Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2023 – 06:46 PM EDT

PDB ID	:	8DK7
Title	:	Crystal structure of theophylline aptamer soaked with TAL2
Authors	:	Menichelli, E.; Spraggon, G.
Deposited on	:	2022-07-04
Resolution	:	2.46 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

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

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

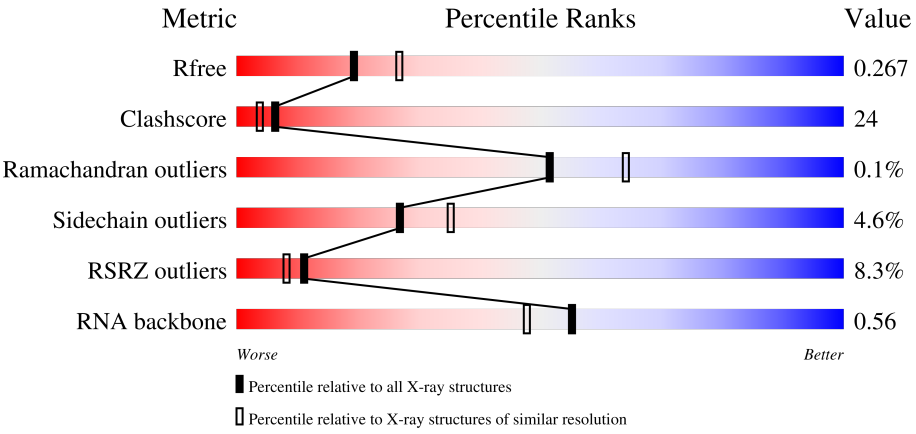
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.46 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)
RNA backbone	3102	1001 (2.80-2.12)

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	11% 56% 40%
1	E	214	6% 52% 43%
2	B	229	5% 76% 21%
2	D	229	5% 76% 20%

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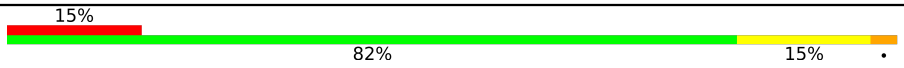
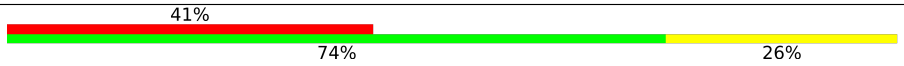
Mol	Chain	Length	Quality of chain
3	C	34	
3	F	34	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8052 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 FAB light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1611	1007	270	329	5			
1	E	211	Total	C	N	O	S	0	0	0
			1620	1013	272	330	5			

- Molecule 2 is a protein called FAB heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	223	Total	C	N	O	S	0	0	0
			1666	1049	285	327	5			
2	D	223	Total	C	N	O	S	0	0	0
			1666	1049	285	327	5			

- Molecule 3 is a RNA chain called RNA (34-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	34	Total	C	N	O	P	0	0	0
			723	324	134	232	33			
3	F	34	Total	C	N	O	P	0	0	0
			723	324	134	232	33			

- Molecule 4 is water.

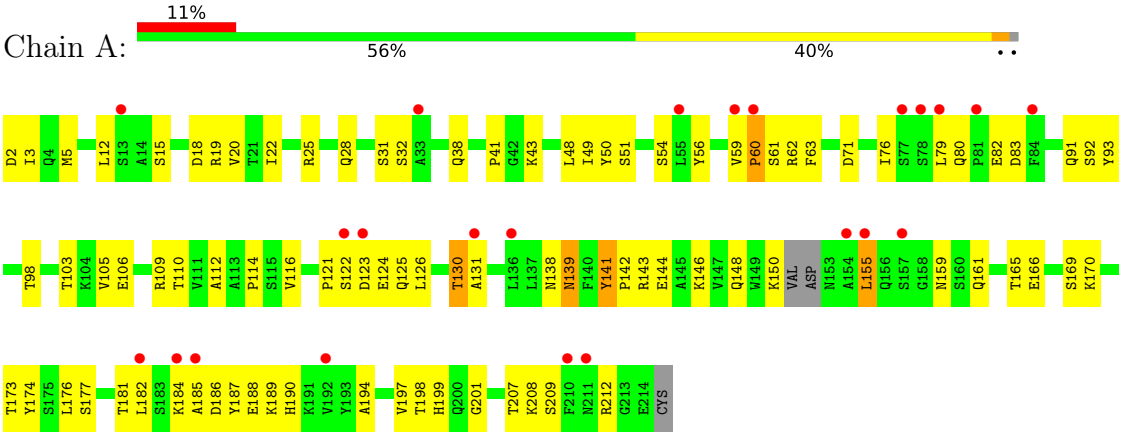
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		
4	B	19	Total	O	0	0
			19	19		
4	D	19	Total	O	0	0
			19	19		
4	E	3	Total	O	0	0
			3	3		

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.

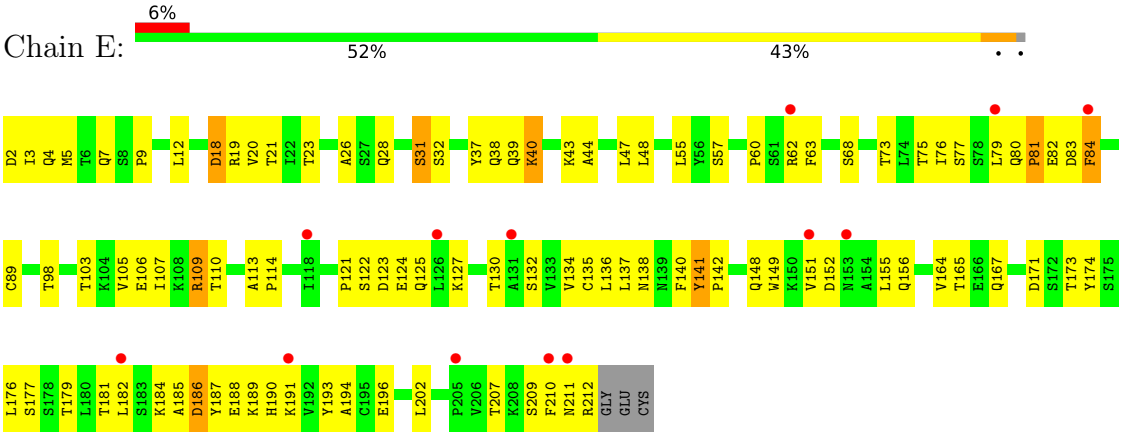
• Molecule 1: FAB light chain

Chain A:



