



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:29 PM UTC

PDB ID : 4FTB / pdb_00004ftb
Title : Crystal structure of the authentic Flock House virus particle
Authors : Speir, J.A.; Chen, Z.; Reddy, V.S.; Johnson, J.E.
Deposited on : 2012-06-27
Resolution : 2.70 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
Mogul : 2022.3.0, CSD as543be (2022)
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

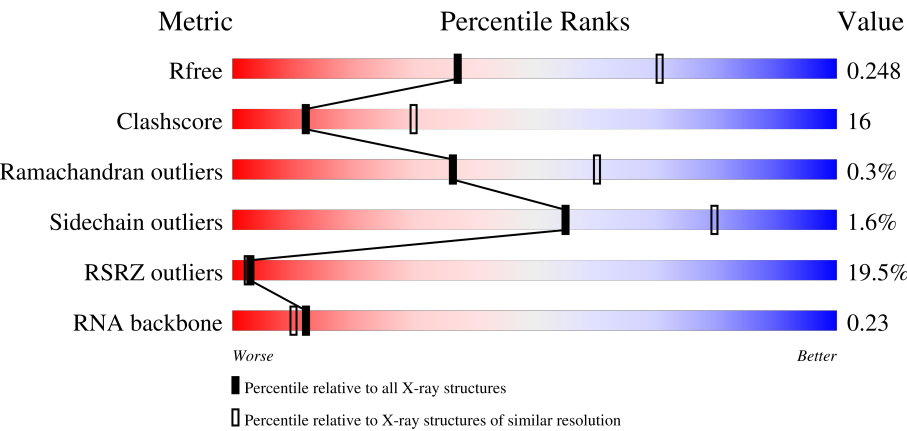
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

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	363	17% 64% 22% • 12%
1	B	363	11% 61% 23% • 14%
1	C	363	10% 65% 19% • 15%
2	D	44	39% 23% 25% 52%

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Mol	Chain	Length	Quality of chain
2	E	44	41%25%18%57%
2	F	44	18%36%9%55%
3	R	15	100%33%47%20%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8321 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 Capsid protein beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2407	1531	398	468	10			
1	B	311	Total	C	N	O	S	0	0	0
			2325	1481	381	452	11			
1	C	309	Total	C	N	O	S	0	0	0
			2312	1473	379	450	10			

- Molecule 2 is a protein called Capsid protein gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	21	Total	C	N	O	S	0	0	0
			157	99	28	29	1			
2	E	19	Total	C	N	O	S	0	0	0
			141	89	25	26	1			
2	F	20	Total	C	N	O	S	0	0	0
			149	93	27	28	1			

- Molecule 3 is a RNA chain called Flock House virus genomic RNA.

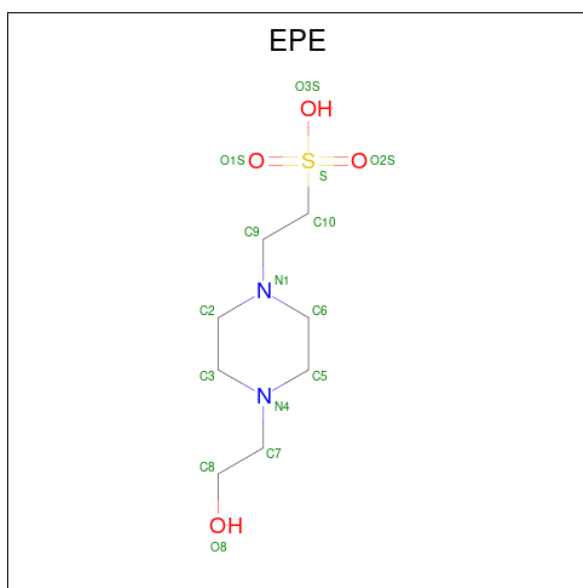
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	15	Total	C	N	O	P	0	0	0
			302	136	36	115	15			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Ca	0	0
			3	3		
4	B	1	Total	Ca	0	0
			1	1		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD

ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	162	Total	O	0	0
			162	162		
7	D	5	Total	O	0	0
			5	5		
7	B	144	Total	O	0	0
			144	144		
7	E	4	Total	O	0	0
			4	4		
7	C	157	Total	O	0	0
			157	157		

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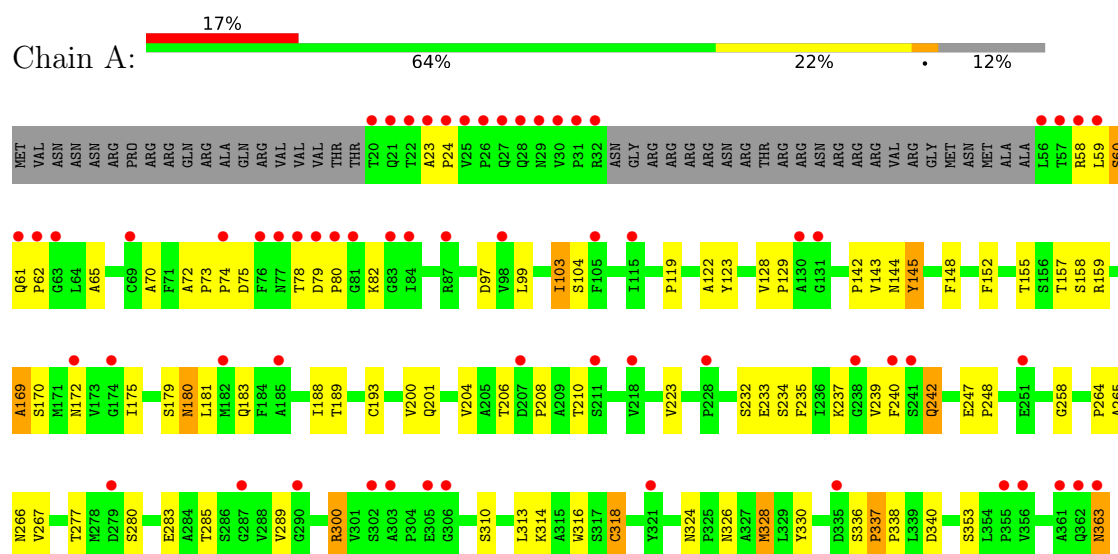
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	F	5	Total	O	0	0
			5	5		
7	R	1	Total	O	0	0
			1	1		

