE3	1:A:90:LEU:HD12	1.56	0.88
1:E:30:GLU:OE2	1:E:32:ASN:HB2	1.74	0.86
1:C:91:ASP:HB3	1:C:117:TRP:O	1.75	0.85
1:E:132:VAL:HG22	1:E:232:THR:HG22	1.57	0.85
1:A:30:GLU:HG3	1:A:31:LYS:H	0.69	0.84
1:E:157:ILE:HD13	1:E:249:LEU:HD23	1.61	0.83
2:D:32:SER:OG	2:D:35:GLU:HG3	1.78	0.83
1:C:47:VAL:CG2	1:C:64:GLN:HE21	1.91	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:50:ILE:HG22	2:D:51:ILE:H	1.43	0.82
2:B:50:ILE:HG22	2:B:51:ILE:H	1.44	0.82
1:A:154:ASN:HD22	1:A:242:VAL:HG11	1.45	0.81
1:C:157:ILE:CD1	1:C:249:LEU:HD23	2.10	0.81
2:F:31:VAL:HG23	2:F:35:GLU:HB2	1.60	0.81
1:A:142:ALA:HB2	1:A:168:PHE:CD2	2.16	0.81
2:B:79:ASP:CG	2:B:80:THR:H	1.85	0.81
1:A:210:GLY:HA3	1:A:213:SER:HA	1.62	0.80
1:C:141:SER:O	1:C:217:TRP:HZ3	1.64	0.80
1:C:144:HIS:ND1	1:C:144:HIS:O	2.15	0.79
2:F:79:ASP:CG	2:F:80:THR:H	1.85	0.79
1:E:36:ASN:HD22	1:E:37:CYS:N	1.80	0.78
2:B:50:ILE:HG22	2:B:51:ILE:N	1.97	0.77
2:D:79:ASP:CG	2:D:80:THR:H	1.88	0.77
1:C:142:ALA:HB2	1:C:168:PHE:CD2	2.20	0.77
1:E:47:VAL:HG23	1:E:64:GLN:NE2	1.98	0.76
1:A:36:ASN:HD22	1:A:37:CYS:N	1.83	0.76
1:A:47:VAL:CG2	1:A:64:GLN:HE21	1.98	0.76
1:E:46:TYR:HB3	2:F:21:VAL:CG2	2.16	0.75
1:A:154:ASN:ND2	1:A:242:VAL:HG11	2.00	0.75
1:C:89:ILE:O	1:C:91:ASP:N	2.19	0.75
1:C:50:ALA:HB3	1:C:53:TYR:HD2	1.52	0.75
1:C:132:VAL:HG22	1:C:232:THR:HG22	1.67	0.74
1:C:143:SER:H	1:C:217:TRP:HH2	1.34	0.74
1:C:143:SER:HA	1:C:159:LYS:HB2	1.69	0.74
1:C:163:PRO:O	1:C:164:VAL:HG12	1.87	0.73
2:B:100:PRO:HB2	2:B:101:PRO:HD2	1.69	0.73
2:D:50:ILE:HG22	2:D:51:ILE:N	2.04	0.73
1:C:89:ILE:O	1:C:89:ILE:HD13	1.89	0.72
1:C:163:PRO:HG2	1:C:166:TRP:CE2	2.24	0.72
1:E:163:PRO:O	1:E:164:VAL:HG12	1.89	0.72
1:E:157:ILE:CD1	1:E:249:LEU:HD23	2.21	0.71
1:E:66:LEU:HD21	2:F:47:LYS:HE3	1.70	0.71
1:C:229:LEU:HD12	1:C:249:LEU:HD11	1.72	0.71
1:E:213:SER:O	1:E:214:LEU:HG	1.90	0.71
1:A:163:PRO:O	1:A:164:VAL:HG12	1.90	0.71
1:E:89:ILE:O	1:E:89:ILE:HD13	1.90	0.70
1:A:47:VAL:CG2	1:A:64:GLN:HG2	2.21	0.70
2:D:31:VAL:CG2	2:D:35:GLU:HB2	2.20	0.70
2:F:17:ASN:O	2:F:19:PRO:HD3	1.91	0.70
1:A:143:SER:HA	1:A:159:LYS:HB2	1.73	0.69
1:E:141:SER:O	1:E:217:TRP:HZ3	1.75	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:53:TYR:CZ	1:A:63:LYS:HD2	2.27	0.69
1:A:46:TYR:HB3	2:B:21:VAL:CG2	2.20	0.69
1:E:65:HIS:HA	1:E:69:LEU:HD12	1.74	0.69
2:F:37:LEU:HD13	2:F:96:PHE:HB3	1.76	0.67
1:A:157:ILE:HD13	1:A:249:LEU:HD23	1.76	0.67
2:F:78:ILE:HD13	2:F:78:ILE:O	1.95	0.67
1:A:89:ILE:O	1:A:91:ASP:N	2.27	0.67
1:C:90:LEU:O	1:C:92:ALA:N	2.26	0.67
1:A:154:ASN:HD22	1:A:242:VAL:CG1	2.08	0.67
1:C:88:LYS:CE	1:C:90:LEU:HD12	2.25	0.67
1:C:76:LYS:HD2	2:D:22:ILE:HD12	1.76	0.67
1:A:62:MSE:HE2	1:A:84:TYR:HE2	1.60	0.66
1:A:162:ILE:CG2	1:A:163:PRO:HD2	2.25	0.66
1:E:76:LYS:HD2	2:F:22:ILE:HD12	1.77	0.66
2:F:18:THR:O	2:F:18:THR:HG23	1.95	0.65
2:F:32:SER:OG	2:F:35:GLU:HG3	1.96	0.65