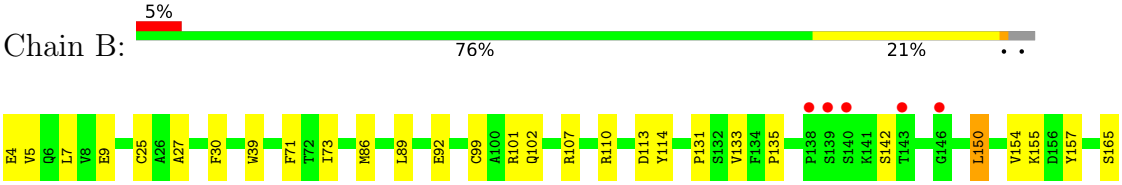
• Molecule 1: FAB light chain

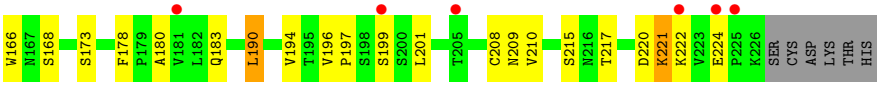
Chain E:



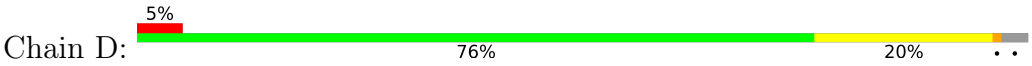
• Molecule 2: FAB heavy chain

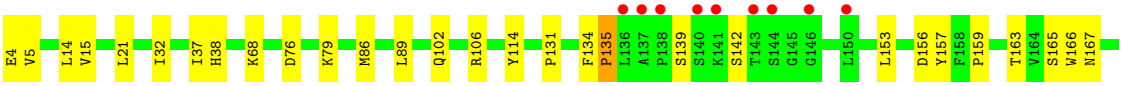
Chain B:

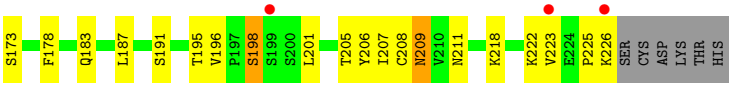




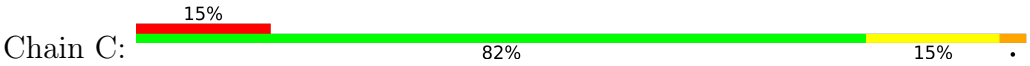
• Molecule 2: FAB heavy chain

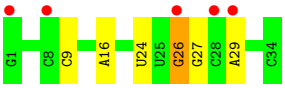




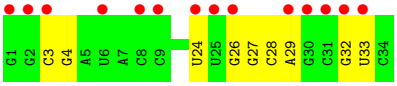


• Molecule 3: RNA (34-MER)





• Molecule 3: RNA (34-MER)



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	38.39Å 90.11Å 93.75Å 83.53° 89.40° 84.57°	Depositor
Resolution (Å)	89.14 – 2.46 93.15 – 2.46	Depositor EDS
% Data completeness (in resolution range)	92.1 (89.14-2.46) 86.6 (93.15-2.46)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.246 , 0.270 0.245 , 0.267	Depositor DCC
R_{free} test set	2106 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	44.8	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 52.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8052	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.44	2/1645 (0.1%)	0.61	1/2232 (0.0%)
1	E	0.33	1/1655 (0.1%)	0.55	1/2247 (0.0%)
2	B	3.66	1/1707 (0.1%)	1.36	3/2323 (0.1%)
2	D	0.64	2/1707 (0.1%)	0.61	2/2323 (0.1%)
3	C	0.13	0/808	0.68	0/1258
3	F	0.12	0/808	0.67	0/1258
All	All	1.70	6/8330 (0.1%)	0.82	7/11641 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	197	PRO	N-CD	150.65	3.58	1.47
2	D	135	PRO	N-CD	21.66	1.78	1.47
2	D	225	PRO	N-CD	-10.88	1.32	1.47
1	A	41	PRO	N-CD	-8.01	1.36	1.47
1	E	81	PRO	N-CD	-6.37	1.39	1.47
1	A	60	PRO	N-CD	-5.46	1.40	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	197	PRO	N-CD-CG	-54.07	22.09	103.20
2	B	197	PRO	CA-N-CD	-24.17	77.66	111.50
2	B	196	VAL	C-N-CD	12.22	154.06	128.40
2	D	135	PRO	CA-N-CD	-11.44	95.49	111.50
2	D	135	PRO	N-CD-CG	-6.04	94.14	103.20
1	E	152	ASP	CB-CG-OD2	5.21	122.98	118.30
1	A	155	LEU	CA-CB-CG	-5.00	103.79	115.30