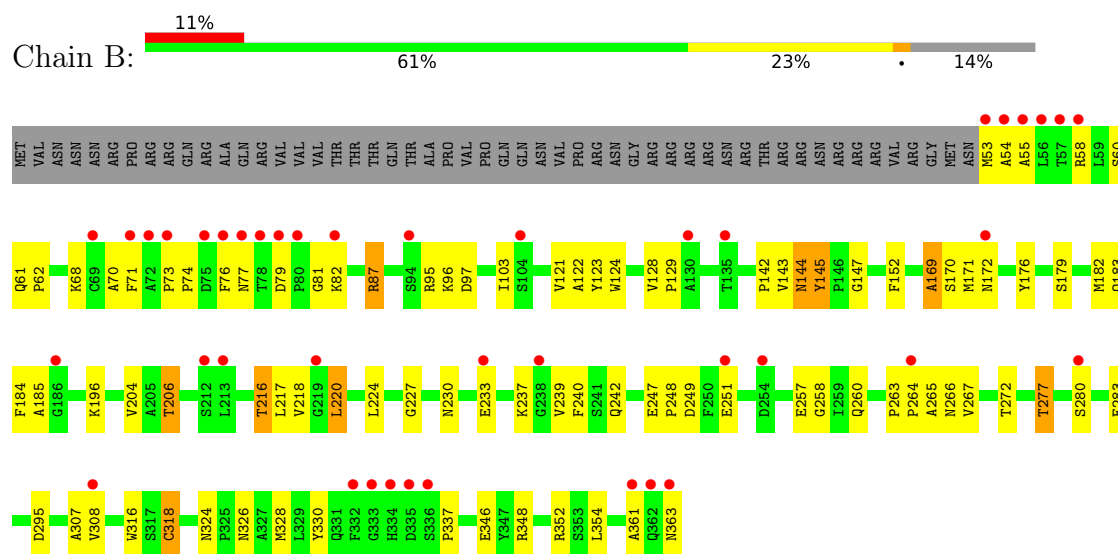
3 Residue-property plots [i](#)

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: Capsid protein beta

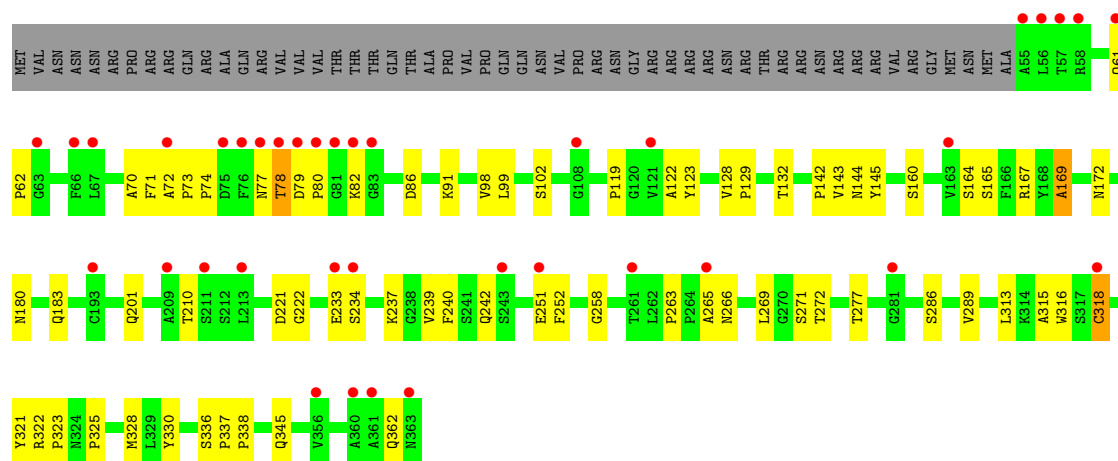


- Molecule 1: Capsid protein beta

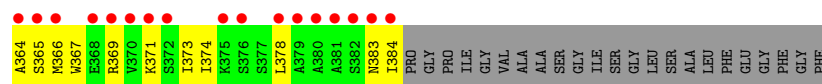


- Molecule 1: Capsid protein beta

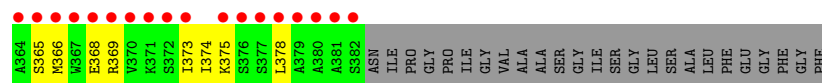




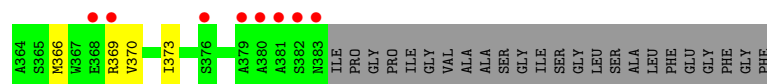
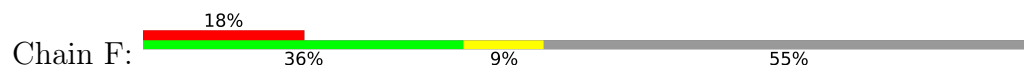
● Molecule 2: Capsid protein gamma