2:D:37:LEU:HD13	2:D:96:PHE:HB3	1.78	0.65
1:C:47:VAL:HG23	1:C:64:GLN:NE2	2.10	0.65
1:E:90:LEU:O	1:E:92:ALA:N	2.21	0.65
1:E:36:ASN:ND2	1:E:38:ILE:H	1.94	0.65
1:E:143:SER:O	1:E:144:HIS:HB3	1.96	0.65
2:D:49:ASN:HD22	2:D:50:ILE:H	1.44	0.64
1:C:143:SER:O	1:C:144:HIS:HB3	1.96	0.64
1:C:46:TYR:HB3	2:D:21:VAL:CG2	2.27	0.64
2:F:49:ASN:HD22	2:F:50:ILE:H	1.46	0.64
2:B:91:ARG:HG2	2:B:91:ARG:HH11	1.63	0.63
1:E:139:ILE:O	1:E:139:ILE:HD12	1.98	0.63
1:E:169:VAL:HG22	1:E:170:HIS:N	2.13	0.63
1:E:24:VAL:HG21	2:F:28:PRO:HB2	1.80	0.63
2:B:78:ILE:O	2:B:78:ILE:HD13	1.98	0.63
1:E:39:VAL:HG11	2:F:28:PRO:HB3	1.79	0.63
1:E:71:MSE:HE2	2:F:88:GLN:HG2	1.80	0.63
1:A:132:VAL:HG22	1:A:232:THR:HG22	1.81	0.62
1:A:119:HIS:HE1	2:B:25:THR:OG1	1.82	0.62
2:B:49:ASN:HD22	2:B:50:ILE:H	1.48	0.62
1:E:218:VAL:HG13	1:E:223:GLU:C	2.19	0.62
1:A:66:LEU:HD22	2:B:82:LEU:CD2	2.29	0.62
1:A:157:ILE:CD1	1:A:249:LEU:HD23	2.30	0.62
1:A:210:GLY:HA3	1:A:213:SER:CA	2.30	0.61
1:A:88:LYS:CE	1:A:90:LEU:HD12	2.30	0.61
1:A:143:SER:H	1:A:217:TRP:HH2	1.46	0.61
1:A:23:GLN:HE21	1:A:25:THR:HA	1.66	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:62:MSE:O	1:E:66:LEU:HB2	2.00	0.61
2:D:50:ILE:CG2	2:D:51:ILE:H	2.12	0.61
1:C:47:VAL:CG2	1:C:64:GLN:HG2	2.30	0.61
2:F:52:ASP:CG	2:F:78:ILE:N	2.54	0.61
1:E:157:ILE:HD13	1:E:249:LEU:CD2	2.29	0.61
1:E:119:HIS:HE1	2:F:25:THR:OG1	1.84	0.61
1:C:29:ASP:C	1:C:30:GLU:HG3	2.20	0.61
1:A:142:ALA:O	1:A:143:SER:HB3	2.00	0.61
1:C:218:VAL:HG13	1:C:223:GLU:C	2.22	0.61
1:C:36:ASN:HD22	1:C:37:CYS:N	1.98	0.61
1:E:90:LEU:C	1:E:92:ALA:H	2.03	0.61
1:A:218:VAL:HG13	1:A:223:GLU:C	2.21	0.61
1:A:143:SER:O	1:A:144:HIS:HB3	2.00	0.60
1:C:47:VAL:HG23	1:C:64:GLN:HG2	1.84	0.60
1:C:49:LEU:HD21	1:C:57:PRO:HB3	1.83	0.60
2:D:49:ASN:ND2	2:D:50:ILE:H	1.99	0.60
1:A:141:SER:O	1:A:217:TRP:HZ3	1.84	0.60
1:C:142:ALA:O	1:C:143:SER:HB3	2.01	0.60
1:C:28:ILE:HA	1:C:35:SER:HA	1.83	0.60
1:A:80:VAL:HB	1:A:125:TRP:HB3	1.83	0.60
1:C:120:VAL:HG22	1:C:121:ASN:N	2.16	0.60
1:A:140:GLN:HE22	1:A:225:ILE:HG12	1.67	0.60
1:E:48:SER:HA	1:E:115:PHE:CD1	2.37	0.59
1:E:46:TYR:HB3	2:F:21:VAL:HG23	1.83	0.59
1:C:162:ILE:CG2	1:C:163:PRO:HD2	2.32	0.59
1:C:71:MSE:HE2	2:D:88:GLN:HG2	1.84	0.59
1:C:88:LYS:HE2	1:C:90:LEU:HD12	1.84	0.59
2:B:79:ASP:CG	2:B:80:THR:N	2.56	0.59
1:A:47:VAL:HG23	1:A:64:GLN:HG2	1.83	0.59
1:C:88:LYS:HG2	1:C:90:LEU:HB2	1.84	0.59
1:E:67:ASN:N	1:E:68:PRO:CD	2.66	0.59
1:A:62:MSE:HE2	1:A:84:TYR:CE2	2.37	0.59
2:F:79:ASP:CG	2:F:80:THR:N	2.54	0.59
1:A:30:GLU:CG	1:A:31:LYS:N	2.28	0.58
2:B:49:ASN:HD22	2:B:50:ILE:N	2.01	0.58
2:F:17:ASN:N	2:F:17:ASN:HD22	2.01	0.58
1:E:224:PRO:O	1:E:225:ILE:C	2.42	0.58
1:A:47:VAL:HG21	1:A:64:GLN:HG2	1.84	0.57
1:C:62:MSE:HE2	1:C:84:TYR:HE2	1.67	0.57
1:E:132:VAL:CG2	1:E:232:THR:HG22	2.33	0.57
1:A:162:ILE:HG22	1:A:163:PRO:HD2	1.86	0.57