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	1611	0	1552	113	0
1	E	1620	0	1570	150	0
2	B	1666	0	1628	59	0
2	D	1666	0	1625	67	0
3	C	723	0	372	3	0
3	F	723	0	372	0	0
4	A	2	0	0	0	0
4	B	19	0	0	7	0
4	D	19	0	0	0	0
4	E	3	0	0	0	0
All	All	8052	0	7119	364	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (364) 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:E:151:VAL:CG2	1:E:156:GLN:HE21	1.29	1.42
1:E:189:LYS:HD3	1:E:190:HIS:CD2	1.56	1.39
2:D:135:PRO:CD	2:D:135:PRO:N	1.78	1.36
1:E:23:THR:HG22	1:E:73:THR:CG2	1.58	1.30
1:E:23:THR:CG2	1:E:73:THR:HG22	1.62	1.29
2:B:107:ARG:O	2:B:107:ARG:HD3	1.19	1.28
1:E:151:VAL:HG22	1:E:156:GLN:NE2	0.95	1.26
1:A:25:ARG:HH21	1:A:71:ASP:CG	1.40	1.22
1:A:15:SER:O	1:A:18:ASP:OD2	1.57	1.22
1:A:25:ARG:NH2	1:A:71:ASP:OD2	1.74	1.20
2:B:107:ARG:HD3	2:B:107:ARG:C	1.59	1.17
1:A:25:ARG:NH2	1:A:71:ASP:CG	1.98	1.17
1:A:126:LEU:CA	1:A:184:LYS:HE3	1.62	1.17
1:E:191:LYS:CG	1:E:211:ASN:HD21	1.56	1.16
1:E:151:VAL:CG2	1:E:156:GLN:NE2	1.91	1.15
1:E:151:VAL:N	1:E:156:GLN:HE22	1.45	1.14
1:E:127:LYS:HD2	1:E:127:LYS:O	1.45	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ARG:HH12	1:A:112:ALA:HB2	1.02	1.13
1:E:171:ASP:OD1	1:E:173:THR:HG23	1.49	1.12
2:B:30:PHE:N	4:B:301:HOH:O	1.82	1.11
1:A:25:ARG:NE	1:A:71:ASP:OD2	1.82	1.11
1:E:19:ARG:HG3	1:E:77:SER:HA	1.16	1.11
1:E:23:THR:HG22	1:E:73:THR:HG23	1.30	1.11
1:A:25:ARG:NH2	1:A:71:ASP:OD1	1.84	1.11
2:D:211:ASN:OD1	2:D:218:LYS:HD3	1.50	1.10
1:E:127:LYS:HD2	1:E:127:LYS:C	1.70	1.10
1:A:62:ARG:NH1	1:A:82:GLU:OE2	1.86	1.09
1:A:150:LYS:CB	1:A:194:ALA:O	2.01	1.08
1:E:23:THR:CG2	1:E:73:THR:CG2	2.22	1.07
1:E:191:LYS:HG2	1:E:211:ASN:HD21	1.14	1.06
1:A:25:ARG:CZ	1:A:71:ASP:OD2	2.03	1.06
2:D:178:PHE:CE2	1:E:177:SER:HB3	1.89	1.06
1:E:23:THR:HG23	1:E:73:THR:HG22	1.35	1.05
2:B:30:PHE:CD1	4:B:301:HOH:O	2.09	1.05
2:D:205:THR:HG22	2:D:222:LYS:NZ	1.70	1.04
1:E:5:MET:HE2	1:E:26:ALA:HA	1.39	1.04
1:E:188:GLU:O	1:E:212:ARG:NH2	1.65	1.04
1:E:191:LYS:HG2	1:E:211:ASN:ND2	1.74	1.03
1:A:109:ARG:NH1	1:A:112:ALA:HB2	1.74	1.02
1:A:126:LEU:HA	1:A:184:LYS:CE	1.89	1.01
1:A:126:LEU:HA	1:A:184:LYS:HE3	1.04	1.01
2:B:133:VAL:HG22	2:B:154:VAL:HG12	1.37	1.00
1:A:186:ASP:HA	1:A:189:LYS:HE2	1.42	1.00
2:D:205:THR:HG22	2:D:222:LYS:HZ1	1.25	1.00
1:E:151:VAL:H	1:E:156:GLN:HE22	1.07	0.98
2:D:205:THR:CG2	2:D:222:LYS:NZ	2.27	0.98
1:E:189:LYS:NZ	1:E:190:HIS:NE2	2.09	0.98
2:D:205:THR:CB	2:D:222:LYS:NZ	2.27	0.97
1:E:189:LYS:HD3	1:E:190:HIS:HD2	1.23	0.97
1:E:9:PRO:O	1:E:103:THR:HG22	1.66	0.96
1:A:76:ILE:HD11	1:A:83:ASP:OD1	1.67	0.94
1:A:109:ARG:HH12	1:A:112:ALA:CB	1.79	0.94
1:E:55:LEU:HD11	1:E:63:PHE:O	1.68	0.94
2:D:32:ILE:HG22	2:D:37:ILE:HD11	1.49	0.93
2:D:205:THR:CG2	2:D:222:LYS:HZ3	1.79	0.93
1:A:22:ILE:HD11	1:A:103:THR:HG21	1.50	0.92
2:D:226:LYS:HE3	1:E:123:ASP:OD1	1.69	0.92
2:B:107:ARG:O	2:B:107:ARG:CD	2.15	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ILE:HG23	1:A:54:SER:O	1.70	0.92
1:A:50:TYR:HD1	1:A:51:SER:HG	1.19	0.90
1:E:62:ARG:HH11	1:E:80:GLN:HG3	1.36	0.90
1:E:189:LYS:CD	1:E:190:HIS:CD2	2.51	0.90
1:A:62:ARG:HH11	1:A:80:GLN:HG3	1.33	0.90
2:D:178:PHE:CD1	1:E:165:THR:HG23	2.07	0.89
2:D:205:THR:HB	2:D:222:LYS:NZ	1.88	0.89
1:E:193:TYR:HB2	1:E:210:PHE:CZ	2.08	0.89
2:B:9:GLU:OE1	2:B:99:CYS:N	2.06	0.87
2:D:205:THR:CB	2:D:222:LYS:HZ3	1.88	0.87
1:A:76:ILE:CD1	1:A:83:ASP:OD1	2.22	0.87
1:A:116:VAL:HG21	1:A:197:VAL:HG11	1.56	0.85
1:E:191:LYS:CG	1:E:211:ASN:ND2	2.33	0.85
1:E:151:VAL:H	1:E:156:GLN:NE2	1.75	0.85
1:E:23:THR:HG22	1:E:73:THR:HG22	1.30	0.84
1:A:38:GLN:HB2	1:A:48:LEU:HD11	1.59	0.83
1:A:188:GLU:HA	1:A:212:ARG:NH1	1.94	0.83
1:A:5:MET:CE	1:A:91:GLN:HB3	2.07	0.83
1:A:20:VAL:HG23	1:A:76:ILE:HG22	1.61	0.83
1:E:5:MET:CE	1:E:26:ALA:HA	2.09	0.83
1:A:144:GLU:OE1	1:A:144:GLU:N	2.14	0.81
2:B:133:VAL:HG21	2:B:210:VAL:HG11	1.61	0.81
1:A:15:SER:N	1:A:18:ASP:OD2	2.13	0.81
1:A:22:ILE:CD1	1:A:103:THR:HG21	2.12	0.80
2:D:86:MET:HB3	2:D:89:LEU:HD11	1.63	0.79
2:B:133:VAL:HG22	2:B:154:VAL:CG1	2.12	0.79
1:E:189:LYS:HD3	1:E:190:HIS:NE2	1.96	0.79
1:A:92:SER:O	2:B:110:ARG:NH1	2.15	0.79
2:B:92:GLU:N	2:B:92:GLU:OE1	2.15	0.79