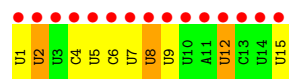
● Molecule 2: Capsid protein gamma



● Molecule 2: Capsid protein gamma



● Molecule 3: Flock House virus genomic RNA



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	327.66Å 327.66Å 774.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.70 40.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	82.2 (40.00-2.70) 82.3 (40.00-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.240 , (Not available) 0.243 , 0.248	Depositor DCC
R_{free} test set	34853 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	52.5	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	0.000 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k +1/3*l 0.000 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/ 3*k+1/3*l 0.000 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+ 1/3*l,-4/3*h+4/3*k+1/3*l 0.000 for 1/3*h+2/3*k-1/3*l,-k,-8/3*h-4/3* k-1/3*l 0.000 for -1/3*h-2/3*k+1/3*l,-2/3*h-1/3*k- 1/3*l,4/3*h-4/3*k-1/3*l 0.000 for -h,2/3*h+1/3*k+1/3*l,4/3*h+8/3 *k-1/3*l 0.000 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.42	EDS
Total number of atoms	8321	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.32% 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

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, CL, CA

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	0.58	0/2471	1.06	14/3384 (0.4%)
1	B	0.56	0/2387	1.07	17/3267 (0.5%)
1	C	0.55	0/2374	1.04	12/3250 (0.4%)
2	D	0.47	0/158	0.99	0/211
2	E	0.41	0/142	1.00	0/189
2	F	0.44	0/150	0.80	0/200
3	R	0.30	0/332	0.65	0/511
All	All	0.55	0/8014	1.04	43/11012 (0.4%)

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	271	SER	N-CA-C	-8.51	102.90	113.28
1	A	330	TYR	N-CA-C	7.72	119.69	111.28
1	B	73	PRO	N-CA-C	7.57	119.94	110.70
1	C	269	LEU	N-CA-C	-7.42	100.76	110.33
1	B	144	ASN	N-CA-C	7.21	121.16	110.48
1	B	60	SER	N-CA-C	-7.10	100.97	110.55
1	B	145	TYR	N-CA-C	-6.52	100.61	110.39
1	A	181	LEU	N-CA-C	6.44	118.30	111.28
1	A	152	PHE	N-CA-C	6.21	120.48	112.41
1	A	145	TYR	N-CA-C	-6.16	101.15	110.39
1	C	336	SER	N-CA-C	-5.96	101.55	109.84
1	A	159	ARG	N-CA-C	5.90	119.30	111.75
1	B	77	ASN	N-CA-C	-5.80	105.03	111.36
1	A	337	PRO	O-C-N	5.80	123.88	121.15
1	C	277	THR	N-CA-C	5.77	119.12	109.95
1	A	258	GLY	N-CA-C	5.71	122.94	115.40
1	B	152	PHE	N-CA-C	5.67	119.77	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	SER	N-CA-C	-5.66	101.98	109.84
1	A	180	ASN	N-CA-C	-5.56	103.36	110.53
1	B	169	ALA	N-CA-C	-5.56	105.53	112.93
1	B	328	MET	CA-C-N	5.56	128.28	120.28
1	B	328	MET	C-N-CA	5.56	128.28	120.28
1	C	258	GLY	N-CA-C	5.55	122.75	115.47
1	C	142	PRO	N-CA-C	5.55	120.00	111.57
1	B	58	ARG	N-CA-C	-5.52	106.39	113.23
1	B	337	PRO	O-C-N	5.44	123.81	121.31
1	C	169	ALA	N-CA-C	-5.43	106.71	113.55
1	B	230	ASN	N-CA-C	5.37	116.44	108.60
1	A	70	ALA	N-CA-C	5.34	117.18	111.36
1	C	337	PRO	O-C-N	5.33	123.76	121.31
1	A	169	ALA	N-CA-C	-5.32	106.92	113.41
1	B	277	THR	N-CA-C	5.28	118.35	109.95
1	C	71	PHE	N-CA-C	5.27	120.72	113.97
1	A	328	MET	N-CA-C	-5.25	106.87	113.28
1	C	78	THR	N-CA-C	5.25	116.26	108.60
1	B	206	THR	N-CA-C	-5.24	102.25	110.17
1	B	71	PHE	N-CA-C	5.24	121.06	114.31
1	B	330	TYR	N-CA-C	5.16	116.90	111.28
1	B	258	GLY	N-CA-C	5.15	122.46	115.30
1	C	102	SER	N-CA-C	-5.15	102.07	110.20
1	A	277	THR	N-CA-C	5.14	118.12	109.95
1	C	70	ALA	N-CA-C	5.12	116.55	111.07
1	A	193	CYS	N-CA-C	5.09	117.83	110.14

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	2407	0	2341	81	0
1	B	2325	0	2260	76	0
1	C	2312	0	2246	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	157	0	167	8	0
2	E	141	0	150	12	0
2	F	149	0	156	4	0
3	R	302	0	155	18	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
5	A	15	0	17	1	0
5	B	15	0	17	2	0
5	C	15	0	17	0	0
6	B	1	0	0	0	0
7	A	162	0	0	3	0
7	B	144	0	0	1	0
7	C	157	0	0	4	0
7	D	5	0	0	0	0
7	E	4	0	0	0	0
7	F	5	0	0	0	0
7	R	1	0	0	0	0
All	All	8321	0	7526	240	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 16.