1:E:26:ASN:HB3	1:E:36:ASN:O	2.03	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:80:THR:O	2:F:80:THR:HG22	2.03	0.57
1:A:61:VAL:O	1:A:64:GLN:HB3	2.04	0.57
1:A:46:TYR:HB3	2:B:21:VAL:HG22	1.86	0.57
1:C:139:ILE:O	1:C:139:ILE:HD12	2.04	0.57
1:A:67:ASN:O	1:A:68:PRO:C	2.43	0.57
2:B:50:ILE:CG2	2:B:51:ILE:N	2.68	0.57
2:B:37:LEU:HD13	2:B:96:PHE:HB3	1.87	0.57
1:C:162:ILE:HG23	1:C:163:PRO:HD2	1.87	0.56
2:B:32:SER:OG	2:B:35:GLU:HG3	2.04	0.56
2:D:82:LEU:O	2:D:86:ILE:HG13	2.06	0.56
1:E:89:ILE:O	1:E:91:ASP:N	2.38	0.56
1:A:90:LEU:O	1:A:92:ALA:N	2.34	0.56
1:E:137:ILE:HD11	1:E:225:ILE:HG13	1.87	0.56
1:E:211:ASN:HD21	1:E:214:LEU:CD1	2.13	0.56
1:E:211:ASN:ND2	1:E:214:LEU:HD12	2.14	0.56
1:A:120:VAL:HG22	1:A:121:ASN:N	2.21	0.56
1:C:67:ASN:O	1:C:68:PRO:C	2.41	0.56
1:A:112:PRO:O	1:A:113:PHE:HB2	2.04	0.56
2:B:50:ILE:O	2:B:51:ILE:HB	2.05	0.56
1:E:162:ILE:HG23	1:E:163:PRO:HD2	1.88	0.56
1:A:120:VAL:HG22	1:A:121:ASN:H	1.71	0.56
1:A:84:TYR:HB2	1:A:120:VAL:HG21	1.87	0.55
1:C:25:THR:HA	1:C:128:GLN:HE22	1.71	0.55
1:E:66:LEU:HD21	2:F:47:LYS:CE	2.36	0.55
1:C:140:GLN:HE22	1:C:225:ILE:HG12	1.71	0.55
1:E:91:ASP:OD2	1:E:117:TRP:HB3	2.07	0.55
1:C:224:PRO:O	1:C:225:ILE:C	2.45	0.55
1:E:50:ALA:HB3	1:E:53:TYR:HD2	1.70	0.55
1:C:66:LEU:HD22	2:D:82:LEU:HD22	1.88	0.55
1:A:57:PRO:O	1:A:61:VAL:HG23	2.07	0.55
2:B:88:GLN:O	2:B:91:ARG:HB2	2.07	0.55
1:C:66:LEU:HD22	2:D:82:LEU:CD2	2.36	0.55
2:B:52:ASP:OD1	2:B:78:ILE:N	2.25	0.55
1:A:73:TYR:CD1	1:A:74:ASN:N	2.75	0.55
1:C:144:HIS:CG	1:C:144:HIS:O	2.60	0.55
1:E:21:LYS:NZ	1:E:23:GLN:NE2	2.55	0.55
1:A:66:LEU:HD22	2:B:82:LEU:HD22	1.89	0.55
1:E:71:MSE:HE1	1:E:153:PHE:CE2	2.41	0.55
1:E:169:VAL:CG2	1:E:170:HIS:N	2.69	0.54
1:C:67:ASN:N	1:C:68:PRO:CD	2.70	0.54
1:A:46:TYR:HB2	1:A:117:TRP:CH2	2.43	0.54
2:F:17:ASN:ND2	2:F:17:ASN:N	2.56	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:157:ILE:HD13	1:A:249:LEU:CD2	2.37	0.54
2:B:50:ILE:CG2	2:B:51:ILE:H	2.15	0.54
1:E:141:SER:O	1:E:143:SER:N	2.40	0.54
1:A:50:ALA:HB3	1:A:53:TYR:CD2	2.42	0.54
1:C:92:ALA:O	1:C:93:ASP:HB2	2.07	0.54
1:A:142:ALA:HB2	1:A:168:PHE:CE2	2.42	0.54
1:A:59:GLN:NE2	1:A:59:GLN:HA	2.22	0.54
1:A:47:VAL:HG23	1:A:64:GLN:HE21	1.71	0.54
1:E:66:LEU:O	1:E:70:VAL:HG23	2.08	0.54
1:A:53:TYR:OH	1:A:63:LYS:HD2	2.06	0.54
1:A:242:VAL:HG12	1:A:243:VAL:O	2.08	0.54
1:A:172:ASP:HB2	1:A:214:LEU:CD1	2.37	0.54
2:F:78:ILE:CD1	2:F:82:LEU:HD22	2.38	0.53
2:D:79:ASP:CG	2:D:80:THR:N	2.57	0.53
1:A:147:LEU:HB2	1:A:155:ALA:HB3	1.89	0.53
2:B:91:ARG:HG2	2:B:91:ARG:NH1	2.23	0.53
1:C:154:ASN:HD22	1:C:242:VAL:HG11	1.74	0.53
1:A:67:ASN:N	1:A:68:PRO:CD	2.71	0.53
1:C:50:ALA:HB3	1:C:53:TYR:CD2	2.38	0.53
1:E:126:GLN:O	1:E:126:GLN:HG2	2.08	0.53
1:A:171:ASN:C	1:A:210:GLY:H	2.12	0.53
1:A:140:GLN:HE22	1:A:225:ILE:CG1	2.22	0.53
1:A:27:PRO:HD2	2:B:30:HIS:CE1	2.44	0.53