2:D:178:PHE:CE1	1:E:165:THR:HG23	2.17	0.78
1:A:62:ARG:CZ	1:A:82:GLU:OE2	2.32	0.78
2:D:205:THR:HB	2:D:222:LYS:HZ3	1.44	0.78
1:A:15:SER:C	1:A:18:ASP:OD2	2.22	0.77
1:E:19:ARG:HG3	1:E:77:SER:CA	2.06	0.76
1:E:151:VAL:HG12	1:E:193:TYR:CE1	2.20	0.76
1:A:22:ILE:HD11	1:A:103:THR:CG2	2.16	0.76
1:A:56:TYR:O	1:A:59:VAL:HG22	1.85	0.76
2:B:150:LEU:HD11	2:B:194:VAL:CG1	2.16	0.76
1:A:5:MET:HE1	1:A:91:GLN:HB3	1.69	0.75
2:B:30:PHE:CG	4:B:301:HOH:O	2.34	0.75
1:E:189:LYS:O	1:E:189:LYS:HG2	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ARG:NH2	1:A:82:GLU:OE2	2.23	0.72
2:D:76:ASP:OD2	2:D:79:LYS:HE2	1.89	0.72
2:D:178:PHE:CD2	1:E:177:SER:HB3	2.24	0.71
2:B:30:PHE:CA	4:B:301:HOH:O	2.28	0.71
1:E:84:PHE:O	1:E:84:PHE:CD1	2.43	0.71
1:E:60:PRO:HG2	1:E:62:ARG:HH21	1.55	0.71
2:D:135:PRO:HD2	1:E:122:SER:HB3	1.73	0.70
1:A:139:ASN:OD1	1:A:173:THR:OG1	2.04	0.70
1:A:49:ILE:CD1	1:A:54:SER:O	2.38	0.70
1:A:106:GLU:OE2	1:A:174:TYR:OH	2.10	0.70
1:E:60:PRO:HG2	1:E:62:ARG:HE	1.56	0.69
1:E:4:GLN:O	1:E:5:MET:CE	2.40	0.68
1:E:19:ARG:CG	1:E:77:SER:HA	2.09	0.68
1:A:5:MET:HE2	1:A:91:GLN:HB3	1.73	0.68
1:E:4:GLN:O	1:E:5:MET:HE3	1.94	0.68
2:D:134:PHE:CE2	1:E:125:GLN:HG3	2.29	0.67
1:A:186:ASP:HA	1:A:189:LYS:CE	2.23	0.67
2:B:150:LEU:CD1	2:B:194:VAL:CG1	2.72	0.67
2:B:30:PHE:O	4:B:301:HOH:O	2.11	0.67
1:E:81:PRO:HD2	1:E:82:GLU:OE1	1.95	0.67
2:D:135:PRO:HD2	1:E:122:SER:CB	2.25	0.67
1:A:109:ARG:HD3	1:A:110:THR:O	1.96	0.66
1:E:151:VAL:HG12	1:E:193:TYR:HE1	1.61	0.66
1:E:127:LYS:C	1:E:127:LYS:CD	2.48	0.66
1:A:165:THR:HG22	1:A:166:GLU:N	2.11	0.65
1:E:38:GLN:HB2	1:E:48:LEU:HD11	1.77	0.65
2:B:39:TRP:HD1	2:B:73:ILE:HD12	1.62	0.65
2:D:178:PHE:HD1	1:E:165:THR:HG23	1.62	0.65
1:E:62:ARG:HH11	1:E:80:GLN:CG	2.08	0.65
1:E:60:PRO:CG	1:E:62:ARG:HH21	2.09	0.65
1:E:171:ASP:CG	1:E:173:THR:HG23	2.18	0.65
1:E:189:LYS:CE	1:E:190:HIS:NE2	2.60	0.65
2:D:167:ASN:HA	2:D:207:ILE:HG12	1.78	0.64
1:E:191:LYS:HG3	1:E:211:ASN:HD21	1.55	0.64
1:A:130:THR:O	1:A:184:LYS:HE2	1.97	0.64
2:D:15:VAL:HG11	2:D:21:LEU:HG	1.79	0.64
2:B:168:SER:H	2:B:209:ASN:HD21	1.46	0.64
1:A:122:SER:HB3	2:B:135:PRO:HD2	1.80	0.63
1:E:5:MET:CE	1:E:5:MET:HA	2.29	0.63
2:B:27:ALA:O	2:D:79:LYS:NZ	2.32	0.63
1:E:62:ARG:O	1:E:76:ILE:HG13	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:167:ASN:HD21	2:D:206:TYR:HA	1.63	0.63
1:E:136:LEU:HD21	1:E:138:ASN:HD22	1.64	0.63
2:B:7:LEU:HD22	2:B:25:CYS:SG	2.38	0.62
1:E:82:GLU:OE1	1:E:82:GLU:N	2.32	0.62
1:A:15:SER:CA	1:A:18:ASP:OD2	2.47	0.62
2:D:135:PRO:CD	1:E:122:SER:HB3	2.28	0.62
1:E:121:PRO:HB3	1:E:132:SER:H	1.63	0.62
2:B:107:ARG:C	2:B:107:ARG:CD	2.41	0.62
2:D:135:PRO:HD2	2:D:135:PRO:O	1.98	0.62
1:A:161:GLN:HE22	2:B:183:GLN:HA	1.65	0.62
2:B:215:SER:OG	2:B:217:THR:OG1	2.15	0.61
2:B:113:ASP:OD2	2:B:114:TYR:HD2	1.83	0.61
2:D:135:PRO:HG2	2:D:226:LYS:NZ	2.15	0.61
2:D:226:LYS:HE3	1:E:123:ASP:CG	2.21	0.60
1:A:62:ARG:HH11	1:A:80:GLN:CG	2.11	0.60
2:B:113:ASP:OD2	2:B:114:TYR:CD2	2.54	0.60
1:E:189:LYS:CD	1:E:190:HIS:NE2	2.63	0.60
2:B:150:LEU:HD11	2:B:194:VAL:HG13	1.84	0.60
1:A:20:VAL:CG2	1:A:76:ILE:HG22	2.32	0.60
1:E:12:LEU:HD11	1:E:105:VAL:HG13	1.84	0.59
1:A:49:ILE:HD12	1:A:54:SER:O	1.71	0.59
1:A:123:ASP:HA	1:A:126:LEU:HD23	1.85	0.59
1:A:176:LEU:HD23	1:A:177:SER:N	2.18	0.59
2:B:71:PHE:CZ	2:B:86:MET:HG2	2.38	0.59
1:E:137:LEU:HD22	1:E:176:LEU:HD22	1.84	0.59
1:E:62:ARG:NH1	1:E:80:GLN:CB	2.66	0.59
2:B:131:PRO:HB3	2:B:157:TYR:HB3	1.84	0.58
2:D:211:ASN:OD1	2:D:218:LYS:CD	2.41	0.58
1:E:62:ARG:NH1	1:E:80:GLN:HB2	2.18	0.58
2:D:5:VAL:HG12	2:D:114:TYR:CD2	2.39	0.58
1:E:84:PHE:CD1	1:E:84:PHE:C	2.77	0.58
1:E:148:GLN:HG2	1:E:155:LEU:CD1	2.33	0.58
1:E:62:ARG:NH1	1:E:80:GLN:HG3	2.14	0.57
2:D:131:PRO:HB3	2:D:157:TYR:HB3	1.85	0.57
2:D:142:SER:OG	2:D:201:LEU:O	2.21	0.57
1:E:5:MET:HE2	1:E:5:MET:HA	1.86	0.57
1:E:31:SER:OG	1:E:32:SER:N	2.38	0.57
1:E:188:GLU:HA	1:E:212:ARG:CD	2.28	0.57
2:B:150:LEU:CD1	2:B:194:VAL:HG12	2.35	0.57
1:E:39:GLN:HA	1:E:43:LYS:HD2	1.85	0.57
2:B:30:PHE:C	4:B:301:HOH:O	2.42	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:153:LEU:HD23	2:D:191:SER:OG	2.05	0.56
1:E:4:GLN:C	1:E:5:MET:HE3	2.25	0.56
