



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:19 AM UTC

PDB ID : 8DK7 / pdb_00008dk7
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

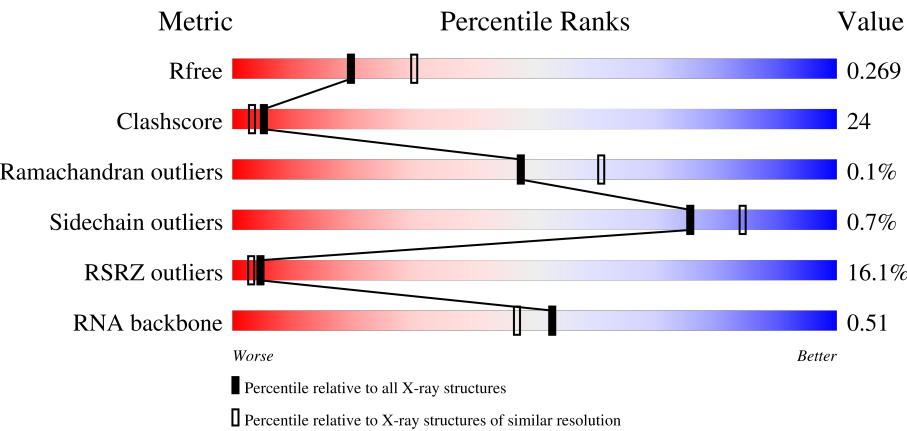
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)
RNA backbone	3983	1023 (2.72-2.20)

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 $\leq 5\%$. 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	21% 57% 39% ..
1	E	214	19% 54% 44% .
2	B	229	10% 76% 22% .
2	D	229	12% 77% 19% ..

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Mol	Chain	Length	Quality of chain
3	C	34	21% 82% 15%
3	F	34	18% 74% 26%

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			

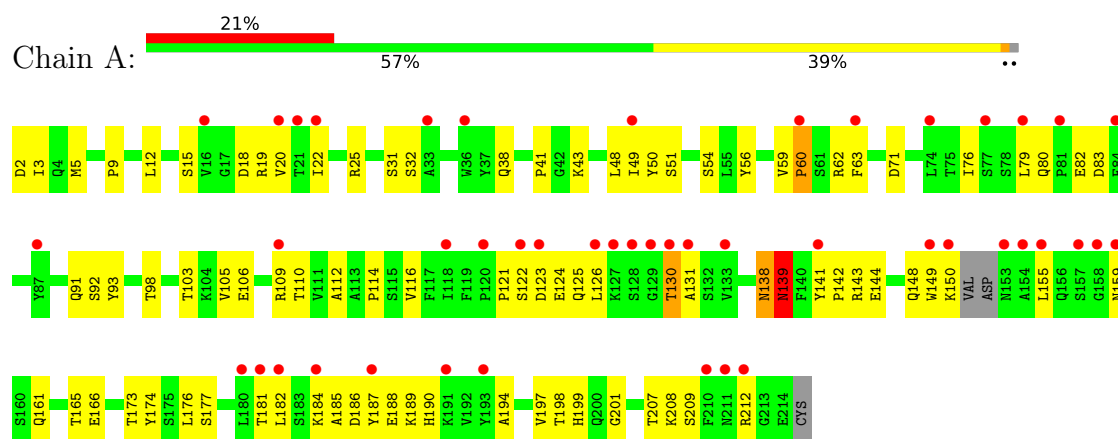
- Molecule 4 is water.

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		

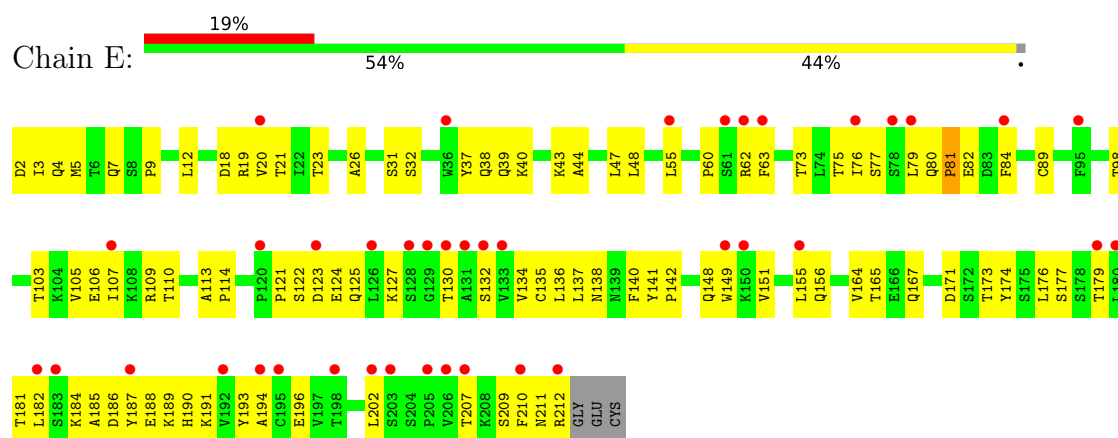
3 Residue-property plots [i](#)

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.