1:E:144:HIS:O	1:E:144:HIS:ND1	2.41	0.53
1:E:141:SER:O	1:E:217:TRP:CZ3	2.60	0.53
1:C:76:LYS:NZ	2:D:20:VAL:O	2.42	0.53
1:A:234:ARG:HH11	1:A:248:THR:HG21	1.72	0.53
1:A:62:MSE:HA	1:A:65:HIS:HB2	1.91	0.52
1:A:162:ILE:HG23	1:A:163:PRO:HD2	1.91	0.52
1:C:163:PRO:HB2	1:C:166:TRP:CD1	2.44	0.52
1:C:88:LYS:HE3	1:C:90:LEU:HD12	1.92	0.52
1:E:30:GLU:OE1	1:E:32:ASN:N	2.41	0.52
1:A:66:LEU:HD21	2:B:47:LYS:HD2	1.92	0.52
1:A:23:GLN:CG	1:A:25:THR:HA	2.39	0.52
1:A:32:ASN:N	1:A:32:ASN:HD22	2.06	0.52
1:E:42:PRO:HG3	1:E:121:ASN:OD1	2.09	0.52
1:A:76:LYS:HD2	2:B:22:ILE:HD12	1.92	0.52
1:C:89:ILE:C	1:C:91:ASP:N	2.63	0.52
1:A:47:VAL:HG23	1:A:64:GLN:NE2	2.24	0.52
2:D:50:ILE:CG2	2:D:51:ILE:N	2.71	0.52
1:E:120:VAL:HG22	1:E:121:ASN:N	2.25	0.52
2:D:78:ILE:CD1	2:D:82:LEU:HD22	2.40	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:66:LEU:C	1:A:68:PRO:HD2	2.29	0.52
1:C:142:ALA:HB2	1:C:168:PHE:CE2	2.45	0.52
1:A:28:ILE:HA	1:A:35:SER:HA	1.91	0.52
1:E:146:GLY:O	1:E:147:LEU:HD23	2.10	0.52
1:C:171:ASN:HB2	1:C:214:LEU:HB2	1.92	0.52
1:E:24:VAL:O	1:E:25:THR:C	2.48	0.51
1:A:139:ILE:O	1:A:139:ILE:HD12	2.10	0.51
1:A:210:GLY:CA	1:A:213:SER:HA	2.36	0.51
2:B:36:VAL:HG13	2:B:37:LEU:N	2.24	0.51
1:A:144:HIS:O	1:A:144:HIS:CG	2.63	0.51
2:F:49:ASN:ND2	2:F:50:ILE:H	2.08	0.51
2:B:27:LEU:HD23	2:B:28:PRO:O	2.10	0.51
1:C:51:PRO:HA	1:C:54:LEU:HD23	1.92	0.51
1:A:157:ILE:HG13	1:A:157:ILE:O	2.11	0.51
1:E:238:THR:O	1:E:239:THR:HB	2.11	0.51
1:C:46:TYR:HB3	2:D:21:VAL:HG22	1.92	0.50
1:E:241:ARG:HG3	1:E:241:ARG:HH11	1.76	0.50
1:A:46:TYR:O	2:B:20:VAL:HG23	2.11	0.50
1:A:141:SER:O	1:A:217:TRP:CZ3	2.64	0.50
1:A:53:TYR:OH	1:A:63:LYS:CD	2.60	0.50
1:E:38:ILE:HD12	1:E:38:ILE:N	2.27	0.50
1:E:142:ALA:O	1:E:217:TRP:CH2	2.65	0.50
1:C:126:GLN:HG2	1:C:126:GLN:O	2.12	0.50
1:A:66:LEU:HD22	2:B:82:LEU:HD21	1.93	0.50
1:A:26:ASN:HD22	2:B:30:HIS:CE1	2.30	0.50
1:E:154:ASN:ND2	1:E:242:VAL:HG11	2.27	0.49
1:A:140:GLN:NE2	1:A:225:ILE:HG12	2.27	0.49
2:F:49:ASN:HD22	2:F:50:ILE:N	2.09	0.49
1:C:63:LYS:HG3	1:C:63:LYS:O	2.12	0.49
1:A:89:ILE:C	1:A:89:ILE:HD13	2.32	0.49
1:A:89:ILE:C	1:A:91:ASP:H	2.16	0.49
2:F:36:VAL:HG13	2:F:37:LEU:N	2.28	0.49
1:E:137:ILE:CD1	1:E:225:ILE:HG13	2.43	0.49
1:E:165:ASP:OD1	1:E:220:SER:HB3	2.13	0.49
1:A:50:ALA:HB3	1:A:53:TYR:HD2	1.78	0.49
1:C:86:GLY:O	1:C:87:LEU:C	2.52	0.48
1:E:51:PRO:HA	1:E:54:LEU:HD23	1.94	0.48
1:E:66:LEU:HD22	2:F:82:LEU:CD2	2.43	0.48
1:E:36:ASN:HD22	1:E:36:ASN:C	2.10	0.48
1:C:26:ASN:HD22	2:D:30:HIS:CE1	2.31	0.48
1:C:65:HIS:O	1:C:69:LEU:HB2	2.13	0.48
1:A:62:MSE:O	1:A:66:LEU:HB2	2.12	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:163:PRO:HG2	1:A:166:TRP:CE2	2.48	0.48
1:A:36:ASN:HD22	1:A:36:ASN:C	2.12	0.48
1:A:48:SER:HA	1:A:115:PHE:CD1	2.48	0.48
1:E:36:ASN:HD21	1:E:38:ILE:H	1.61	0.48
1:C:157:ILE:HD13	1:C:249:LEU:CD2	2.29	0.48
