Full wwPDB X-ray Structure Validation Report (i)

Apr 29, 2025 – 07:31 AM EDT

PDB ID	:	2RF4 / pdb_00002rf4
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 X-ray Structure Validation Report for a publicly released PDB entry.

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

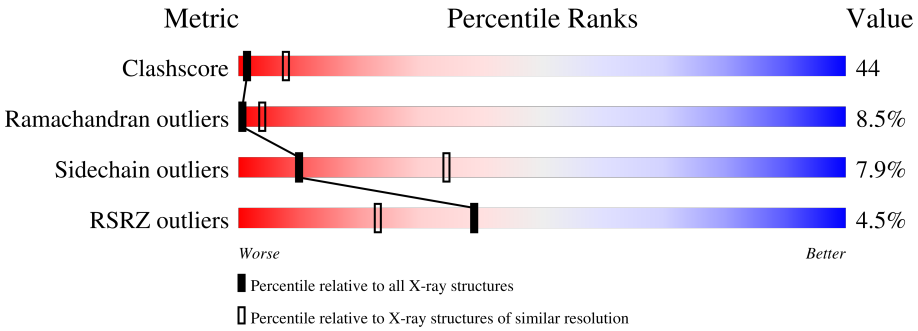
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	214	4% 28% 39% 12% • 19%
1	C	214	4% 33% 38% 6% • 20%
1	E	214	4% 31% 36% 12% • 18%
2	B	87	% 34% 24% 9% • 30%
2	D	87	% 34% 25% 7% • 31%
2	F	87	2% 30% 28% 11% 31%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5530 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 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.

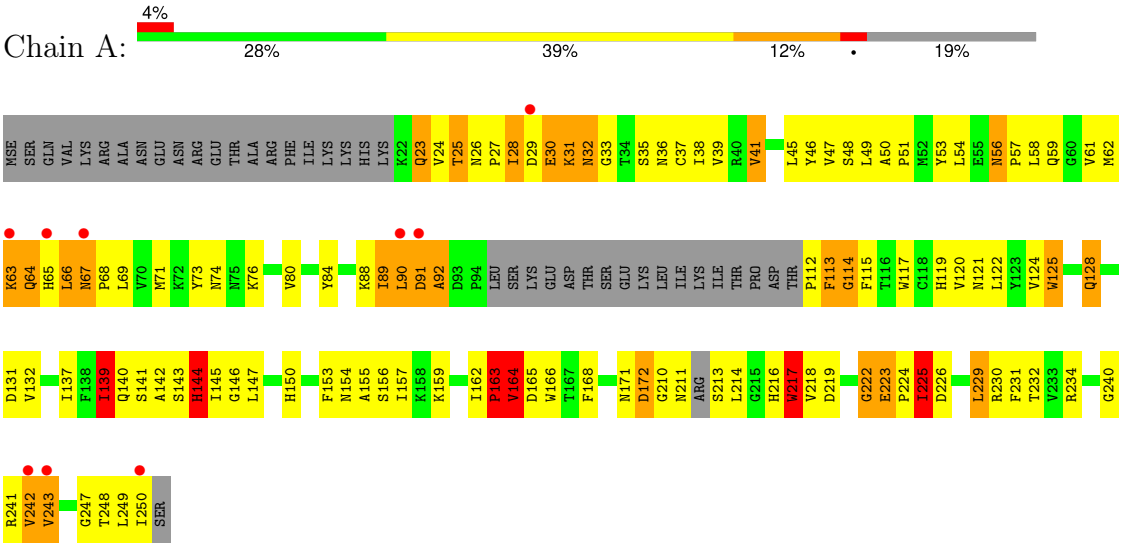
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	61	Total	C	N	O	0	0	0
			488	309	82	97			
2	D	60	Total	C	N	O	0	0	0
			480	303	81	96			
2	F	60	Total	C	N	O	0	0	0
			480	303	81	96			

3 Residue-property plots (i)

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

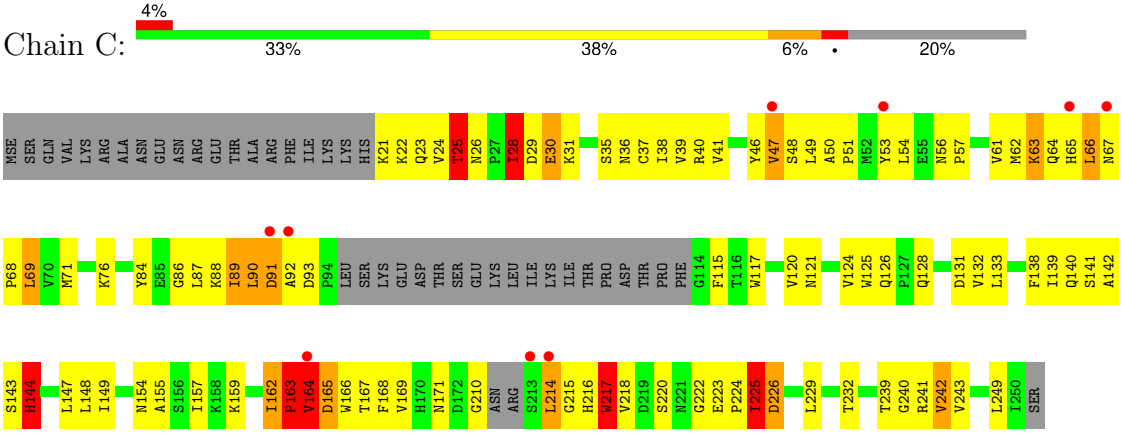
• Molecule 1: DNA-directed RNA polymerase I subunit RPA4

Chain A:



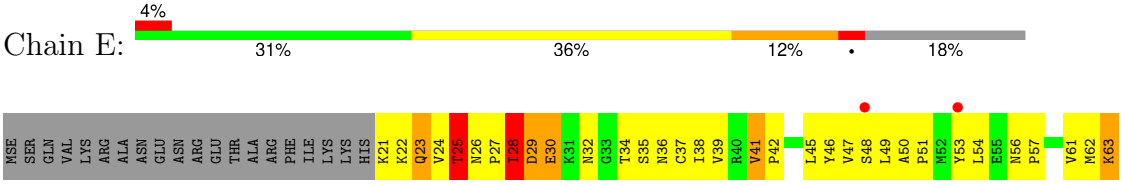
• Molecule 1: DNA-directed RNA polymerase I subunit RPA4

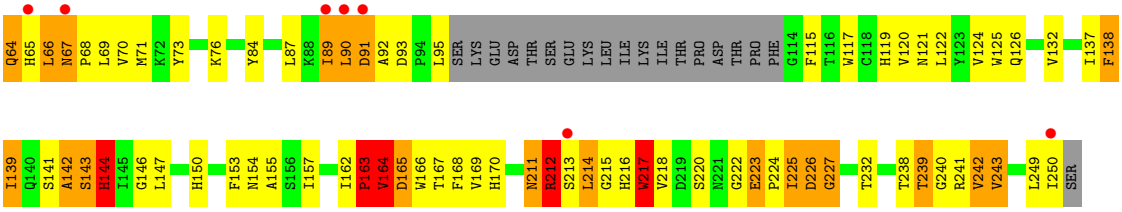
Chain C:



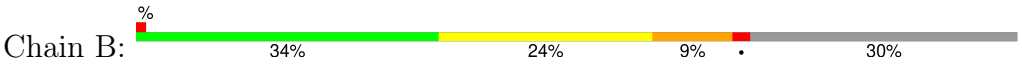
• Molecule 1: DNA-directed RNA polymerase I subunit RPA4

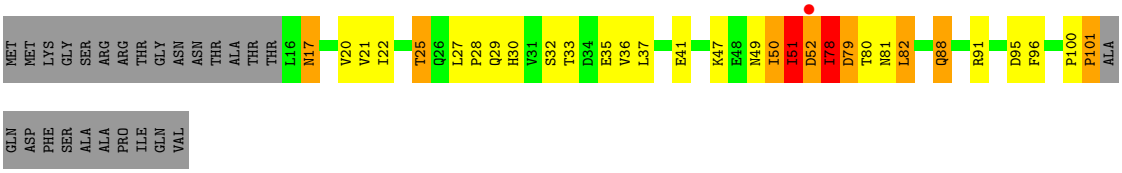
Chain E:



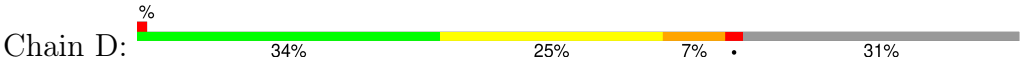


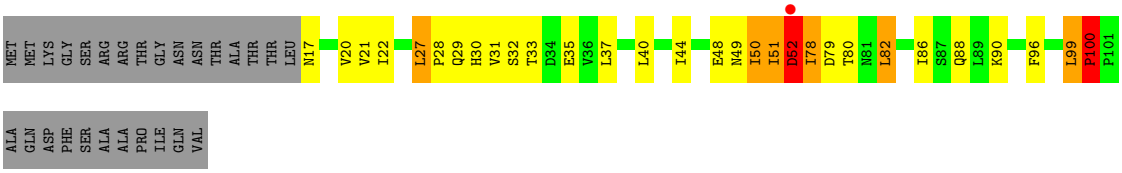
• Molecule 2: DNA-directed RNA polymerase I subunit RPA4



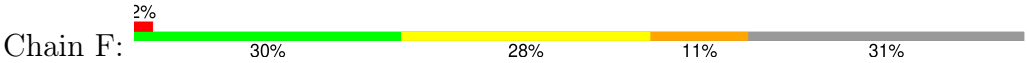


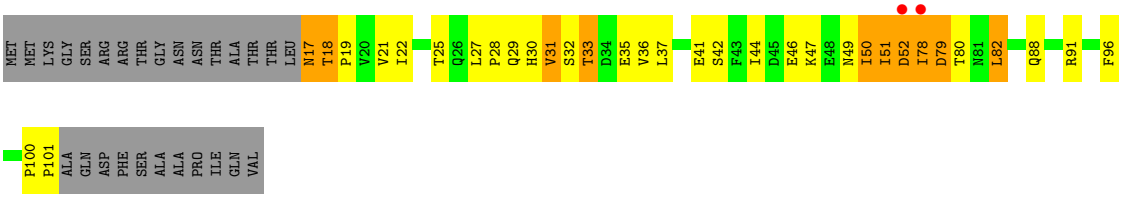
• Molecule 2: DNA-directed RNA polymerase I subunit RPA4





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





4 Data and refinement statistics (i)

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 30.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-3.10) 99.5 (30.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	5.35 (at 3.11Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.252 , 0.285 0.252 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	77.2	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 58.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.064 for -h,l,k	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.57	0/1394	1.43	22/1894 (1.2%)
1	C	0.56	0/1375	1.22	17/1867 (0.9%)
1	E	0.58	0/1403	1.27	20/1906 (1.0%)
2	B	0.65	0/496	1.22	5/674 (0.7%)
2	D	0.56	0/488	1.31	6/663 (0.9%)
2	F	0.58	0/488	1.14	7/663 (1.1%)
All	All	0.58	0/5644	1.29	77/7667 (1.0%)

There are no bond length outliers.