2:D:226:LYS:O	2:D:226:LYS:HG3	2.05	0.56
2:B:221:LYS:CA	2:B:221:LYS:HE2	2.34	0.56
1:A:143:ARG:HG3	1:A:174:TYR:CD2	2.40	0.56
1:E:171:ASP:OD1	1:E:171:ASP:C	2.44	0.56
1:A:122:SER:O	1:A:126:LEU:HD22	2.05	0.56
1:A:188:GLU:HA	1:A:212:ARG:CZ	2.35	0.56
1:A:194:ALA:HB2	1:A:209:SER:HB3	1.86	0.56
2:B:110:ARG:HD3	3:C:16:A:C5	2.41	0.56
2:B:142:SER:OG	2:B:201:LEU:O	2.22	0.55
2:D:205:THR:HB	2:D:222:LYS:HZ2	1.70	0.55
1:E:113:ALA:HB1	1:E:202:LEU:CD2	2.36	0.55
1:E:151:VAL:N	1:E:156:GLN:NE2	2.29	0.55
2:D:198:SER:HA	2:D:201:LEU:CD2	2.36	0.55
1:A:207:THR:HG23	1:A:207:THR:O	2.07	0.55
1:E:60:PRO:CG	1:E:62:ARG:HE	2.20	0.55
2:D:178:PHE:CD1	1:E:165:THR:CG2	2.87	0.54
1:E:2:ASP:N	1:E:2:ASP:OD1	2.41	0.54
1:E:151:VAL:CB	1:E:156:GLN:NE2	2.68	0.54
2:D:205:THR:CA	2:D:222:LYS:NZ	2.71	0.54
1:E:191:LYS:HG3	1:E:211:ASN:ND2	2.18	0.54
1:E:148:GLN:HG2	1:E:155:LEU:HD13	1.89	0.53
1:E:107:ILE:O	1:E:167:GLN:NE2	2.41	0.53
1:A:177:SER:HB3	2:B:178:PHE:CE1	2.43	0.53
2:D:135:PRO:HD2	1:E:122:SER:OG	2.09	0.53
1:E:60:PRO:C	1:E:62:ARG:H	2.09	0.53
1:A:76:ILE:HG23	1:A:76:ILE:O	2.07	0.53
1:A:109:ARG:HD3	1:A:110:THR:N	2.24	0.53
2:D:106:ARG:O	2:D:106:ARG:HG2	2.08	0.52
2:D:205:THR:CB	2:D:222:LYS:HZ2	2.21	0.52
1:E:43:LYS:HD3	1:E:44:ALA:O	2.10	0.52
1:E:60:PRO:HG2	1:E:62:ARG:NH2	2.23	0.52
1:A:62:ARG:O	1:A:76:ILE:HA	2.10	0.52
1:A:122:SER:CB	2:B:135:PRO:HD2	2.40	0.52
2:B:150:LEU:HD12	2:B:150:LEU:O	2.09	0.52
2:B:166:TRP:CH2	2:B:208:CYS:HB3	2.45	0.52
1:A:22:ILE:CD1	1:A:103:THR:CG2	2.83	0.52
1:A:199:HIS:CD2	1:A:201:GLY:H	2.28	0.52
1:A:2:ASP:OD2	1:A:2:ASP:N	2.41	0.52
1:A:186:ASP:CA	1:A:189:LYS:HE2	2.29	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:113:ALA:HB1	1:E:202:LEU:HD21	1.92	0.52
2:B:209:ASN:HA	2:B:220:ASP:OD1	2.11	0.51
2:D:183:GLN:HG3	2:D:187:LEU:O	2.10	0.51
1:E:193:TYR:HB2	1:E:210:PHE:CE1	2.46	0.51
1:A:60:PRO:HG2	1:A:63:PHE:HE1	1.76	0.51
1:A:31:SER:OG	1:A:32:SER:N	2.41	0.51
1:E:5:MET:HE1	1:E:26:ALA:CB	2.41	0.51
1:A:62:ARG:NH1	1:A:80:GLN:HG3	2.15	0.51
1:A:15:SER:O	1:A:18:ASP:CG	2.44	0.51
2:D:167:ASN:HA	2:D:207:ILE:CG1	2.40	0.50
2:D:167:ASN:ND2	2:D:207:ILE:H	2.09	0.50
2:B:150:LEU:HD12	2:B:194:VAL:HG12	1.93	0.50
2:B:150:LEU:HD12	2:B:150:LEU:C	2.32	0.50
1:A:82:GLU:HG2	1:A:83:ASP:OD2	2.12	0.50
1:A:181:THR:OG1	1:A:182:LEU:N	2.45	0.50
2:B:113:ASP:OD2	2:B:113:ASP:C	2.50	0.50
1:E:21:THR:HG22	1:E:75:THR:OG1	2.10	0.50
1:E:109:ARG:HD3	1:E:110:THR:O	2.12	0.50
2:D:32:ILE:CG2	2:D:37:ILE:HD11	2.31	0.50
1:A:165:THR:HG22	1:A:166:GLU:H	1.77	0.50
2:D:166:TRP:CZ3	2:D:223:VAL:HG21	2.46	0.50
1:A:3:ILE:HD12	1:A:91:GLN:NE2	2.27	0.49
1:A:12:LEU:HD11	1:A:105:VAL:HG22	1.94	0.49
1:E:135:CYS:HB2	1:E:149:TRP:CH2	2.48	0.49
2:B:221:LYS:HE2	2:B:221:LYS:HA	1.94	0.49
2:D:195:THR:CG2	1:E:138:ASN:ND2	2.76	0.49
1:E:141:TYR:CD2	1:E:142:PRO:N	2.80	0.49
2:B:155:LYS:HE2	2:B:183:GLN:HE22	1.78	0.48
1:A:38:GLN:HB2	1:A:48:LEU:CD1	2.39	0.48
1:A:109:ARG:CZ	1:A:112:ALA:HB2	2.38	0.48
1:E:141:TYR:CD2	1:E:141:TYR:C	2.87	0.48
2:B:39:TRP:CD1	2:B:73:ILE:HD12	2.46	0.48
1:A:131:ALA:HB2	1:A:184:LYS:HD3	1.96	0.48
2:D:135:PRO:CD	1:E:122:SER:CB	2.88	0.48
1:E:7:GLN:OE1	1:E:89:CYS:N	2.39	0.48
1:A:123:ASP:OD1	1:A:124:GLU:N	2.46	0.48
1:E:186:ASP:OD1	1:E:186:ASP:N	2.46	0.48
1:A:50:TYR:HD1	1:A:51:SER:OG	1.88	0.48
1:A:76:ILE:HG21	1:A:79:LEU:HD12	1.95	0.48
2:B:101:ARG:NH2	4:B:303:HOH:O	2.31	0.48
1:E:4:GLN:O	1:E:5:MET:HE2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:135:PRO:HG2	2:D:226:LYS:HZ2	1.78	0.48
1:E:63:PHE:CE1	1:E:76:ILE:HD12	2.49	0.47
1:A:25:ARG:CZ	1:A:71:ASP:CG	2.66	0.47
1:A:20:VAL:CG2	1:A:76:ILE:CG2	2.92	0.47
1:E:60:PRO:HG2	1:E:62:ARG:NE	2.26	0.47
1:A:121:PRO:HB2	1:A:184:LYS:NZ	2.29	0.47
1:E:62:ARG:O	1:E:76:ILE:HA	2.15	0.47
1:A:114:PRO:HD3	1:A:199:HIS:CD2	2.50	0.47
1:A:141:TYR:HD1	1:A:142:PRO:CA	2.28	0.47
1:E:114:PRO:HB3	1:E:140:PHE:CD2	2.50	0.47
1:E:193:TYR:CB	1:E:210:PHE:CZ	2.90	0.47
1:E:135:CYS:HB2	1:E:149:TRP:CZ2	2.50	0.47
1:E:194:ALA:HA	1:E:209:SER:HA	1.97	0.47
1:A:138:ASN:OD1	1:A:139:ASN:N	2.48	0.47
2:D:5:VAL:CG1	2:D:114:TYR:CD2	2.98	0.47
2:D:134:PHE:CD2	1:E:125:GLN:HG3	2.50	0.47
1:A:165:THR:CG2	1:A:166:GLU:N	2.77	0.46