1:C:89:ILE:C	1:C:91:ASP:H	2.17	0.48
1:A:36:ASN:ND2	1:A:38:ILE:H	2.12	0.48
1:E:218:VAL:HG12	1:E:222:GLY:HA2	1.94	0.48
2:D:32:SER:HG	2:D:35:GLU:HG3	1.77	0.48
1:C:87:LEU:HD13	1:C:87:LEU:C	2.34	0.48
1:C:90:LEU:C	1:C:92:ALA:H	2.17	0.48
1:E:218:VAL:HG13	1:E:223:GLU:O	2.13	0.48
1:E:47:VAL:HG22	1:E:48:SER:N	2.29	0.48
1:C:91:ASP:HB3	1:C:117:TRP:C	2.33	0.47
2:F:17:ASN:O	2:F:19:PRO:CD	2.61	0.47
1:C:46:TYR:O	2:D:20:VAL:HG23	2.14	0.47
1:A:241:ARG:HH11	1:A:241:ARG:HG3	1.79	0.47
1:C:62:MSE:O	1:C:66:LEU:HB2	2.14	0.47
2:F:41:GLU:HA	2:F:41:GLU:OE1	2.13	0.47
1:C:165:ASP:OD1	1:C:220:SER:HB3	2.14	0.47
1:C:91:ASP:OD1	1:C:91:ASP:O	2.32	0.47
1:E:26:ASN:ND2	2:F:30:HIS:CE1	2.82	0.47
1:C:154:ASN:ND2	1:C:242:VAL:HG11	2.29	0.47
1:E:120:VAL:HG22	1:E:121:ASN:H	1.79	0.47
1:A:89:ILE:C	1:A:91:ASP:N	2.68	0.47
1:A:71:MSE:HE2	2:B:88:GLN:HG2	1.97	0.47
1:C:26:ASN:ND2	2:D:30:HIS:HE1	2.13	0.47
1:E:132:VAL:O	1:E:132:VAL:HG12	2.13	0.47
1:E:93:ASP:C	1:E:95:LEU:H	2.17	0.47
1:A:58:LEU:HD13	1:A:89:ILE:HG22	1.97	0.47
2:D:49:ASN:HD22	2:D:50:ILE:N	2.12	0.47
1:E:162:ILE:CG2	1:E:163:PRO:HD2	2.44	0.47
1:C:141:SER:O	1:C:217:TRP:CZ3	2.56	0.47
2:F:50:ILE:HG13	2:F:51:ILE:HG13	1.96	0.47
1:E:67:ASN:O	1:E:68:PRO:C	2.54	0.47
1:A:33:GLY:HA3	1:A:230:ARG:NH1	2.30	0.47
2:D:44:ILE:HD13	2:D:90:LYS:HG2	1.97	0.47
1:A:211:ASN:N	1:A:213:SER:HA	2.30	0.46
1:C:47:VAL:HG22	1:C:48:SER:N	2.30	0.46
2:B:49:ASN:ND2	2:B:50:ILE:N	2.64	0.46
1:A:140:GLN:OE1	1:A:225:ILE:HD11	2.14	0.46
1:E:87:LEU:HD23	1:E:120:VAL:HB	1.96	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:17:ASN:O	2:B:17:ASN:CG	2.53	0.46
1:E:90:LEU:C	1:E:92:ALA:N	2.67	0.46
1:C:218:VAL:HG12	1:C:222:GLY:HA2	1.97	0.46
2:D:48:GLU:OE2	2:D:90:LYS:NZ	2.44	0.46
2:F:49:ASN:ND2	2:F:50:ILE:N	2.64	0.46
1:C:36:ASN:HD22	1:C:36:ASN:C	2.19	0.46
1:C:171:ASN:HB2	1:C:214:LEU:H	1.81	0.46
1:C:120:VAL:CG2	1:C:121:ASN:N	2.79	0.46
2:B:80:THR:O	2:B:82:LEU:N	2.49	0.46
1:C:89:ILE:HD13	1:C:89:ILE:C	2.36	0.46
1:A:172:ASP:C	1:A:214:LEU:HD12	2.36	0.46
1:A:141:SER:O	1:A:142:ALA:C	2.55	0.45
1:A:144:HIS:CD2	1:A:156:SER:HB2	2.50	0.45
1:E:168:PHE:CZ	1:E:215:GLY:HA3	2.50	0.45
2:D:49:ASN:ND2	2:D:50:ILE:N	2.64	0.45
1:A:36:ASN:C	1:A:36:ASN:ND2	2.70	0.45
1:A:47:VAL:CG2	1:A:64:GLN:NE2	2.74	0.45
1:A:53:TYR:CE1	1:A:63:LYS:NZ	2.84	0.45
1:A:218:VAL:HG12	1:A:222:GLY:HA2	1.98	0.45
1:E:147:LEU:HB2	1:E:155:ALA:HB3	1.97	0.45
2:D:27:LEU:HD23	2:D:28:PRO:O	2.16	0.45
1:A:224:PRO:O	1:A:225:ILE:C	2.54	0.45
1:C:87:LEU:HD13	1:C:88:LYS:N	2.32	0.45
1:A:66:LEU:O	1:A:67:ASN:C	2.56	0.45
1:E:66:LEU:HG	1:E:84:TYR:OH	2.17	0.45
1:E:239:THR:HG23	1:E:239:THR:O	2.17	0.45
1:A:48:SER:HA	1:A:115:PHE:HD1	1.81	0.45
1:C:65:HIS:CE1	1:C:120:VAL:HG11	2.52	0.45
1:A:49:LEU:HD21	1:A:57:PRO:HB3	1.99	0.45
2:D:31:VAL:CG2	2:D:35:GLU:CB	2.92	0.45
1:E:61:VAL:O	1:E:64:GLN:HB3	2.17	0.44