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	24	VAL	N-CA-C	-23.34	73.91	107.99
1	A	113	PHE	N-CA-C	12.78	132.18	113.40
1	E	216	HIS	N-CA-C	12.18	128.03	111.71
2	D	99	LEU	CA-C-N	11.93	132.66	120.38
2	D	99	LEU	C-N-CA	11.93	132.66	120.38
1	C	216	HIS	N-CA-C	10.92	126.34	111.71
2	B	52	ASP	N-CA-C	10.91	123.72	110.19
1	A	29	ASP	N-CA-C	10.52	123.25	108.74
1	A	216	HIS	N-CA-C	10.40	128.25	112.54
1	E	124	VAL	N-CA-C	10.03	122.62	107.77
1	A	23	GLN	N-CA-C	9.87	125.10	108.13
1	A	64	GLN	N-CA-C	-9.36	102.96	114.75
2	F	82	LEU	N-CA-C	-8.65	102.16	112.89
2	F	52	ASP	N-CA-C	8.61	123.07	110.59
2	B	82	LEU	N-CA-C	-8.46	102.40	112.89
2	D	82	LEU	N-CA-C	-8.39	103.05	113.28
1	A	124	VAL	N-CA-C	8.32	120.08	107.77
1	E	64	GLN	N-CA-C	-8.20	104.14	114.56
1	E	28	ILE	N-CA-C	-8.07	98.24	109.21
1	A	125	TRP	N-CA-C	-7.99	97.02	109.25
2	D	100	PRO	N-CA-C	7.98	120.44	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	165	ASP	N-CA-C	-7.80	102.84	113.30
1	E	165	ASP	N-CA-C	-7.64	103.03	112.88
1	C	125	TRP	N-CA-C	-7.57	96.92	108.96
1	E	217	TRP	N-CA-C	7.56	126.91	110.80
1	C	138	PHE	N-CA-C	-7.49	98.47	109.63
1	C	217	TRP	N-CA-C	7.36	126.48	110.80
1	E	138	PHE	N-CA-C	-7.36	98.39	109.94
1	A	217	TRP	N-CA-C	7.22	126.18	110.80
2	F	51	ILE	N-CA-C	-7.19	94.39	109.34
1	C	144	HIS	N-CA-C	7.10	125.92	110.80
1	E	63	LYS	N-CA-C	-7.08	103.96	112.59
1	C	63	LYS	N-CA-C	-7.05	103.99	112.59
1	E	22	LYS	N-CA-C	-6.82	99.07	109.85
1	A	56	ASN	CA-C-N	6.77	126.40	119.56
1	A	56	ASN	C-N-CA	6.77	126.40	119.56
1	A	63	LYS	N-CA-C	-6.70	103.42	112.26
1	C	23	GLN	N-CA-C	6.66	119.26	108.41
1	C	28	ILE	N-CA-C	-6.61	100.22	109.21
1	C	165	ASP	N-CA-C	-6.59	103.65	112.94
1	E	125	TRP	N-CA-C	-6.24	100.17	109.15
1	A	222	GLY	N-CA-C	6.21	127.89	113.18
1	E	144	HIS	N-CA-C	6.13	123.85	110.80
1	A	67	ASN	N-CA-C	-6.12	105.69	113.77
2	B	17	ASN	N-CA-C	6.08	123.75	110.80
2	D	27	LEU	N-CA-C	-6.08	102.39	109.93
1	E	67	ASN	N-CA-C	-6.08	105.35	113.25
1	A	114	GLY	N-CA-C	6.04	127.48	113.18
1	A	229	LEU	N-CA-C	5.81	118.95	109.59
2	B	51	ILE	N-CA-C	-5.81	97.26	109.34
2	B	25	THR	N-CA-C	-5.70	106.31	113.72
1	E	143	SER	N-CA-C	-5.70	98.99	108.34
1	A	139	ILE	N-CA-C	5.59	115.62	106.72
1	E	29	ASP	N-CA-C	5.58	115.75	107.88
1	C	69	LEU	N-CA-C	5.52	120.50	113.55
1	C	31	LYS	N-CA-C	5.50	117.13	111.03
2	D	52	ASP	N-CA-C	5.48	122.48	110.80
2	F	27	LEU	N-CA-C	-5.46	102.77	110.31
1	E	223	GLU	CA-C-N	-5.43	113.96	119.83
1	E	223	GLU	C-N-CA	-5.43	113.96	119.83
1	C	162	ILE	CA-C-N	5.37	126.55	119.84
1	C	162	ILE	C-N-CA	5.37	126.55	119.84
1	E	30	GLU	N-CA-C	5.33	119.13	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	44	ILE	N-CA-C	-5.31	105.43	110.42
1	C	22	LYS	N-CA-C	-5.27	98.72	107.99
1	A	113	PHE	CB-CA-C	-5.26	101.43	111.06
1	C	124	VAL	N-CA-C	5.24	116.26	108.46
1	E	27	PRO	N-CA-C	5.23	118.71	110.50
1	A	144	HIS	N-CA-C	5.23	121.93	110.80
1	A	223	GLU	N-CA-C	-5.18	101.55	109.64
2	F	27	LEU	CA-C-N	5.17	126.30	119.84
2	F	27	LEU	C-N-CA	5.17	126.30	119.84
1	C	226	ASP	N-CA-C	5.15	121.77	110.80
1	E	30	GLU	CB-CA-C	-5.11	109.71	115.79
1	C	47	VAL	N-CA-C	5.10	117.02	109.17
1	A	69	LEU	N-CA-C	5.08	119.47	113.12
1	E	150	HIS	N-CA-C	-5.01	104.72	111.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1363	0	1350	153	0
1	C	1346	0	1340	119	0
1	E	1373	0	1371	123	0
2	B	488	0	491	47	0
2	D	480	0	480	39	0
2	F	480	0	480	45	0
All	All	5530	0	5512	482	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 44.