All (240) 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)
3:R:1:U:H2'	3:R:2:U:C5'	1.42	1.45
3:R:1:U:C2'	3:R:2:U:H5''	1.47	1.42
1:A:180:ASN:OD1	1:A:183:GLN:HG2	1.42	1.16
1:C:128:VAL:HG13	1:C:129:PRO:HD2	1.38	1.04
3:R:7:U:H2'	3:R:8:U:H4'	1.39	1.04
1:A:155:THR:HG22	1:A:157:THR:H	1.21	1.03
1:A:326:ASN:HD22	1:C:222:GLY:HA2	1.33	0.94
1:A:60:SER:OG	1:A:340:ASP:OD1	1.86	0.93
1:B:87:ARG:HG3	1:B:87:ARG:HH11	1.34	0.93
1:B:218:VAL:HG13	1:C:160:SER:HB2	1.51	0.92
1:C:128:VAL:HG12	1:C:132:THR:OG1	1.70	0.92
1:C:128:VAL:CG1	1:C:132:THR:OG1	2.21	0.89
1:A:180:ASN:OD1	1:A:183:GLN:CG	2.20	0.89
1:C:128:VAL:HG13	1:C:129:PRO:CD	2.04	0.87
3:R:7:U:C2'	3:R:8:U:H4'	2.05	0.86
1:C:128:VAL:CG1	1:C:129:PRO:HD2	2.06	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:ARG:HH11	1:A:300:ARG:HG2	1.40	0.84
1:A:247:GLU:HG3	1:A:248:PRO:HD2	1.59	0.83
3:R:7:U:H2'	3:R:8:U:C4'	2.09	0.82
3:R:1:U:H2'	3:R:2:U:C4'	2.08	0.82
1:A:82:LYS:O	1:A:82:LYS:HD3	1.80	0.82
1:B:53:MET:HG2	1:B:54:ALA:H	1.45	0.80
1:B:247:GLU:HG3	1:B:248:PRO:HD2	1.66	0.78
1:C:128:VAL:CG1	1:C:129:PRO:CD	2.63	0.76
1:C:77:ASN:O	1:C:78:THR:HG22	1.85	0.76
3:R:1:U:C3'	3:R:2:U:H5''	2.16	0.74
1:B:79:ASP:HB3	1:B:96:LYS:HD2	1.69	0.73
3:R:1:U:C2'	3:R:2:U:C5'	2.30	0.72
1:A:72:ALA:HB1	1:A:75:ASP:OD2	1.89	0.71
1:A:61:GLN:HB3	7:A:543:HOH:O	1.91	0.71
1:A:300:ARG:HG2	1:A:300:ARG:NH1	1.98	0.71
1:B:352:ARG:CG	1:B:352:ARG:O	2.39	0.70
1:C:77:ASN:C	1:C:78:THR:CG2	2.65	0.70
1:B:352:ARG:O	1:B:352:ARG:HG2	1.92	0.70
1:A:123:TYR:CZ	1:A:143:VAL:HG21	2.27	0.69
1:B:260:GLN:HG3	5:B:403:EPE:H61	1.74	0.69
1:A:353:SER:HB2	2:D:373:ILE:HD13	1.76	0.68
1:B:218:VAL:HG13	1:C:160:SER:CB	2.22	0.68
1:A:233:GLU:HG3	1:A:234:SER:N	2.07	0.68
1:A:155:THR:HB	1:A:158:SER:OG	1.93	0.68
1:B:263:PRO:HD2	1:B:277:THR:HG23	1.74	0.67
1:C:61:GLN:HB3	1:C:62:PRO:HD3	1.76	0.67
1:A:300:ARG:HH11	1:A:300:ARG:CG	2.08	0.66
1:B:216:THR:HG21	1:B:272:THR:O	1.95	0.66
2:D:374:ILE:O	2:D:378:LEU:HB2	1.96	0.66
1:C:82:LYS:O	1:C:82:LYS:HG3	1.95	0.65
3:R:1:U:H2'	3:R:2:U:H5''	0.68	0.65
3:R:8:U:H5'	3:R:9:U:H5	1.62	0.65
1:C:263:PRO:HB3	1:C:272:THR:HG21	1.78	0.65
1:C:345:GLN:NE2	1:C:345:GLN:HA	2.12	0.65
1:A:363:ASN:O	1:A:363:ASN:ND2	2.30	0.64
1:C:73:PRO:N	1:C:74:PRO:HD2	2.12	0.64
1:A:78:THR:HG22	1:A:79:ASP:N	2.13	0.64
1:C:77:ASN:C	1:C:78:THR:HG23	2.22	0.64
1:C:86:ASP:OD2	1:C:167:ARG:NH1	2.28	0.64
1:C:122:ALA:HA	1:C:145:TYR:CE1	2.32	0.64
1:C:72:ALA:C	1:C:74:PRO:HD2	2.22	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:ARG:HH11	1:B:87:ARG:CG	2.09	0.63
1:B:196:LYS:HE3	1:C:165:SER:OG	1.98	0.63
1:A:200:VAL:HA	1:B:257:GLU:O	1.98	0.63
1:C:77:ASN:O	1:C:78:THR:CG2	2.46	0.62
1:A:206:THR:OG1	1:A:210:THR:HG23	2.00	0.62
1:B:172:ASN:HB2	1:B:316:TRP:CE3	2.35	0.62
1:A:144:ASN:ND2	1:A:285:THR:O	2.32	0.62
1:B:147:GLY:HA2	7:B:590:HOH:O	1.99	0.62
1:A:142:PRO:HG3	1:A:280:SER:HA	1.80	0.62
1:B:295:ASP:OD1	1:C:322:ARG:NH2	2.32	0.62
1:B:172:ASN:HB2	1:B:316:TRP:HE3	1.64	0.62
1:B:53:MET:HG2	1:B:54:ALA:N	2.15	0.61
1:C:362:GLN:NE2	2:F:369:ARG:HH22	1.98	0.61
1:A:155:THR:HG22	1:A:157:THR:N	2.05	0.61
1:A:61:GLN:HA	1:A:61:GLN:NE2	2.15	0.61
1:B:263:PRO:HB3	1:B:272:THR:HG21	1.83	0.61
1:B:87:ARG:HG3	1:B:87:ARG:NH1	2.10	0.61
3:R:7:U:C3'	3:R:8:U:H4'	2.31	0.60
1:A:188:ILE:HG13	1:A:235:PHE:HA	1.82	0.60
1:B:216:THR:HG23	1:B:272:THR:HB	1.84	0.60
1:A:103:ILE:HG13	1:A:104:SER:N	2.17	0.59
1:B:123:TYR:CZ	1:B:143:VAL:HG21	2.37	0.59
1:B:79:ASP:CB	1:B:96:LYS:HD2	2.33	0.59
1:C:321:TYR:O	1:C:323:PRO:HD3	2.02	0.59
1:A:233:GLU:CG	1:A:237:LYS:HD2	2.33	0.59
1:C:128:VAL:HG12	1:C:129:PRO:N	2.18	0.59