1:E:53:TYR:OH	1:E:63:LYS:HD2	2.17	0.44
1:A:159:LYS:HA	1:A:162:ILE:HD12	1.99	0.44
1:A:76:LYS:NZ	2:B:20:VAL:O	2.51	0.44
1:E:84:TYR:HB3	1:E:122:LEU:HD23	2.00	0.44
1:A:26:ASN:HB3	1:A:36:ASN:O	2.18	0.44
1:E:169:VAL:HG22	1:E:170:HIS:O	2.18	0.44
1:A:41:VAL:HG13	1:A:122:LEU:HB2	1.98	0.44
1:A:249:LEU:O	1:A:250:ILE:C	2.55	0.44
1:E:36:ASN:C	1:E:36:ASN:ND2	2.70	0.44
1:A:50:ALA:HB1	1:A:51:PRO:HD2	1.99	0.44
1:E:65:HIS:HB3	1:E:84:TYR:CE1	2.52	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:36:ASN:ND2	1:A:37:CYS:N	2.61	0.44
1:A:128:GLN:HB2	1:A:128:GLN:HE21	1.51	0.44
2:F:91:ARG:HG2	2:F:91:ARG:HH11	1.83	0.44
2:B:36:VAL:HG11	2:B:96:PHE:CE2	2.52	0.44
1:C:171:ASN:C	1:C:210:GLY:N	2.71	0.44
2:B:41:GLU:HA	2:B:41:GLU:OE1	2.17	0.44
1:A:84:TYR:HB2	1:A:120:VAL:CG2	2.48	0.43
1:E:34:THR:HG23	1:E:132:VAL:O	2.18	0.43
1:C:61:VAL:HG12	1:C:65:HIS:CD2	2.52	0.43
1:E:26:ASN:HD22	2:F:30:HIS:CE1	2.37	0.43
1:A:23:GLN:NE2	1:A:25:THR:HA	2.32	0.43
1:E:41:VAL:HG22	1:E:41:VAL:O	2.17	0.43
1:C:40:ARG:NH2	1:C:121:ASN:ND2	2.65	0.43
1:C:66:LEU:HG	1:C:84:TYR:OH	2.18	0.43
1:E:47:VAL:CG2	1:E:64:GLN:HG2	2.48	0.43
1:C:62:MSE:HE2	1:C:84:TYR:CE2	2.51	0.43
1:C:38:ILE:HD12	1:C:38:ILE:N	2.33	0.43
1:A:143:SER:N	1:A:217:TRP:HH2	2.14	0.43
1:C:168:PHE:CZ	1:C:215:GLY:HA3	2.54	0.43
1:A:23:GLN:HG3	1:A:128:GLN:NE2	2.33	0.43
1:A:73:TYR:C	1:A:73:TYR:CD1	2.92	0.43
1:E:226:ASP:CG	1:E:227:GLY:N	2.71	0.43
1:E:29:ASP:C	1:E:30:GLU:HG3	2.39	0.43
1:C:242:VAL:HG12	1:C:243:VAL:O	2.19	0.43
1:C:147:LEU:HB2	1:C:155:ALA:HB3	2.01	0.43
1:E:57:PRO:O	1:E:61:VAL:HG23	2.19	0.43
1:A:217:TRP:O	1:A:225:ILE:HG13	2.18	0.43
1:C:163:PRO:O	1:C:164:VAL:CG1	2.63	0.43
1:A:231:PHE:CD1	1:A:247:GLY:HA3	2.53	0.43
2:B:50:ILE:O	2:B:51:ILE:CB	2.67	0.43
1:E:89:ILE:C	1:E:91:ASP:H	2.23	0.43
1:A:163:PRO:O	1:A:164:VAL:CG1	2.64	0.42
1:E:49:LEU:HD21	1:E:57:PRO:HB3	2.00	0.42
1:E:163:PRO:HG2	1:E:166:TRP:CE2	2.54	0.42
1:E:242:VAL:HG12	1:E:243:VAL:O	2.19	0.42
2:D:99:LEU:HA	2:D:100:PRO:HD3	1.75	0.42
1:E:28:ILE:HA	1:E:35:SER:HA	2.00	0.42
1:C:47:VAL:HG21	1:C:64:GLN:HG2	2.01	0.42
2:F:52:ASP:CG	2:F:78:ILE:H	2.20	0.42
1:C:143:SER:N	1:C:217:TRP:HH2	2.07	0.42
1:E:142:ALA:C	1:E:217:TRP:CH2	2.93	0.42
1:C:128:GLN:N	1:C:131:ASP:OD2	2.48	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:47:LYS:HA	2:F:47:LYS:HD3	1.78	0.42
2:F:29:GLN:HE21	2:F:29:GLN:HB2	1.66	0.42
1:C:48:SER:HA	1:C:115:PHE:CD1	2.55	0.42
1:C:61:VAL:O	1:C:64:GLN:HB3	2.20	0.42
1:A:91:ASP:O	1:A:117:TRP:HB2	2.20	0.42
2:F:33:THR:O	2:F:36:VAL:HG12	2.20	0.42
1:E:53:TYR:CE2	1:E:63:LYS:HD3	2.55	0.42
1:C:241:ARG:HH11	1:C:241:ARG:HG3	1.83	0.42
1:C:84:TYR:HB2	1:C:120:VAL:HG21	2.02	0.42
1:E:89:ILE:C	1:E:89:ILE:HD13	2.40	0.42
1:C:218:VAL:CG1	1:C:223:GLU:N	2.83	0.42
1:C:133:LEU:HD13	1:C:149:ILE:HD13	2.01	0.42
1:E:47:VAL:HG23	1:E:64:GLN:HG2	2.00	0.42