1:A:49:ILE:HG23	1:A:54:SER:C	2.35	0.46
1:A:138:ASN:OD1	1:A:139:ASN:HB2	2.14	0.46
2:B:7:LEU:HD22	2:B:99:CYS:SG	2.56	0.46
2:D:165:SER:OG	2:D:209:ASN:OD1	2.28	0.46
1:A:142:PRO:HB2	1:A:144:GLU:OE1	2.15	0.46
1:A:159:ASN:N	1:A:159:ASN:OD1	2.49	0.46
1:E:181:THR:OG1	1:E:182:LEU:N	2.49	0.46
1:A:49:ILE:CG2	1:A:50:TYR:N	2.78	0.46
1:A:190:HIS:O	1:A:212:ARG:NH1	2.49	0.46
1:E:141:TYR:CD2	1:E:142:PRO:CA	2.99	0.46
1:E:188:GLU:HA	1:E:212:ARG:HD2	1.98	0.46
1:E:196:GLU:HA	1:E:207:THR:HA	1.98	0.46
1:E:130:THR:HG22	1:E:184:LYS:HZ2	1.80	0.46
1:E:5:MET:CE	1:E:26:ALA:CA	2.91	0.46
1:A:188:GLU:O	1:A:212:ARG:NH2	2.48	0.45
2:B:150:LEU:CD1	2:B:194:VAL:HG13	2.42	0.45
1:E:18:ASP:OD1	1:E:18:ASP:N	2.49	0.45
1:A:122:SER:O	1:A:125:GLN:N	2.46	0.45
1:A:187:TYR:O	1:A:212:ARG:NH1	2.50	0.45
1:A:148:GLN:HG2	1:A:155:LEU:HD13	1.98	0.45
1:E:81:PRO:CD	1:E:82:GLU:OE1	2.65	0.45
1:E:171:ASP:OD1	1:E:173:THR:N	2.49	0.45
1:A:109:ARG:NH1	1:A:112:ALA:CB	2.56	0.44
1:A:76:ILE:O	1:A:76:ILE:CG2	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:LEU:CD1	1:E:105:VAL:HG13	2.45	0.44
2:D:135:PRO:HG2	2:D:226:LYS:HZ1	1.81	0.44
1:E:185:ALA:C	1:E:187:TYR:H	2.21	0.44
2:B:180:ALA:HA	2:B:190:LEU:HB3	2.00	0.44
2:B:190:LEU:C	2:B:190:LEU:HD12	2.38	0.44
1:E:62:ARG:NH1	1:E:80:GLN:CG	2.79	0.43
2:D:205:THR:HA	2:D:222:LYS:NZ	2.33	0.43
1:E:134:VAL:HG22	1:E:179:THR:HG22	2.00	0.43
2:D:135:PRO:HD2	1:E:122:SER:HG	1.83	0.43
2:D:178:PHE:CD2	1:E:177:SER:CB	2.99	0.43
1:E:60:PRO:CG	1:E:62:ARG:NH2	2.81	0.43
1:A:109:ARG:NH1	1:A:110:THR:O	2.44	0.43
2:D:195:THR:CG2	1:E:138:ASN:HD21	2.30	0.43
1:A:82:GLU:N	1:A:82:GLU:OE1	2.52	0.43
1:A:19:ARG:HG2	1:A:19:ARG:HH11	1.84	0.43
2:B:150:LEU:HD12	2:B:194:VAL:CG1	2.48	0.43
2:B:221:LYS:HA	2:B:221:LYS:CE	2.47	0.43
1:E:37:TYR:CE1	1:E:47:LEU:HD13	2.53	0.43
1:E:76:ILE:HD13	1:E:79:LEU:HD23	2.01	0.42
2:B:222:LYS:HE3	2:B:224:GLU:HG3	2.00	0.42
3:C:9:C:H42	3:C:26:G:H22	1.67	0.42
2:D:38:HIS:NE2	2:D:102:GLN:OE1	2.50	0.42
1:E:107:ILE:HB	1:E:167:GLN:NE2	2.34	0.42
2:D:14:LEU:HD22	2:D:159:PRO:HG3	2.00	0.42
1:E:141:TYR:CD2	1:E:142:PRO:HA	2.55	0.42
2:B:86:MET:HB3	2:B:89:LEU:HD21	2.02	0.42
2:D:156:ASP:OD1	2:D:183:GLN:NE2	2.53	0.42
1:E:106:GLU:OE2	1:E:174:TYR:OH	2.31	0.42
1:E:190:HIS:O	1:E:191:LYS:HB3	2.20	0.42
1:E:23:THR:HG23	1:E:73:THR:CG2	2.18	0.42
1:A:177:SER:HB3	2:B:178:PHE:CD1	2.55	0.42
2:D:166:TRP:HA	2:D:207:ILE:O	2.20	0.41
1:A:116:VAL:HG12	1:A:208:LYS:HG3	2.02	0.41
1:E:62:ARG:HH11	1:E:80:GLN:CB	2.29	0.41
1:A:19:ARG:HG2	1:A:19:ARG:NH1	2.34	0.41
2:B:4:GLU:CG	2:B:5:VAL:N	2.83	0.41
1:A:43:LYS:HA	1:A:43:LYS:HD3	1.78	0.41
1:A:91:GLN:OE1	1:A:93:TYR:N	2.50	0.41
1:E:5:MET:CE	1:E:5:MET:CA	2.99	0.41
1:A:49:ILE:HD13	1:A:56:TYR:H	1.78	0.41
2:D:135:PRO:CD	2:D:135:PRO:O	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:163:THR:OG1	2:D:211:ASN:HB2	2.21	0.41
1:E:164:VAL:HG22	1:E:176:LEU:HD12	2.02	0.41
1:A:49:ILE:HD13	1:A:49:ILE:HA	1.89	0.41
1:A:176:LEU:HD23	1:A:176:LEU:C	2.41	0.41
1:E:40:LYS:HG3	1:E:43:LYS:HE2	2.01	0.41
1:E:123:ASP:OD1	1:E:124:GLU:N	2.54	0.41
1:E:140:PHE:CD1	1:E:140:PHE:C	2.94	0.41
2:B:4:GLU:HG3	2:B:5:VAL:H	1.86	0.41
1:E:3:ILE:O	1:E:98:THR:HG21	2.21	0.40
1:E:113:ALA:HB1	1:E:202:LEU:HD23	2.03	0.40
1:E:130:THR:HA	1:E:184:LYS:HZ2	1.86	0.40
1:E:189:LYS:HZ3	1:E:190:HIS:CE1	2.19	0.40
1:A:185:ALA:O	1:A:189:LYS:HG3	2.21	0.40
1:E:107:ILE:H	1:E:167:GLN:HE22	1.68	0.40
1:E:109:ARG:HG3	1:E:141:TYR:CD1	2.56	0.40
2:B:165:SER:HG	2:B:209:ASN:HD22	1.62	0.40
2:B:110:ARG:HD3	3:C:16:A:N7	2.36	0.40
2:D:196:VAL:HG11	2:D:206:TYR:CE1	2.57	0.40
2:D:207:ILE:O	2:D:207:ILE:HG13	2.21	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	207/214 (97%)	193 (93%)	13 (6%)	1 (0%)	29 34
1	E	209/214 (98%)	195 (93%)	14 (7%)	0	100 100
2	B	221/229 (96%)	216 (98%)	5 (2%)	0	100 100
2	D	221/229 (96%)	215 (97%)	6 (3%)	0	100 100
All	All	858/886 (97%)	819 (96%)	38 (4%)	1 (0%)	51 64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	184/189 (97%)	175 (95%)	9 (5%)	25	32
1	E	187/189 (99%)	175 (94%)	12 (6%)	17	21
2	B	184/190 (97%)	178 (97%)	6 (3%)	38	49
2	D	184/190 (97%)	177 (96%)	7 (4%)	33	43
All	All	739/758 (98%)	705 (95%)	34 (5%)	27	35