2:E:365:SER:HB3	2:E:368:GLU:HG2	1.86	0.58
2:F:366:MET:O	2:F:370:VAL:HG23	2.02	0.58
1:A:170:SER:OG	1:A:318:CYS:HB2	2.04	0.58
1:B:142:PRO:HG3	1:B:280:SER:HA	1.84	0.58
1:B:169:ALA:HB3	1:B:318:CYS:HB3	1.85	0.57
1:C:73:PRO:HG2	1:C:74:PRO:HD3	1.86	0.57
1:A:363:ASN:ND2	1:A:363:ASN:C	2.59	0.57
2:D:364:ALA:CB	2:D:367:TRP:HB3	2.34	0.57
3:R:1:U:H3'	3:R:1:U:C6	2.39	0.57
1:A:201:GLN:NE2	1:B:264:PRO:HB3	2.20	0.57
1:A:363:ASN:C	1:A:363:ASN:HD22	2.10	0.57
1:C:73:PRO:N	1:C:74:PRO:CD	2.68	0.57
1:B:55:ALA:HB1	2:E:378:LEU:HD13	1.85	0.57
1:B:61:GLN:HB3	1:B:62:PRO:HD3	1.87	0.56
1:B:68:LYS:HD3	1:B:76:PHE:CZ	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ALA:HA	1:B:170:SER:HB3	1.86	0.56
1:A:99:LEU:O	1:A:314:LYS:HA	2.05	0.56
2:D:364:ALA:HB3	2:D:367:TRP:HB3	1.86	0.56
1:A:326:ASN:HD22	1:C:222:GLY:CA	2.13	0.56
1:C:79:ASP:N	1:C:80:PRO:CD	2.69	0.55
1:C:128:VAL:CG1	1:C:129:PRO:N	2.69	0.55
1:C:82:LYS:O	1:C:82:LYS:CG	2.55	0.54
1:B:233:GLU:CG	1:B:237:LYS:HD2	2.38	0.54
3:R:7:U:N3	3:R:8:U:O2	2.40	0.54
1:A:313:LEU:C	1:A:313:LEU:HD23	2.32	0.54
1:C:265:ALA:O	1:C:266:ASN:HB2	2.07	0.54
1:A:324:ASN:HB3	1:A:326:ASN:ND2	2.23	0.54
1:B:172:ASN:ND2	1:B:242:GLN:HB3	2.23	0.54
2:F:369:ARG:O	2:F:373:ILE:HG13	2.08	0.54
1:B:87:ARG:CG	1:B:87:ARG:NH1	2.68	0.53
1:C:128:VAL:HG11	1:C:132:THR:OG1	2.05	0.53
1:B:179:SER:HB3	1:B:183:GLN:HG3	1.91	0.53
3:R:1:U:C3'	3:R:1:U:C6	2.91	0.53
1:C:128:VAL:HG12	1:C:132:THR:HG1	1.74	0.53
1:A:122:ALA:HA	1:A:145:TYR:CE2	2.44	0.53
1:A:78:THR:CG2	1:A:79:ASP:N	2.71	0.53
1:B:74:PRO:HG3	1:B:316:TRP:CZ2	2.45	0.52
1:A:233:GLU:HG3	1:A:234:SER:H	1.73	0.52
1:B:55:ALA:CB	2:E:378:LEU:HD13	2.39	0.52
1:C:172:ASN:OD1	1:C:242:GLN:HB3	2.09	0.52
1:C:233:GLU:HG3	1:C:234:SER:N	2.25	0.52
1:B:183:GLN:HB2	1:B:308:VAL:HB	1.91	0.52
1:A:73:PRO:HD2	1:A:74:PRO:HD3	1.93	0.51
1:C:362:GLN:HE22	2:F:369:ARG:HH22	1.56	0.51
1:C:144:ASN:HD21	1:C:286:SER:HB2	1.75	0.51
1:B:184:PHE:C	1:B:184:PHE:CD2	2.88	0.51
1:B:185:ALA:HB3	1:B:307:ALA:CB	2.40	0.51
3:R:1:U:H3'	3:R:1:U:H6	1.76	0.51
1:A:172:ASN:OD1	1:A:242:GLN:HB3	2.12	0.50
2:D:367:TRP:NE1	2:D:371:LYS:HD2	2.26	0.50
1:A:201:GLN:CD	1:B:264:PRO:HB3	2.37	0.50
1:C:78:THR:C	1:C:80:PRO:HD3	2.36	0.50
7:A:541:HOH:O	1:B:251:GLU:HB3	2.11	0.50
1:C:233:GLU:CG	1:C:237:LYS:HD2	2.41	0.50
1:C:169:ALA:HB3	1:C:318:CYS:HB3	1.95	0.49
1:A:208:PRO:O	1:A:210:THR:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:THR:O	1:A:80:PRO:HD3	2.13	0.49
1:C:345:GLN:HA	1:C:345:GLN:HE21	1.78	0.49
1:A:180:ASN:OD1	1:A:183:GLN:CB	2.60	0.49
1:A:79:ASP:OD1	1:A:79:ASP:O	2.29	0.48
2:D:383:ASN:O	2:D:384:ILE:C	2.56	0.48
1:B:354:LEU:HD22	2:E:366:MET:HE1	1.94	0.48
1:B:55:ALA:HA	2:E:378:LEU:HD13	1.96	0.48
1:A:58:ARG:NH1	7:A:639:HOH:O	2.47	0.48
1:B:264:PRO:HG2	1:B:267:VAL:HG21	1.95	0.48
1:A:179:SER:HG	1:A:310:SER:H	1.60	0.48
1:A:175:ILE:HB	1:A:239:VAL:HG12	1.96	0.48
2:E:374:ILE:O	2:E:378:LEU:HB2	2.14	0.47
1:A:61:GLN:N	1:A:62:PRO:HD2	2.28	0.47
1:B:55:ALA:CA	2:E:378:LEU:HD13	2.44	0.47
2:E:369:ARG:O	2:E:373:ILE:HG13	2.13	0.47
1:B:247:GLU:HG2	1:C:251:GLU:OE2	2.15	0.47
2:E:368:GLU:OE2	2:E:368:GLU:HA	2.14	0.47
1:B:55:ALA:HB3	2:E:375:LYS:HG2	1.97	0.47
1:C:86:ASP:C	1:C:86:ASP:OD1	2.55	0.47
1:A:65:ALA:HB1	1:A:80:PRO:O	2.15	0.47
1:A:73:PRO:N	1:A:74:PRO:HD3	2.29	0.47
1:B:176:TYR:HE1	1:B:363:ASN:ND2	2.13	0.47
1:A:119:PRO:HB2	1:A:289:VAL:CG2	2.45	0.47
1:A:264:PRO:HB3	1:C:201:GLN:CD	2.40	0.46
1:A:128:VAL:HB	1:A:129:PRO:HD2	1.97	0.46
1:C:239:VAL:HG22	1:C:240:PHE:N	2.30	0.46
1:B:239:VAL:HG22	1:B:240:PHE:N	2.29	0.46
2:D:364:ALA:C	2:D:366:MET:H	2.24	0.46
1:C:98:VAL:HA	1:C:315:ALA:O	2.16	0.46