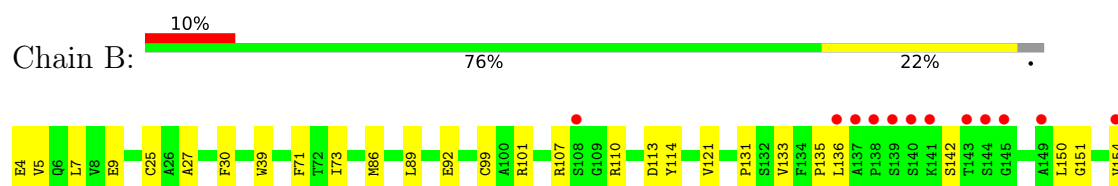
• Molecule 1: FAB light chain

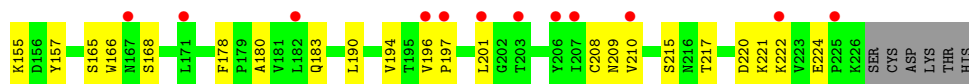


• Molecule 1: FAB light chain

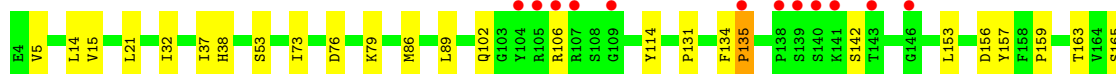
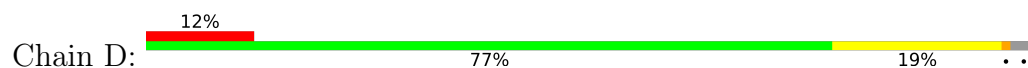


• Molecule 2: FAB heavy chain

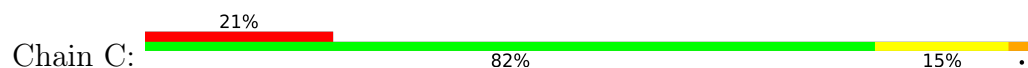




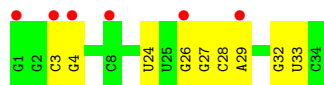
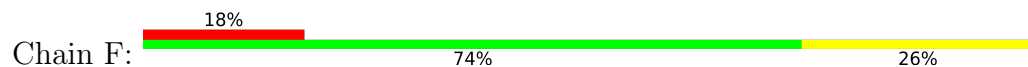
• Molecule 2: FAB heavy chain



• Molecule 3: RNA (34-MER)



• Molecule 3: RNA (34-MER)



4 Data and refinement statistics

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 89.14 – 2.46	Depositor EDS
% Data completeness (in resolution range)	92.1 (89.14-2.46) 86.5 (89.14-2.46)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.246 , 0.270 0.246 , 0.269	Depositor DCC
R_{free} test set	2106 reflections (4.54%)	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 , 63.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.42	2/1645 (0.1%)	0.53	3/2232 (0.1%)
1	E	0.23	1/1655 (0.1%)	0.40	0/2247
2	B	3.65	1/1707 (0.1%)	1.28	3/2323 (0.1%)
2	D	0.60	2/1707 (0.1%)	0.45	2/2323 (0.1%)
3	C	0.06	0/808	0.16	0/1258
3	F	0.07	0/808	0.18	0/1258
All	All	1.69	6/8330 (0.1%)	0.68	8/11641 (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	150.72	3.58	1.47
2	D	135	PRO	N-CD	21.73	1.78	1.47
2	D	225	PRO	N-CD	-10.80	1.32	1.47
1	A	41	PRO	N-CD	-7.93	1.36	1.47
1	E	81	PRO	N-CD	-6.30	1.39	1.47
1	A	60	PRO	N-CD	-5.38	1.40	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	197	PRO	N-CD-CG	-54.07	22.09	103.20
2	B	197	PRO	CA-N-CD	-24.53	77.66	112.00
2	D	135	PRO	CA-N-CD	-11.79	95.49	112.00
2	B	196	VAL	C-N-CD	7.09	154.06	125.00
2	D	135	PRO	N-CD-CG	-6.04	94.14	103.20
1	A	138	ASN	N-CA-C	5.97	119.12	110.28
1	A	139	ASN	N-CA-C	5.47	122.45	110.80
1	A	149	TRP	N-CA-C	5.08	117.04	108.96