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	61	SER
1	A	98	THR
1	A	130	THR
1	A	141	TYR
1	A	146	LYS
1	A	169	SER
1	A	170	LYS
1	A	198	THR
2	B	102	GLN
2	B	150	LEU
2	B	173	SER
2	B	190	LEU
2	B	199	SER
2	B	221	LYS
2	D	4	GLU
2	D	68	LYS
2	D	139	SER
2	D	173	SER

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Mol	Chain	Res	Type
2	D	198	SER
2	D	208	CYS
2	D	209	ASN
1	E	18	ASP
1	E	20	VAL
1	E	28	GLN
1	E	31	SER
1	E	40	LYS
1	E	57	SER
1	E	68	SER
1	E	83	ASP
1	E	84	PHE
1	E	109	ARG
1	E	141	TYR
1	E	186	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	GLN
1	A	199	HIS
2	B	16	GLN
2	B	85	GLN
2	B	183	GLN
2	D	16	GLN
2	D	167	ASN
2	D	204	GLN
1	E	138	ASN
1	E	156	GLN
1	E	211	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	33/34 (97%)	4 (12%)	0
3	F	33/34 (97%)	8 (24%)	1 (3%)
All	All	66/68 (97%)	12 (18%)	1 (1%)

All (12) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	24	U
3	C	26	G
3	C	27	G
3	C	29	A
3	F	3	C
3	F	4	G
3	F	24	U
3	F	26	G
3	F	27	G
3	F	28	C
3	F	29	A
3	F	33	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	F	32	G