1:A:78:THR:HG22	1:A:79:ASP:OD1	2.15	0.46
1:B:217:LEU:HB2	1:B:220:LEU:HD22	1.97	0.46
2:E:378:LEU:HD23	2:E:378:LEU:O	2.16	0.46
1:C:123:TYR:CZ	1:C:143:VAL:HG21	2.51	0.45
1:B:121:VAL:HG22	1:B:144:ASN:ND2	2.30	0.45
1:B:242:GLN:HE22	1:B:354:LEU:HD13	1.81	0.45
1:A:73:PRO:CD	1:A:74:PRO:HD3	2.46	0.45
1:B:171:MET:C	1:B:172:ASN:HD22	2.25	0.45
1:B:204:VAL:HG12	1:B:206:THR:HG23	1.99	0.45
1:A:264:PRO:HB3	1:C:201:GLN:NE2	2.32	0.45
3:R:6:C:H2'	3:R:7:U:C6	2.52	0.45
1:A:97:ASP:HB3	1:A:145:TYR:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ALA:O	1:A:266:ASN:HB2	2.17	0.44
1:B:95:ARG:NH1	1:B:97:ASP:OD1	2.50	0.44
1:C:91:LYS:HE3	1:C:330:TYR:OH	2.17	0.44
1:A:264:PRO:HG2	1:A:267:VAL:HG21	2.00	0.44
1:C:119:PRO:HB2	1:C:289:VAL:CG2	2.48	0.44
1:A:103:ILE:CG1	1:A:104:SER:N	2.76	0.44
1:B:324:ASN:HB3	1:B:326:ASN:OD1	2.17	0.44
1:C:180:ASN:HD21	1:C:183:GLN:HG3	1.82	0.44
1:A:204:VAL:HG11	1:C:210:THR:CG2	2.47	0.44
1:A:189:THR:HG23	1:A:232:SER:OG	2.18	0.44
1:B:247:GLU:OE1	1:C:252:PHE:HB2	2.18	0.44
1:B:265:ALA:O	1:B:266:ASN:HB2	2.18	0.44
1:C:78:THR:HA	7:C:571:HOH:O	2.18	0.44
1:C:328:MET:SD	1:C:328:MET:C	3.01	0.44
1:A:73:PRO:N	1:A:74:PRO:CD	2.80	0.44
1:A:328:MET:HE2	1:A:328:MET:HA	2.00	0.43
1:B:70:ALA:HA	1:B:170:SER:CB	2.48	0.43
1:A:74:PRO:HG3	1:A:316:TRP:CH2	2.53	0.43
1:A:169:ALA:HB3	1:A:318:CYS:HB3	1.99	0.43
1:A:337:PRO:HA	1:A:338:PRO:HD3	1.80	0.43
1:A:204:VAL:HG12	1:A:206:THR:HG23	2.00	0.43
1:B:82:LYS:HD2	1:B:82:LYS:HA	1.51	0.43
1:B:283:GLU:H	5:B:403:EPE:H81	1.83	0.43
1:C:61:GLN:CB	1:C:62:PRO:HD3	2.44	0.43
1:C:172:ASN:OD1	1:C:242:GLN:CB	2.67	0.43
1:A:172:ASN:OD1	1:A:242:GLN:CB	2.67	0.43
1:C:345:GLN:HB2	7:C:537:HOH:O	2.18	0.43
1:B:128:VAL:HB	1:B:129:PRO:CD	2.48	0.43
3:R:8:U:H3'	3:R:9:U:C6	2.53	0.43
2:E:365:SER:HB3	2:E:368:GLU:CG	2.49	0.42
1:B:249:ASP:HB3	7:C:568:HOH:O	2.18	0.42
1:C:61:GLN:NE2	3:R:12:U:O2'	2.52	0.42
1:C:338:PRO:HD3	7:C:522:HOH:O	2.19	0.42
1:A:180:ASN:CG	1:A:183:GLN:HG2	2.32	0.42
1:B:218:VAL:HG12	1:C:164:SER:HB2	2.02	0.42
1:A:148:PHE:CD2	1:A:148:PHE:C	2.97	0.42
2:D:369:ARG:O	2:D:373:ILE:HG13	2.19	0.42
1:B:227:GLY:HA3	1:C:325:PRO:HB3	2.01	0.42
1:B:233:GLU:HG3	1:B:237:LYS:HD2	2.01	0.42
1:C:99:LEU:HD22	1:C:122:ALA:CB	2.49	0.42
1:A:99:LEU:HD22	1:A:122:ALA:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:ASN:HB3	1:A:326:ASN:HD21	1.85	0.41
1:B:124:TRP:CZ2	1:B:142:PRO:HB3	2.54	0.41
1:A:300:ARG:CG	1:A:300:ARG:O	2.65	0.41
1:B:122:ALA:HA	1:B:145:TYR:CE1	2.56	0.41
1:A:223:VAL:O	1:A:223:VAL:HG12	2.20	0.41
1:B:185:ALA:HB3	1:B:307:ALA:HB2	2.01	0.41
1:B:348:ARG:HA	1:B:348:ARG:HD3	1.95	0.41
1:B:61:GLN:HA	1:B:61:GLN:NE2	2.36	0.41
1:C:313:LEU:C	1:C:313:LEU:HD23	2.45	0.41
1:B:182:MET:HE2	1:B:182:MET:HB3	1.96	0.41
1:A:283:GLU:OE1	5:A:404:EPE:H32	2.21	0.41
1:A:23:ALA:HA	1:A:24:PRO:HD3	1.86	0.40
1:A:363:ASN:HD22	1:A:363:ASN:N	2.20	0.40
1:B:224:LEU:N	1:B:224:LEU:HD23	2.37	0.40
1:A:239:VAL:HG22	1:A:240:PHE:N	2.35	0.40
1:A:326:ASN:ND2	1:C:221:ASP:C	2.79	0.40
1:B:124:TRP:CE2	1:B:142:PRO:HB3	2.56	0.40
1:B:346:GLU:OE2	1:B:346:GLU:HA	2.22	0.40
1:C:98:VAL:HG12	1:C:316:TRP:CD1	2.57	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	317/363 (87%)	308 (97%)	9 (3%)	0	100	100
1	B	309/363 (85%)	294 (95%)	13 (4%)	2 (1%)	21	44
1	C	307/363 (85%)	299 (97%)	8 (3%)	0	100	100
2	D	19/44 (43%)	17 (90%)	1 (5%)	1 (5%)	1	3
2	E	17/44 (39%)	17 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	18/44 (41%)	18 (100%)	0	0	100	100
All	All	987/1221 (81%)	953 (97%)	31 (3%)	3 (0%)	36	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	81	GLY
2	D	365	SER
1	B	361	ALA