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1611	0	1552	115	0
1	E	1620	0	1570	151	0
2	B	1666	0	1628	61	0
2	D	1666	0	1625	68	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	370	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 (370) 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:A:25:ARG:HH21	1:A:71:ASP:CG	1.40	1.27
1:E:151:VAL:HG22	1:E:156:GLN:NE2	0.95	1.26
1:A:15:SER:O	1:A:18:ASP:OD2	1.57	1.22
2:B:107:ARG:HD3	2:B:107:ARG:C	1.59	1.22
1:A:25:ARG:NH2	1:A:71:ASP:CG	1.98	1.22
1:A:25:ARG:NH2	1:A:71:ASP:OD2	1.74	1.20
1:E:127:LYS:HD2	1:E:127:LYS:C	1.70	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:A:5:MET:HE2	1:A:91:GLN:HB3	1.19	1.15
1:E:151:VAL:CG2	1:E:156:GLN:NE2	1.91	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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
1:A:50:TYR:HD1	1:A:51:SER:HG	1.11	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
1:E:5:MET:HE2	1:E:5:MET:HA	1.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:49:ILE:HG23	1:A:54:SER:O	1.70	0.92
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
1:E:5:MET:HE1	1:E:26:ALA:HA	1.53	0.88
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:E:4:GLN:O	1:E:5:MET:HE2	1.75	0.86
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
2:B:215:SER:HG	2:B:217:THR:HG1	1.23	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: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:15:SER:C	1:A:18:ASP:OD2	2.22	0.82
1:A:5:MET:CE	1:A:91:GLN:HB3	2.07	0.81
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
1:E:5:MET:HE1	1:E:26:ALA:CB	2.10	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
1:E:5:MET:HE1	1:E:26:ALA:CA	2.13	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:B:107:ARG:C	2:B:107:ARG:CD	2.41	0.71
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:106:GLU:OE2	1:A:174:TYR:OH	2.10	0.70
1:E:171:ASP:CG	1:E:173:THR:HG23	2.18	0.69
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:49:ILE:CD1	1:A:54:SER:O	2.38	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:A:165:THR:HG22	1:A:166:GLU:N	2.11	0.65
2:D:226:LYS:HE3	1:E:123:ASP:CG	2.21	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: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:E:5:MET:HE2	1:E:5:MET:CA	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:SER:H	2:B:209:ASN:HD21	1.46	0.64
1:E:127:LYS:C	1:E:127:LYS:CD	2.48	0.63
1:A:122:SER:HB3	2:B:135:PRO:HD2	1.80	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
2:B:30:PHE:C	4:B:301:HOH:O	2.42	0.63
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:E:84:PHE:CD1	1:E:84:PHE:C	2.77	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: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
1:E:171:ASP:OD1	1:E:171:ASP:C	2.44	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
1:E:3:ILE:HG22	1:E:5:MET:HE3	1.82	0.61
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:25:ARG:CZ	1:A:71:ASP:CG	2.66	0.59
1:E:130:THR:HG22	1:E:184:LYS:HZ2	1.65	0.59
1:E:60:PRO:C	1:E:62:ARG:H	2.09	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:153:LEU:HD23	2:D:191:SER:OG	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:A:122:SER:O	1:A:126:LEU:HD22	2.05	0.56