All (482) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:GLU:CG	1:A:31:LYS:H	1.52	1.19
1:E:47:VAL:HG23	1:E:64:GLN:HE21	1.16	1.07
1:A:30:GLU:HG3	1:A:31:LYS:N	1.53	1.02
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:HD13	1:A:89:ILE:O	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
2:F:79:ASP:CG	2:F:80:THR:H	1.85	0.85
1:A:30:GLU:HG3	1:A:31:LYS:H	0.69	0.84
2:B:79:ASP:CG	2:B:80:THR:H	1.85	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
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
2:D:79:ASP:CG	2:D:80:THR:H	1.88	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
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:O	1:C:144:HIS:ND1	2.15	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:53:TYR:CZ	1:A:63:LYS:HD2	2.27	0.69
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
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:E:218:VAL:HG13	1:E:223:GLU:C	2.19	0.67
1:C:76:LYS:HD2	2:D:22:ILE:HD12	1.76	0.67
1:C:88:LYS:CE	1:C:90:LEU:HD12	2.25	0.67
1:C:29:ASP:C	1:C:30:GLU:HG3	2.20	0.66
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:52:ASP:CG	2:F:78:ILE:N	2.54	0.66
1:C:218:VAL:HG13	1:C:223:GLU:C	2.22	0.65
1:A:218:VAL:HG13	1:A:223:GLU:C	2.21	0.65
1:E:90:LEU:C	1:E:92:ALA:H	2.03	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:37:LEU:HD13	2:D:96:PHE:HB3	1.78	0.65
2:F:18:THR:HG23	2:F:18:THR:O	1.95	0.65
2:F:32:SER:OG	2:F:35:GLU:HG3	1.96	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:24:VAL:HG21	2:F:28:PRO:HB2	1.80	0.63
1:E:139:ILE:HD12	1:E:139:ILE:O	1.98	0.63
1:E:169:VAL:HG22	1:E:170:HIS:N	2.13	0.63
2:B:78:ILE:HD13	2:B:78:ILE:O	1.98	0.63
2:B:79:ASP:CG	2:B:80:THR:N	2.56	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:119:HIS:HE1	2:B:25:THR:OG1	1.82	0.62
1:A:132:VAL:HG22	1:A:232:THR:HG22	1.81	0.62
1:E:224:PRO:O	1:E:225:ILE:C	2.42	0.62
2:B:49:ASN:HD22	2:B:50:ILE:H	1.48	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:67:ASN:O	1:A:68:PRO:C	2.43	0.61
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:23:GLN:HE21	1:A:25:THR:HA	1.66	0.61
1:A:143:SER:H	1:A:217:TRP:HH2	1.46	0.61
2:D:50:ILE:CG2	2:D:51:ILE:H	2.12	0.61
1:E:62:MSE:O	1:E:66:LEU:HB2	2.00	0.61
1:C:47:VAL:CG2	1:C:64:GLN:HG2	2.30	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:A:142:ALA:O	1:A:143:SER:HB3	2.00	0.61
1:C:36:ASN:HD22	1:C:37:CYS:N	1.98	0.61
1:C:67:ASN:O	1:C:68:PRO:C	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:SER:O	1:A:217:TRP:HZ3	1.84	0.60
2:D:49:ASN:ND2	2:D:50:ILE:H	1.99	0.60
1:C:142:ALA:O	1:C:143:SER:HB3	2.01	0.60
1:A:80:VAL:HB	1:A:125:TRP:HB3	1.83	0.60
1:C:28:ILE:HA	1:C:35:SER:HA	1.83	0.60
1:A:140:GLN:HE22	1:A:225:ILE:HG12	1.67	0.60
1:C:120:VAL:HG22	1:C:121:ASN:N	2.16	0.60
1:C:224:PRO:O	1:C:225:ILE:C	2.45	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:71:MSE:HE2	2:D:88:GLN:HG2	1.84	0.59
1:C:162:ILE:CG2	1:C:163:PRO:HD2	2.32	0.59
1:C:88:LYS:HE2	1:C:90:LEU:HD12	1.84	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
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:D:79:ASP:CG	2:D:80:THR:N	2.57	0.58
2:F:17:ASN:N	2:F:17:ASN:HD22	2.01	0.58
1:A:47:VAL:HG21	1:A:64:GLN:HG2	1.84	0.57
1:A:162:ILE:HG22	1:A:163:PRO:HD2	1.86	0.57
1:A:171:ASN:C	1:A:210:GLY:H	2.12	0.57
1:C:62:MSE:HE2	1:C:84:TYR:HE2	1.67	0.57
1:E:26:ASN:HB3	1:E:36:ASN:O	2.03	0.57
1:E:132:VAL:CG2	1:E:232:THR:HG22	2.33	0.57
2:F:80:THR:HG22	2:F:80:THR:O	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:A:66:LEU:C	1:A:68:PRO:HD2	2.29	0.57
1:C:139:ILE:HD12	1:C:139:ILE:O	2.04	0.57
2:B:37:LEU:HD13	2:B:96:PHE:HB3	1.87	0.57
2:B:50:ILE:CG2	2:B:51:ILE:N	2.68	0.57
1:C:89:ILE:C	1:C:91:ASP:N	2.63	0.57
2:B:32:SER:OG	2:B:35:GLU:HG3	2.04	0.56
1:C:162:ILE:HG23	1:C:163:PRO:HD2	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:24:VAL:O	1:E:25:THR:C	2.48	0.56
1:E:211:ASN:HD21	1:E:214:LEU:CD1	2.13	0.56
1:A:112:PRO:O	1:A:113:PHE:HB2	2.04	0.56
1:A:120:VAL:HG22	1:A:121:ASN:N	2.21	0.56
1:E:211:ASN:ND2	1:E:214:LEU:HD12	2.14	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:E:50:ALA:HB3	1:E:53:TYR:HD2	1.70	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:HD22	1.88	0.55
1:A:73:TYR:CD1	1:A:74:ASN:N	2.75	0.55
2:B:52:ASP:OD1	2:B:78:ILE:N	2.25	0.55
1:C:66:LEU:HD22	2:D:82:LEU:CD2	2.36	0.55
1:C:144:HIS:O	1:C:144:HIS:CG	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
2:F:79:ASP:CG	2:F:80:THR:N	2.54	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
1:A:50:ALA:HB3	1:A:53:TYR:CD2	2.42	0.54
1:A:89:ILE:HD13	1:A:89:ILE:C	2.32	0.54
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:C:92:ALA:O	1:C:93:ASP:HB2	2.07	0.54
1:E:141:SER:O	1:E:143:SER:N	2.40	0.54
1:A:59:GLN:NE2	1:A:59:GLN:HA	2.22	0.54
1:A:142:ALA:HB2	1:A:168:PHE:CE2	2.42	0.54
1:A:47:VAL:HG23	1:A:64:GLN:HE21	1.71	0.54
1:A:53:TYR:OH	1:A:63:LYS:HD2	2.06	0.54
1:E:66:LEU:O	1:E:70:VAL:HG23	2.08	0.54
1:A:89:ILE:C	1:A:91:ASP:H	2.16	0.54
1:A:172:ASP:HB2	1:A:214:LEU:CD1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:VAL:HG12	1:A:243:VAL:O	2.08	0.54
2:F:78:ILE:CD1	2:F:82:LEU:HD22	2.38	0.53