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	268/305 (88%)	261 (97%)	7 (3%)	40	70
1	B	257/305 (84%)	252 (98%)	5 (2%)	50	77
1	C	256/305 (84%)	255 (100%)	1 (0%)	84	93
2	D	17/31 (55%)	17 (100%)	0	100	100
2	E	15/31 (48%)	15 (100%)	0	100	100
2	F	16/31 (52%)	16 (100%)	0	100	100
All	All	829/1008 (82%)	816 (98%)	13 (2%)	55	80

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LEU
1	A	60	SER
1	A	103	ILE
1	A	242	GLN
1	A	300	ARG
1	A	318	CYS
1	A	363	ASN
1	B	87	ARG

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Mol	Chain	Res	Type
1	B	103	ILE
1	B	216	THR
1	B	220	LEU
1	B	318	CYS
1	C	318	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	109	GLN
1	A	162	GLN
1	A	266	ASN
1	A	324	ASN
1	A	326	ASN
1	A	334	HIS
1	A	345	GLN
1	A	363	ASN
2	D	383	ASN
1	B	61	GLN
1	B	109	GLN
1	B	162	GLN
1	B	253	ASN
1	B	324	ASN
1	B	363	ASN
1	C	61	GLN
1	C	109	GLN
1	C	144	ASN
1	C	266	ASN
1	C	334	HIS
1	C	345	GLN
1	C	362	GLN
2	F	383	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	R	14/15 (93%)	6 (42%)	0

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	R	2	U
3	R	4	C
3	R	5	U
3	R	8	U
3	R	12	U
3	R	15	U

There are no RNA pucker outliers to report.