1:A:5:MET:HE2	1:A:91:GLN:CB	2.13	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
1:A:15:SER:O	1:A:18:ASP:CG	2.44	0.55
2:B:142:SER:OG	2:B:201:LEU:O	2.22	0.55
2:B:150:LEU:C	2:B:150:LEU:HD12	2.32	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
2:D:226:LYS:O	2:D:226:LYS:HG3	2.05	0.55
1:E:151:VAL:N	1:E:156:GLN:NE2	2.29	0.55
2:D:135:PRO:HG2	2:D:226:LYS:HZ1	1.69	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
2:B:113:ASP:OD2	2:B:113:ASP:C	2.50	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:5:MET:HA	1:E:5:MET:CE	2.29	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:141:TYR:C	1:E:141:TYR:CD2	2.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:49:ILE:HG23	1:A:54:SER:C	2.35	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:A:62:ARG:NH1	1:A:80:GLN:HG3	2.15	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
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
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:5:MET:HE2	1:E:26:ALA:HA	1.93	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:106:GLU:OE2	1:E:174:TYR:OH	2.31	0.49
1:E:141:TYR:CD2	1:E:142:PRO:N	2.80	0.49
1:E:185:ALA:C	1:E:187:TYR:H	2.21	0.49
2:B:155:LYS:HE2	2:B:183:GLN:HE22	1.78	0.48
2:B:190:LEU:C	2:B:190:LEU:HD12	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:4:GLN:C	1:E:5:MET:HE2	2.37	0.48
1:E:186:ASP:OD1	1:E:186:ASP:N	2.46	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:63:PHE:CE1	1:E:76:ILE:HD12	2.49	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
2:B:86:MET:HE1	2:B:121:VAL:HG11	1.96	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: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
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:A:176:LEU:HD23	1:A:176:LEU:C	2.41	0.45
1:A:188:GLU:O	1:A:212:ARG:NH2	2.48	0.45
1:E:140:PHE:CD1	1:E:140:PHE:C	2.94	0.45
2:B:150:LEU:CD1	2:B:194:VAL:HG13	2.42	0.45
1:A:50:TYR:HD1	1:A:51:SER:OG	1.88	0.45
1:A:122:SER:O	1:A:125:GLN:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:TYR:O	1:A:212:ARG:NH1	2.50	0.45
2:D:165:SER:OG	2:D:209:ASN:OD1	2.28	0.45
1:E:60:PRO:C	1:E:62:ARG:N	2.75	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:E:18:ASP:OD1	1:E:18:ASP: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
1:E:12:LEU:CD1	1:E:105:VAL:HG13	2.45	0.44
2:B:150:LEU:CD1	2:B:150:LEU:C	2.90	0.44
2:B:180:ALA:HA	2:B:190:LEU:HB3	2.00	0.44
1:E:62:ARG:NH1	1:E:80:GLN:CG	2.79	0.43
1:A:9:PRO:O	1:A:103:THR:OG1	2.29	0.43
2:D:135:PRO:CD	2:D:135:PRO:C	2.87	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
2:D:53:SER:C	2:D:73:ILE:HD13	2.45	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:49:ILE:HD13	1:A:56:TYR:H	1.78	0.41
1:A:150:LYS:CB	1:A:194:ALA:C	2.88	0.41
2:D:135:PRO:CD	2:D:135:PRO:O	2.64	0.41
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: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
2:B:4:GLU:HG3	2:B:5:VAL:H	1.86	0.41
1:E:185:ALA:C	1:E:187:TYR:N	2.79	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:A:185:ALA:O	1:A:189:LYS:HG3	2.21	0.40
2:B:136:LEU:HB2	2:B:151:GLY:C	2.45	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