1:A:147:LEU:HB2	1:A:155:ALA:HB3	1.89	0.53
1:C:86:GLY:O	1:C:87:LEU:C	2.52	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:C:89:ILE:C	1:C:91:ASP:H	2.17	0.53
1:A:27:PRO:HD2	2:B:30:HIS:CE1	2.44	0.53
1:A:140:GLN:HE22	1:A:225:ILE:CG1	2.22	0.53
1:E:144:HIS:O	1:E:144:HIS:ND1	2.41	0.53
1:A:234:ARG:HH11	1:A:248:THR:HG21	1.72	0.53
1:C:76:LYS:NZ	2:D:20:VAL:O	2.42	0.53
1:E:141:SER:O	1:E:217:TRP:CZ3	2.60	0.53
1:A:36:ASN:HD22	1:A:36:ASN:C	2.12	0.52
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:88:LYS:HE3	1:C:90:LEU:HD12	1.92	0.52
1:C:163:PRO:HB2	1:C:166:TRP:CD1	2.44	0.52
1:E:30:GLU:OE1	1:E:32:ASN:N	2.41	0.52
1:E:36:ASN:HD22	1:E:36:ASN:C	2.10	0.52
1:E:126:GLN:O	1:E:126:GLN:HG2	2.08	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:A:66:LEU:HD21	2:B:47:LYS:HD2	1.92	0.52
1:C:90:LEU:C	1:C:92:ALA:H	2.17	0.52
1:C:91:ASP:HB3	1:C:117:TRP:C	2.33	0.52
1:E:42:PRO:HG3	1:E:121:ASN:OD1	2.09	0.52
1:A:47:VAL:HG23	1:A:64:GLN:NE2	2.24	0.52
1:A:76:LYS:HD2	2:B:22:ILE:HD12	1.92	0.52
1:C:87:LEU:C	1:C:87:LEU:HD13	2.34	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
1:A:28:ILE:HA	1:A:35:SER:HA	1.91	0.52
1:C:142:ALA:HB2	1:C:168:PHE:CE2	2.45	0.52
2:D:78:ILE:CD1	2:D:82:LEU:HD22	2.40	0.52
1:C:171:ASN:HB2	1:C:214:LEU:HB2	1.92	0.52
1:E:146:GLY:O	1:E:147:LEU:HD23	2.10	0.52
1:A:89:ILE:C	1:A:91:ASP:N	2.68	0.52
1:A:139:ILE:O	1:A:139:ILE:HD12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:GLY:CA	1:A:213:SER:HA	2.36	0.51
1:E:67:ASN:O	1:E:68:PRO:C	2.54	0.51
1:E:93:ASP:C	1:E:95:LEU:H	2.17	0.51
2:B:36:VAL:HG13	2:B:37:LEU:N	2.24	0.51
2:B:17:ASN:CG	2:B:17:ASN:O	2.53	0.51
1:A:144:HIS:O	1:A:144:HIS:CG	2.63	0.51
2:B:27:LEU:HD23	2:B:28:PRO:O	2.10	0.51
2:F:49:ASN:ND2	2:F:50:ILE:H	2.08	0.51
1:C:51:PRO:HA	1:C:54:LEU:HD23	1.92	0.51
2:F:17:ASN:N	2:F:17:ASN:ND2	2.56	0.51
1:A:157:ILE:HG13	1:A:157:ILE:O	2.11	0.51
1:C:36:ASN:HD22	1:C:36:ASN:C	2.19	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:172:ASP:C	1:A:214:LEU:HD12	2.36	0.50
1:C:89:ILE:HD13	1:C:89:ILE:C	2.36	0.50
1:A:141:SER:O	1:A:142:ALA:C	2.55	0.50
1:A:53:TYR:OH	1:A:63:LYS:CD	2.60	0.50
1:A:90:LEU:C	1:A:92:ALA:H	2.20	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:A:224:PRO:O	1:A:225:ILE:C	2.54	0.50
1:C:126:GLN:O	1:C:126:GLN:HG2	2.12	0.50
1:A:26:ASN:HD22	2:B:30:HIS:CE1	2.30	0.50
1:A:36:ASN:C	1:A:36:ASN:ND2	2.70	0.50
1:A:66:LEU:HD22	2:B:82:LEU:HD21	1.93	0.50
1:E:154:ASN:ND2	1:E:242:VAL:HG11	2.27	0.49
1:A:66:LEU:O	1:A:67:ASN:C	2.56	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:O	1:C:63:LYS:HG3	2.12	0.49
1:A:249:LEU:O	1:A:250:ILE:C	2.55	0.49
1:E:90:LEU:C	1:E:92:ALA:N	2.67	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
2:F:36:VAL:HG13	2:F:37:LEU:N	2.28	0.49
2:B:32:SER:HG	2:B:35:GLU:HG3	1.77	0.49
1:A:50:ALA:HB3	1:A:53:TYR:HD2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:ASN:ND2	1:E:36:ASN:C	2.70	0.49
1:E:51:PRO:HA	1:E:54:LEU:HD23	1.94	0.48
1:C:26:ASN:HD22	2:D:30:HIS:CE1	2.31	0.48
1:E:66:LEU:HD22	2:F:82:LEU:CD2	2.43	0.48
1:A:48:SER:HA	1:A:115:PHE:CD1	2.48	0.48
1:A:62:MSE:O	1:A:66:LEU:HB2	2.12	0.48
1:A:163:PRO:HG2	1:A:166:TRP:CE2	2.48	0.48
1:C:65:HIS:O	1:C:69:LEU:HB2	2.13	0.48
1:C:171:ASN:C	1:C:210:GLY:N	2.71	0.48
1:E:36:ASN:HD21	1:E:38:ILE:H	1.61	0.48
1:A:36:ASN:ND2	1:A:38:ILE:H	2.12	0.48
1:C:157:ILE:HD13	1:C:249:LEU:CD2	2.29	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:E:218:VAL:HG13	1:E:223:GLU:O	2.13	0.48
1:E:29:ASP:C	1:E:30:GLU:HG3	2.39	0.48
1:C:46:TYR:O	2:D:20:VAL:HG23	2.14	0.47
2:F:17:ASN:O	2:F:19:PRO:CD	2.61	0.47
2:F:52:ASP:CG	2:F:78:ILE:H	2.20	0.47
1:A:241:ARG:HG3	1:A:241:ARG:HH11	1.79	0.47
1:E:89:ILE:C	1:E:91:ASP:H	2.23	0.47
1:C:62:MSE:O	1:C:66:LEU:HB2	2.14	0.47
1:C:90:LEU:C	1:C:92:ALA:N	2.72	0.47
1:C:165:ASP:OD1	1:C:220:SER:HB3	2.14	0.47
2:F:41:GLU:OE1	2:F:41:GLU:HA	2.13	0.47
1:C:91:ASP:OD1	1:C:91:ASP:O	2.32	0.47
1:C:154:ASN:ND2	1:C:242:VAL:HG11	2.29	0.47
1:E:26:ASN:ND2	2:F:30:HIS:CE1	2.82	0.47
1:E:120:VAL:HG22	1:E:121:ASN:H	1.79	0.47
1:A:71:MSE:HE2	2:B:88:GLN:HG2	1.97	0.47
1:A:73:TYR:CD1	1:A:73:TYR:C	2.92	0.47
1:C:26:ASN:ND2	2:D:30:HIS:HE1	2.13	0.47
1:E:47:VAL:HG22	1:E:48:SER:N	2.29	0.47
1:E:132:VAL:HG12	1:E:132:VAL:O	2.13	0.47
1:E:142:ALA:C	1:E:217:TRP:CH2	2.93	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:A:33:GLY:HA3	1:A:230:ARG:NH1	2.30	0.47
1:C:141:SER:O	1:C:217:TRP:CZ3	2.56	0.47
2:D:44:ILE:HD13	2:D:90:LYS:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:89:ILE:HD13	1:E:89:ILE:C	2.40	0.47
2:F:50:ILE:HG13	2:F:51:ILE:HG13	1.96	0.47
1:A:211:ASN:N	1:A:213:SER:HA	2.30	0.46
1:A:140:GLN:OE1	1:A:225:ILE:HD11	2.14	0.46
2:B:49:ASN:ND2	2:B:50:ILE:N	2.64	0.46
1:C:47:VAL:HG22	1:C:48:SER:N	2.30	0.46
1:E:87:LEU:HD23	1:E:120:VAL:HB	1.96	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:171:ASN:HB2	1:C:214:LEU:H	1.81	0.46
1:C:171:ASN:C	1:C:210:GLY:H	2.23	0.46
2:B:80:THR:O	2:B:82:LEU:N	2.49	0.46
1:C:120:VAL:CG2	1:C:121:ASN:N	2.79	0.46
2:D:52:ASP:C	2:D:52:ASP:OD1	2.59	0.46
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