1:A:157:ILE:CG1	1:A:157:ILE:O	2.68	0.42
1:E:225:ILE:HA	1:E:225:ILE:HD12	1.86	0.41
1:A:157:ILE:HG21	1:A:249:LEU:HD23	2.01	0.41
1:A:51:PRO:HA	1:A:54:LEU:HD23	2.02	0.41
2:F:18:THR:CG2	2:F:18:THR:O	2.66	0.41
2:D:17:ASN:ND2	2:D:17:ASN:O	2.53	0.41
1:A:145:ILE:HG22	1:A:146:GLY:N	2.35	0.41
1:C:217:TRP:O	1:C:225:ILE:HG23	2.20	0.41
2:F:42:SER:O	2:F:46:GLU:HB2	2.19	0.41
1:C:143:SER:N	1:C:217:TRP:CH2	2.86	0.41
1:E:163:PRO:O	1:E:164:VAL:CG1	2.64	0.41
1:E:39:VAL:CG1	2:F:28:PRO:HB3	2.48	0.41
1:E:211:ASN:C	1:E:212:ARG:O	2.57	0.41
2:F:50:ILE:O	2:F:51:ILE:HB	2.20	0.41
1:A:137:ILE:HD13	1:A:225:ILE:HB	2.02	0.41
2:B:100:PRO:CB	2:B:101:PRO:HD2	2.43	0.41
1:C:171:ASN:C	1:C:210:GLY:H	2.23	0.41
1:E:50:ALA:HB3	1:E:53:TYR:CD2	2.54	0.41
2:D:50:ILE:C	2:D:52:ASP:N	2.69	0.41
2:D:52:ASP:OD1	2:D:52:ASP:C	2.59	0.41
1:C:26:ASN:HB3	1:C:36:ASN:O	2.21	0.41
1:A:58:LEU:HD13	1:A:89:ILE:CG2	2.51	0.41
1:A:166:TRP:CD1	1:A:219:ASP:HB2	2.56	0.41
1:C:90:LEU:C	1:C:92:ALA:N	2.72	0.41
1:A:128:GLN:O	1:A:131:ASP:OD2	2.39	0.41
1:A:66:LEU:HA	1:A:66:LEU:HD23	1.87	0.41
1:A:39:VAL:HG21	2:B:28:PRO:HB3	2.03	0.41
1:E:47:VAL:CG2	1:E:64:GLN:NE2	2.68	0.40
1:C:148:LEU:HA	1:C:148:LEU:HD23	1.80	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:46:TYR:HB2	1:A:117:TRP:CZ2	2.56	0.40
1:A:71:MSE:HE1	1:A:153:PHE:CE2	2.55	0.40
2:D:40:LEU:HA	2:D:40:LEU:HD23	1.85	0.40
1:A:31:LYS:O	1:A:31:LYS:HD3	2.21	0.40
1:E:66:LEU:HD22	2:F:82:LEU:HD22	2.03	0.40
1:C:36:ASN:C	1:C:36:ASN:ND2	2.75	0.40
1:E:36:ASN:ND2	1:E:37:CYS:N	2.60	0.40
1:E:53:TYR:HE2	1:E:63:LYS:HD3	1.86	0.40
1:A:159:LYS:HA	1:A:162:ILE:CD1	2.51	0.40
1:C:29:ASP:OD1	1:C:30:GLU:HG3	2.21	0.40
1:C:71:MSE:HE2	2:D:88:GLN:CG	2.50	0.40
1:A:172:ASP:HB2	1:A:214:LEU:HD12	2.03	0.40
2:B:29:GLN:HB2	2:B:29:GLN:HE21	1.68	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	168/214 (78%)	129 (77%)	25 (15%)	14 (8%)	1	9
1	C	166/214 (78%)	130 (78%)	23 (14%)	13 (8%)	1	11
1	E	171/214 (80%)	131 (77%)	21 (12%)	19 (11%)	1	5
2	B	59/87 (68%)	52 (88%)	2 (3%)	5 (8%)	1	9
2	D	58/87 (67%)	49 (84%)	5 (9%)	4 (7%)	2	13
2	F	58/87 (67%)	49 (84%)	6 (10%)	3 (5%)	3	21
All	All	680/903 (75%)	540 (79%)	82 (12%)	58 (8%)	1	9

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	LEU
1	A	164	VAL

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Mol	Chain	Res	Type
1	A	226	ASP
1	C	66	LEU
1	C	90	LEU
1	C	91	ASP
1	C	163	PRO
1	C	164	VAL
1	C	225	ILE
1	E	66	LEU
1	E	90	LEU
1	E	91	ASP
1	E	142	ALA
1	E	164	VAL
1	E	226	ASP
1	A	90	LEU
1	A	114	GLY
1	A	172	ASP
1	A	217	TRP
1	A	225	ILE
1	A	240	GLY
2	B	81	ASN
1	C	226	ASP
1	C	240	GLY
1	E	163	PRO
1	E	217	TRP
1	E	225	ILE
1	E	240	GLY
2	F	50	ILE
2	B	79	ASP
1	C	25	THR
1	C	144	HIS
1	C	217	TRP
2	D	52	ASP
2	D	100	PRO
1	E	25	THR
1	E	139	ILE
1	E	212	ARG
1	E	242	VAL
2	F	18	THR
1	A	144	HIS
1	C	239	THR
1	E	23	GLN