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	207/214 (97%)	193 (93%)	13 (6%)	1 (0%)	24	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	48	61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	ASN

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	184/189 (97%)	181 (98%)	3 (2%)	55	69
1	E	187/189 (99%)	186 (100%)	1 (0%)	81	87
2	B	184/190 (97%)	184 (100%)	0	100	100
2	D	184/190 (97%)	183 (100%)	1 (0%)	81	87
All	All	739/758 (98%)	734 (99%)	5 (1%)	76	84

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	THR
1	A	130	THR
1	A	198	THR
2	D	209	ASN
1	E	20	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	GLN
1	A	199	HIS
2	B	16	GLN
2	B	183	GLN
2	D	16	GLN
2	D	117	GLN
2	D	167	ASN
2	D	204	GLN
1	E	125	GLN
1	E	138	ASN
1	E	139	ASN
1	E	156	GLN
1	E	161	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 oligosaccharides 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, 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	211/214 (98%)	1.36	46 (21%) 2 2	58, 86, 131, 189	0
1	E	211/214 (98%)	1.23	40 (18%) 3 2	50, 84, 137, 166	0
2	B	223/229 (97%)	0.71	24 (10%) 11 9	31, 58, 115, 157	0
2	D	223/229 (97%)	0.66	28 (12%) 8 6	32, 56, 126, 162	0
3	C	34/34 (100%)	1.21	7 (20%) 2 2	70, 151, 188, 204	0
3	F	34/34 (100%)	1.24	6 (17%) 4 3	61, 180, 235, 266	0
All	All	936/954 (98%)	1.00	151 (16%) 4 3	31, 77, 155, 266	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	153	ASN	5.9
1	A	154	ALA	5.2
1	E	205	PRO	5.1
2	B	225	PRO	5.1
1	A	123	ASP	4.6
1	A	182	LEU	4.2
1	E	130	THR	4.1
2	B	139	SER	3.9
1	E	182	LEU	3.8
1	E	187	TYR	3.7
1	A	158	GLY	3.7
1	A	33	ALA	3.7
1	A	126	LEU	3.7
1	A	181	THR	3.6
1	A	180	LEU	3.5
2	D	222	LYS	3.5
1	A	155	LEU	3.4
1	E	63	PHE	3.3
2	B	154	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	77	SER	3.3
2	D	139	SER	3.3
1	A	212	ARG	3.3
1	A	184	LYS	3.3
1	E	210	PHE	3.3
1	E	126	LEU	3.3
1	E	194	ALA	3.3
1	A	210	PHE	3.2
1	A	87	TYR	3.2
2	B	201	LEU	3.2
2	D	223	VAL	3.2
1	E	62	ARG	3.1
2	B	222	LYS	3.1
1	A	79	LEU	3.1
2	D	202	GLY	3.1
1	E	207	THR	3.1
1	E	131	ALA	3.1
2	B	137	ALA	3.1
2	B	196	VAL	3.1
1	A	141	TYR	3.0
1	A	84	PHE	3.0
2	B	207	ILE	3.0
1	A	130	THR	3.0
2	B	143	THR	3.0
1	E	84	PHE	3.0
1	A	122	SER	3.0
2	D	106	ARG	2.9
2	B	108	SER	2.9
2	D	140	SER	2.9
2	B	203	THR	2.9
2	D	203	THR	2.9
1	A	157	SER	2.9
1	A	109	ARG	2.9
2	B	197	PRO	2.9
3	C	34	C	2.8
3	C	29	A	2.8
1	A	129	GLY	2.8
1	A	187	TYR	2.8
1	A	22	ILE	2.8
2	D	105	ARG	2.7
2	B	206	TYR	2.7
1	A	131	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
3	F	29	A	2.7
1	E	149	TRP	2.7
1	A	211	ASN	2.7
2	D	175	VAL	2.7
2	B	149	ALA	2.7
2	D	226	LYS	2.6
1	A	149	TRP	2.6
2	B	138	PRO	2.6
1	E	132	SER	2.6
3	C	8	C	2.6
2	B	141	LYS	2.6
1	E	212	ARG	2.6
1	E	79	LEU	2.6
2	D	196	VAL	2.6
1	A	49	ILE	2.5
1	A	63	PHE	2.5
2	B	167	ASN	2.5
1	A	21	THR	2.5
2	D	200	SER	2.5
1	E	123	ASP	2.5
2	D	207	ILE	2.5
2	D	171	LEU	2.5
3	C	26	G	2.5
3	F	26	G	2.5
2	D	146	GLY	2.5
3	F	1	G	2.5
1	E	107	ILE	2.4
3	F	4	G	2.4
2	D	143	THR	2.4
1	A	120	PRO	2.4
1	A	191	LYS	2.4
2	D	199	SER	2.4
1	E	76	ILE	2.4
1	E	202	LEU	2.4
2	B	136	LEU	2.4
3	C	1	G	2.4
2	D	205	THR	2.3
1	E	78	SER	2.3
1	A	16	VAL	2.3
1	E	192	VAL	2.3
1	E	36	TRP	2.3
1	E	61	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	20	VAL	2.3
2	D	107	ARG	2.3
1	E	155	LEU	2.3
2	B	171	LEU	2.3
1	E	129	GLY	2.3
1	E	183	SER	2.3
2	B	144	SER	2.3
1	A	150	LYS	2.3
2	D	141	LYS	2.3
1	A	159	ASN	2.2
2	D	109	GLY	2.2
2	B	182	LEU	2.2
2	D	138	PRO	2.2
1	A	127	LYS	2.2
1	A	20	VAL	2.2
2	B	210	VAL	2.2
3	F	8	C	2.2
1	E	95	PHE	2.2
2	D	225	PRO	2.2
1	A	133	VAL	2.2
1	A	36	TRP	2.2
1	A	81	PRO	2.2
1	E	128	SER	2.1
1	E	206	VAL	2.1
1	E	179	THR	2.1
2	B	145	GLY	2.1
1	E	195	CYS	2.1
1	A	128	SER	2.1
1	E	203	SER	2.1
1	E	55	LEU	2.1
1	A	118	ILE	2.1
2	D	135	PRO	2.1
2	D	197	PRO	2.1
1	E	133	VAL	2.1
1	E	180	LEU	2.1
2	D	201	LEU	2.1
1	E	150	LYS	2.1
2	B	140	SER	2.1
1	A	60	PRO	2.1
2	D	172	THR	2.0
1	E	120	PRO	2.0
2	D	104	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
3	C	28	C	2.0
3	F	3	C	2.0
1	A	74	LEU	2.0
1	E	198	THR	2.0
3	C	7	A	2.0
1	A	193	TYR	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 oligosaccharides 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.