2:D:50:ILE:C	2:D:52:ASP:N	2.69	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:C:36:ASN:C	1:C:36:ASN:ND2	2.75	0.45
2:D:27:LEU:HD23	2:D:28:PRO:O	2.16	0.45
1:E:147:LEU:HB2	1:E:155:ALA:HB3	1.97	0.45
1:C:87:LEU:HD13	1:C:88:LYS:N	2.32	0.45
1:A:48:SER:HA	1:A:115:PHE:HD1	1.81	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:49:LEU:HD21	1:A:57:PRO:HB3	1.99	0.45
1:A:150:HIS:HA	2:B:95:ASP:CG	2.42	0.45
1:C:65:HIS:CE1	1:C:120:VAL:HG11	2.52	0.45
2:D:31:VAL:CG2	2:D:35:GLU:CB	2.92	0.45
1:E:53:TYR:OH	1:E:63:LYS:HD2	2.17	0.44
1:E:61:VAL:O	1:E:64:GLN:HB3	2.17	0.44
1:A:159:LYS:HA	1:A:162:ILE:HD12	1.99	0.44
1:A:26:ASN:HB3	1:A:36:ASN:O	2.18	0.44
1:A:41:VAL:HG13	1:A:122:LEU:HB2	1.98	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:E:169:VAL:HG22	1:E:170:HIS:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:VAL:O	1:C:25:THR:C	2.60	0.44
1:C:171:ASN:CG	1:C:214:LEU:HB2	2.42	0.44
1:E:93:ASP:CG	1:E:93:ASP:O	2.60	0.44
1:E:226:ASP:CG	1:E:227:GLY:N	2.71	0.44
1:A:50:ALA:HB1	1:A:51:PRO:HD2	1.99	0.44
1:E:89:ILE:C	1:E:91:ASP:N	2.76	0.44
1:C:141:SER:O	1:C:142:ALA:C	2.61	0.44
1:E:65:HIS:HB3	1:E:84:TYR:CE1	2.52	0.44
1:A:36:ASN:ND2	1:A:37:CYS:N	2.61	0.44
1:A:128:GLN:HE21	1:A:128:GLN:HB2	1.51	0.44
2:F:91:ARG:HH11	2:F:91:ARG:HG2	1.83	0.44
2:B:36:VAL:HG11	2:B:96:PHE:CE2	2.52	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:A:23:GLN:NE2	1:A:25:THR:HA	2.32	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:E:41:VAL:O	1:E:41:VAL:HG22	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:A:56:ASN:C	1:A:56:ASN:HD22	2.27	0.43
1:C:38:ILE:HD12	1:C:38:ILE:N	2.33	0.43
1:C:62:MSE:HE2	1:C:84:TYR:CE2	2.51	0.43
1:E:47:VAL:CG2	1:E:64:GLN:HG2	2.48	0.43
1:A:23:GLN:HG3	1:A:128:GLN:NE2	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:C:147:LEU:HB2	1:C:155:ALA:HB3	2.01	0.43
1:C:242:VAL:HG12	1:C:243:VAL:O	2.19	0.43
1:A:217:TRP:O	1:A:225:ILE:HG13	2.18	0.43
1:A:231:PHE:CD1	1:A:247:GLY:HA3	2.53	0.43
1:C:89:ILE:O	1:C:90:LEU:C	2.61	0.43
1:C:163:PRO:O	1:C:164:VAL:CG1	2.63	0.43
1:E:57:PRO:O	1:E:61:VAL:HG23	2.19	0.43
2:B:50:ILE:O	2:B:51:ILE:CB	2.67	0.43
1:E:211:ASN:C	1:E:212:ARG:O	2.57	0.43
1:A:163:PRO:O	1:A:164:VAL:CG1	2.64	0.42
1:E:73:TYR:CD1	1:E:73:TYR:C	2.95	0.42
1:A:54:LEU:C	1:A:56:ASN:H	2.25	0.42
2:D:99:LEU:HA	2:D:100:PRO:HD3	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:C:128:GLN:N	1:C:131:ASP:OD2	2.48	0.42
1:C:143:SER:N	1:C:217:TRP:HH2	2.07	0.42
2:F:29:GLN:HE21	2:F:29:GLN:HB2	1.66	0.42
2:F:47:LYS:HA	2:F:47:LYS:HD3	1.78	0.42
1:A:91:ASP:O	1:A:117:TRP:HB2	2.20	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:E:53:TYR:CE2	1:E:63:LYS:HD3	2.55	0.42
2:F:33:THR:O	2:F:36:VAL:HG12	2.20	0.42
1:A:23:GLN:HG3	1:A:128:GLN:CD	2.45	0.42
1:C:241:ARG:HH11	1:C:241:ARG:HG3	1.83	0.42
1:A:241:ARG:O	1:A:242:VAL:C	2.62	0.42
1:C:84:TYR:HB2	1:C:120:VAL:HG21	2.02	0.42
1:C:133:LEU:HD13	1:C:149:ILE:HD13	2.01	0.42
1:C:218:VAL:CG1	1:C:223:GLU:N	2.83	0.42
1:A:157:ILE:O	1:A:157:ILE:CG1	2.68	0.42
1:C:39:VAL:HG23	2:D:29:GLN:C	2.45	0.42
1:E:47:VAL:HG23	1:E:64:GLN:HG2	2.00	0.42
1:E:225:ILE:HD12	1:E:225:ILE:HA	1.86	0.41
1:A:51:PRO:HA	1:A:54:LEU:HD23	2.02	0.41
1:A:90:LEU:C	1:A:92:ALA:N	2.78	0.41
1:A:145:ILE:HG22	1:A:146:GLY:N	2.35	0.41
1:A:157:ILE:HG21	1:A:249:LEU:HD23	2.01	0.41
2:D:17:ASN:O	2:D:17:ASN:ND2	2.53	0.41
2:F:18:THR:O	2:F:18:THR:CG2	2.66	0.41
1:C:217:TRP:O	1:C:225:ILE:HG23	2.20	0.41
1:E:54:LEU:C	1:E:56:ASN:H	2.28	0.41
2:F:42:SER:O	2:F:46:GLU:HB2	2.19	0.41
2:B:80:THR:C	2:B:82:LEU:N	2.77	0.41
1:C:143:SER:N	1:C:217:TRP:CH2	2.86	0.41
1:E:39:VAL:CG1	2:F:28:PRO:HB3	2.48	0.41
1:E:163:PRO:O	1:E:164:VAL:CG1	2.64	0.41
2:F:100:PRO:HA	2:F:101:PRO:C	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:ALA:HB3	1:E:53:TYR:CD2	2.54	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:66:LEU:C	1:A:68:PRO:CD	2.94	0.41
1:A:128:GLN:O	1:A:131:ASP:OD2	2.39	0.41
1:A:166:TRP:CD1	1:A:219:ASP:HB2	2.56	0.41
1:E:93:ASP:C	1:E:95:LEU:N	2.76	0.41
1:E:138:PHE:O	1:E:139:ILE:C	2.64	0.41
1:A:39:VAL:HG21	2:B:28:PRO:HB3	2.03	0.41
1:A:66:LEU:HA	1:A:66:LEU:HD23	1.87	0.41
1:C:241:ARG:O	1:C:242:VAL:C	2.64	0.41
2:B:80:THR:C	2:B:82:LEU:H	2.28	0.40
1:C:148:LEU:HD23	1:C:148:LEU:HA	1.80	0.40
1:E:47:VAL:CG2	1:E:64:GLN:NE2	2.68	0.40
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:HD23	2:D:40:LEU:HA	1.85	0.40
1:E:241:ARG:O	1:E:242:VAL:C	2.63	0.40
1:A:31:LYS:O	1:A:31:LYS:HD3	2.21	0.40
1:C:54:LEU:C	1:C:56:ASN:H	2.28	0.40
1:E:66:LEU:HD22	2:F:82:LEU:HD22	2.03	0.40
2:B:49:ASN:C	2:B:50:ILE:O	2.63	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:A:172:ASP:HB2	1:A:214:LEU:HD12	2.03	0.40
2:B:29:GLN:HE21	2:B:29:GLN:HB2	1.68	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:E:249:LEU:O	1:E:250:ILE:C	2.63	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	168/214 (78%)	129 (77%)	25 (15%)	14 (8%)	0 4
1	C	166/214 (78%)	130 (78%)	23 (14%)	13 (8%)	1 4
1	E	171/214 (80%)	131 (77%)	21 (12%)	19 (11%)	0 2
2	B	59/87 (68%)	52 (88%)	2 (3%)	5 (8%)	0 4
2	D	58/87 (67%)	49 (84%)	5 (9%)	4 (7%)	1 5
2	F	58/87 (67%)	49 (84%)	6 (10%)	3 (5%)	1 10
All	All	680/903 (75%)	540 (79%)	82 (12%)	58 (8%)	0 4