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	211/214 (98%)	0.74	23 (10%) 5 3	58, 86, 131, 189	0
1	E	211/214 (98%)	0.64	13 (6%) 20 17	50, 84, 137, 166	0
2	B	223/229 (97%)	0.43	11 (4%) 29 27	31, 58, 115, 157	0
2	D	223/229 (97%)	0.50	12 (5%) 25 23	32, 56, 126, 162	0
3	C	34/34 (100%)	0.69	5 (14%) 2 1	70, 151, 188, 204	0
3	F	34/34 (100%)	2.09	14 (41%) 0 0	61, 180, 235, 266	0
All	All	936/954 (98%)	0.63	78 (8%) 11 8	31, 77, 155, 266	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	1	G	7.5
1	A	182	LEU	6.4
3	F	30	G	6.4
3	F	33	U	6.2
2	D	140	SER	5.9
3	F	29	A	5.2
3	F	8	C	5.2
2	D	143	THR	5.2
3	C	28	C	5.1
3	F	26	G	4.9
2	B	225	PRO	4.5
2	D	146	GLY	4.3
2	B	143	THR	4.3
2	D	138	PRO	4.1
1	E	182	LEU	4.1
1	A	184	LYS	4.0
3	F	9	C	4.0
1	A	77	SER	3.8
1	E	205	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	153	ASN	3.8
3	F	31	C	3.7
1	A	211	ASN	3.7
2	B	146	GLY	3.6
1	E	84	PHE	3.6
2	D	199	SER	3.5
3	C	26	G	3.5
1	E	210	PHE	3.4
1	A	122	SER	3.4
1	A	84	PHE	3.3
2	D	137	ALA	3.2
1	A	81	PRO	3.2
3	F	32	G	3.2
1	A	155	LEU	3.2
1	A	131	ALA	3.1
2	D	223	VAL	3.1
3	F	6	U	3.0
3	F	24	U	2.9
1	A	154	ALA	2.9
1	A	59	VAL	2.9
1	A	157	SER	2.9
2	B	222	LYS	2.9
1	E	211	ASN	2.9
1	A	79	LEU	2.8
1	A	210	PHE	2.8
2	D	144	SER	2.8
3	C	29	A	2.8
1	A	60	PRO	2.7
2	D	141	LYS	2.7
3	F	3	C	2.7
1	E	126	LEU	2.7
1	A	192	VAL	2.6
3	C	8	C	2.5
2	D	136	LEU	2.4
3	F	25	U	2.4
1	A	55	LEU	2.4
1	A	123	ASP	2.4
2	B	224	GLU	2.4
2	B	138	PRO	2.4
1	E	118	ILE	2.3
1	E	79	LEU	2.3
2	D	150	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	78	SER	2.2
1	A	185	ALA	2.2
1	A	136	LEU	2.2
3	F	2	G	2.2
1	A	13	SER	2.2
1	E	62	ARG	2.1
1	E	151	VAL	2.1
2	B	181	VAL	2.1
2	B	199	SER	2.1
3	C	1	G	2.1
1	E	131	ALA	2.1
1	E	191	LYS	2.1
2	B	205	THR	2.0
2	B	139	SER	2.0
2	B	140	SER	2.0
1	A	33	ALA	2.0
2	D	226	LYS	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.