1	E	214	LEU

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Mol	Chain	Res	Type
1	A	91	ASP
1	E	144	HIS
1	E	239	THR
2	F	79	ASP
1	A	92	ALA
1	A	163	PRO
2	B	50	ILE
1	C	242	VAL
2	B	51	ILE
2	B	78	ILE
2	D	50	ILE
1	A	242	VAL
2	D	51	ILE
1	E	227	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	152/186 (82%)	138 (91%)	14 (9%)	13	45
1	C	150/186 (81%)	138 (92%)	12 (8%)	17	55
1	E	153/186 (82%)	139 (91%)	14 (9%)	13	45
2	B	59/79 (75%)	54 (92%)	5 (8%)	15	51
2	D	58/79 (73%)	55 (95%)	3 (5%)	32	73
2	F	58/79 (73%)	51 (88%)	7 (12%)	7	27
All	All	630/795 (79%)	575 (91%)	55 (9%)	15	49

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	THR
1	A	28	ILE
1	A	30	GLU
1	A	31	LYS
1	A	32	ASN

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Mol	Chain	Res	Type
1	A	36	ASN
1	A	41	VAL
1	A	45	LEU
1	A	56	ASN
1	A	89	ILE
1	A	128	GLN
1	A	163	PRO
1	A	164	VAL
1	A	217	TRP
2	B	33	THR
2	B	49	ASN
2	B	78	ILE
2	B	88	GLN
2	B	101	PRO
1	C	21	LYS
1	C	25	THR
1	C	30	GLU
1	C	36	ASN
1	C	41	VAL
1	C	56	ASN
1	C	89	ILE
1	C	163	PRO
1	C	164	VAL
1	C	167	THR
1	C	217	TRP
1	C	225	ILE
2	D	33	THR
2	D	49	ASN
2	D	78	ILE
1	E	25	THR
1	E	28	ILE
1	E	36	ASN
1	E	45	LEU
1	E	56	ASN
1	E	89	ILE
1	E	143	SER
1	E	163	PRO
1	E	164	VAL
1	E	167	THR
1	E	172	ASP
1	E	211	ASN
1	E	212	ARG

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Mol	Chain	Res	Type
1	E	217	TRP
2	F	17	ASN
2	F	29	GLN
2	F	31	VAL
2	F	33	THR
2	F	49	ASN
2	F	78	ILE
2	F	88	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	26	ASN
1	A	36	ASN
1	A	56	ASN
1	A	59	GLN
1	A	64	GLN
1	A	65	HIS
1	A	119	HIS
1	A	128	GLN
1	A	140	GLN
1	A	154	ASN
1	A	211	ASN
1	A	216	HIS
2	B	29	GLN
2	B	30	HIS
2	B	49	ASN
2	B	93	GLN
1	C	23	GLN
1	C	26	ASN
1	C	36	ASN
1	C	56	ASN
1	C	59	GLN
1	C	64	GLN
1	C	65	HIS
1	C	119	HIS
1	C	126	GLN
1	C	128	GLN
1	C	154	ASN
2	D	17	ASN
2	D	29	GLN

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Mol	Chain	Res	Type
2	D	30	HIS
2	D	49	ASN
2	D	93	GLN
1	E	23	GLN
1	E	26	ASN
1	E	36	ASN
1	E	56	ASN
1	E	59	GLN
1	E	64	GLN
1	E	65	HIS
1	E	119	HIS
1	E	128	GLN
1	E	140	GLN
1	E	154	ASN
1	E	211	ASN
2	F	29	GLN
2	F	30	HIS
2	F	49	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	174/214 (81%)	0.03	2 (1%) 77 22	48, 93, 133, 151	0
1	C	172/214 (80%)	0.02	3 (1%) 67 15	44, 90, 148, 158	0
1	E	175/214 (81%)	-0.08	0 100 100	37, 82, 135, 149	0
2	B	61/87 (70%)	-0.11	1 (1%) 68 15	38, 70, 123, 152	0
2	D	60/87 (68%)	-0.12	1 (1%) 67 15	49, 82, 152, 158	0
2	F	60/87 (68%)	-0.05	3 (5%) 28 4	43, 73, 150, 156	0
All	All	702/903 (77%)	-0.03	10 (1%) 72 17	37, 84, 143, 158	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	17	ASN	3.2
1	A	112	PRO	2.7
2	F	101	PRO	2.7
1	C	241	ARG	2.6
2	F	17	ASN	2.4
1	C	114	GLY	2.2
2	B	101	PRO	2.2
1	A	90	LEU	2.1
1	C	213	SER	2.1
2	F	78	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.