All (58) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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
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 (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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	152/186 (82%)	137 (90%)	15 (10%)	6	24
1	C	150/186 (81%)	137 (91%)	13 (9%)	8	31
1	E	153/186 (82%)	141 (92%)	12 (8%)	10	35
2	B	59/79 (75%)	55 (93%)	4 (7%)	13	40
2	D	58/79 (73%)	56 (97%)	2 (3%)	32	62
2	F	58/79 (73%)	54 (93%)	4 (7%)	13	39
All	All	630/795 (79%)	580 (92%)	50 (8%)	10	34

All (50) 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
1	A	41	VAL
1	A	45	LEU
1	A	89	ILE
1	A	128	GLN
1	A	139	ILE
1	A	163	PRO
1	A	164	VAL
1	A	217	TRP
1	A	225	ILE
1	A	243	VAL
2	B	33	THR
2	B	78	ILE
2	B	88	GLN
2	B	101	PRO
1	C	21	LYS
1	C	25	THR
1	C	28	ILE
1	C	30	GLU
1	C	41	VAL
1	C	89	ILE
1	C	163	PRO
1	C	164	VAL

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Mol	Chain	Res	Type
1	C	167	THR
1	C	169	VAL
1	C	214	LEU
1	C	217	TRP
1	C	225	ILE
2	D	33	THR
2	D	78	ILE
1	E	25	THR
1	E	28	ILE
1	E	41	VAL
1	E	45	LEU
1	E	89	ILE
1	E	163	PRO
1	E	164	VAL
1	E	167	THR
1	E	211	ASN
1	E	212	ARG
1	E	217	TRP
1	E	243	VAL
2	F	17	ASN
2	F	31	VAL
2	F	33	THR
2	F	78	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) 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	75	ASN
1	A	119	HIS
1	A	126	GLN
1	A	128	GLN
1	A	154	ASN
1	A	211	ASN
1	A	216	HIS
1	A	235	ASN

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Mol	Chain	Res	Type
1	A	237	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	75	ASN
1	C	119	HIS
1	C	126	GLN
1	C	128	GLN
1	C	154	ASN
1	C	237	HIS
2	D	17	ASN
2	D	29	GLN
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
1	E	235	ASN
2	F	29	GLN
2	F	30	HIS
2	F	49	ASN
2	F	93	GLN

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 oligosaccharides 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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	171/214 (79%)	0.46	9 (5%)	33	20	48, 93, 133, 151	0
1	C	169/214 (78%)	0.34	9 (5%)	33	20	44, 88, 148, 158	0
1	E	172/214 (80%)	0.21	9 (5%)	34	20	37, 82, 135, 145	0
2	B	61/87 (70%)	0.23	1 (1%)	70	52	38, 70, 123, 152	0
2	D	60/87 (68%)	0.33	1 (1%)	69	50	49, 82, 152, 158	0
2	F	60/87 (68%)	0.18	2 (3%)	49	30	43, 73, 150, 156	0
All	All	693/903 (76%)	0.31	31 (4%)	39	23	37, 84, 143, 158	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	67	ASN	5.3
1	E	48	SER	4.1
1	C	65	HIS	3.9
1	A	65	HIS	3.7
1	E	65	HIS	3.3
1	C	91	ASP	3.3
1	A	67	ASN	3.1
1	A	250	ILE	3.1
1	E	91	ASP	3.0
1	A	242	VAL	3.0
1	C	53	TYR	2.9
1	C	92	ALA	2.9
2	B	52	ASP	2.7
1	E	90	LEU	2.6
1	A	90	LEU	2.5
1	E	89	ILE	2.4
2	F	78	ILE	2.3
1	C	214	LEU	2.3
2	D	52	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	63	LYS	2.3
1	E	53	TYR	2.2
1	C	164	VAL	2.2
1	C	213	SER	2.2
1	E	213	SER	2.1
1	A	91	ASP	2.1
1	C	67	ASN	2.1
2	F	52	ASP	2.1
1	C	47	VAL	2.1
1	A	243	VAL	2.1
1	E	250	ILE	2.0
1	A	29	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.