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](#)

Of 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	EPE	C	401	-	15,15,15	1.75	5 (33%)	19,20,20	2.72	3 (15%)
5	EPE	B	403	-	15,15,15	1.51	3 (20%)	19,20,20	1.69	3 (15%)
5	EPE	A	404	-	15,15,15	1.65	4 (26%)	19,20,20	2.13	2 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EPE	C	401	-	-	3/9/19/19	0/1/1/1
5	EPE	B	403	-	-	2/9/19/19	0/1/1/1
5	EPE	A	404	-	-	0/9/19/19	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	404	EPE	C10-S	2.89	1.81	1.77
5	C	401	EPE	O1S-S	2.74	1.52	1.45
5	C	401	EPE	O2S-S	2.68	1.52	1.45
5	C	401	EPE	C10-S	2.60	1.81	1.77
5	B	403	EPE	O1S-S	2.53	1.52	1.45
5	A	404	EPE	O1S-S	2.30	1.51	1.45
5	C	401	EPE	C7-N4	2.22	1.52	1.47
5	B	403	EPE	C3-N4	2.17	1.52	1.46
5	B	403	EPE	C10-S	2.13	1.80	1.77
5	A	404	EPE	C3-N4	2.04	1.52	1.46
5	C	401	EPE	C3-N4	2.04	1.52	1.46
5	A	404	EPE	C7-N4	2.02	1.52	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	401	EPE	O3S-S-C10	10.88	127.29	106.00
5	A	404	EPE	O3S-S-C10	8.15	121.94	106.00
5	B	403	EPE	O3S-S-O2S	5.51	125.17	111.40
5	A	404	EPE	O2S-S-C10	-2.95	102.27	106.73
5	B	403	EPE	O2S-S-O1S	-2.49	105.72	113.82
5	C	401	EPE	O3S-S-O1S	-2.27	105.71	111.40
5	C	401	EPE	O3S-S-O2S	-2.25	105.77	111.40
5	B	403	EPE	O3S-S-O1S	-2.10	106.15	111.40

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	403	EPE	C9-C10-S-O3S
5	B	403	EPE	C9-C10-S-O1S
5	C	401	EPE	C9-C10-S-O1S
5	C	401	EPE	C9-C10-S-O3S
5	C	401	EPE	N4-C7-C8-O8

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	403	EPE	2	0
5	A	404	EPE	1	0

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	321/363 (88%)	1.39	62 (19%) 3 3	40, 50, 95, 153	0
1	B	311/363 (85%)	1.23	41 (13%) 7 6	39, 50, 88, 156	0
1	C	309/363 (85%)	1.19	37 (11%) 9 7	39, 50, 70, 118	0
2	D	21/44 (47%)	4.28	17 (80%) 0 0	81, 97, 160, 164	0
2	E	19/44 (43%)	4.34	18 (94%) 0 0	99, 114, 154, 155	0
2	F	20/44 (45%)	2.26	8 (40%) 1 0	60, 77, 130, 135	0
3	R	15/15 (100%)	7.06	15 (100%) 0 0	150, 198, 248, 249	0
All	All	1016/1236 (82%)	1.50	198 (19%) 3 2	39, 51, 118, 249	0

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	384	ILE	12.6
1	A	20	THR	12.4
3	R	1	U	10.8
1	A	32	ARG	10.5
3	R	4	C	10.3
2	E	382	SER	9.4
2	D	383	ASN	8.7
2	D	382	SER	8.6
1	B	53	MET	8.6
3	R	3	U	8.4
3	R	15	U	8.2
3	R	5	U	8.1
3	R	2	U	8.0
2	D	381	ALA	8.0
3	R	14	U	7.9
1	A	21	GLN	7.5
1	A	29	ASN	7.1

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Mol	Chain	Res	Type	RSRZ
1	A	23	ALA	6.9
3	R	6	C	6.8
1	B	54	ALA	6.6
1	B	363	ASN	6.6
2	F	383	ASN	6.3
1	B	82	LYS	6.3
3	R	11	A	6.2
2	E	380	ALA	6.0
2	D	365	SER	5.9
2	F	380	ALA	5.9
3	R	10	U	5.8
2	D	379	ALA	5.8
1	A	57	THR	5.8
2	E	364	ALA	5.7
1	C	78	THR	5.7
3	R	7	U	5.6
3	R	8	U	5.6
2	E	378	LEU	5.5
2	E	369	ARG	5.3
3	R	12	U	5.3
2	E	365	SER	5.3
1	B	76	PHE	5.3
2	E	376	SER	5.0
2	F	382	SER	4.9
2	E	379	ALA	4.9
1	A	31	PRO	4.9
1	A	26	PRO	4.8
1	B	78	THR	4.8
1	A	24	PRO	4.7
1	A	22	THR	4.7
2	E	381	ALA	4.6
3	R	13	C	4.5
1	B	333	GLY	4.5
1	A	28	GLN	4.4
1	C	55	ALA	4.4
2	D	375	LYS	4.3
1	C	79	ASP	4.3
2	E	377	SER	4.3
1	A	27	GLN	4.3
1	C	361	ALA	4.2
2	D	380	ALA	4.2
3	R	9	U	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	63	GLY	4.0
1	A	58	ARG	4.0
2	D	364	ALA	4.0
1	A	56	LEU	3.9
1	B	57	THR	3.9
1	C	80	PRO	3.9
1	A	362	GLN	3.9
1	A	30	VAL	3.9
1	B	77	ASN	3.8
2	D	376	SER	3.8
1	A	81	GLY	3.7
1	B	79	ASP	3.7
1	C	211	SER	3.7
2	E	366	MET	3.6
1	B	55	ALA	3.5
2	E	367	TRP	3.5
2	E	375	LYS	3.5
1	A	76	PHE	3.5
1	B	238	GLY	3.5
1	C	81	GLY	3.4
1	A	130	ALA	3.4
1	A	228	PRO	3.4
1	A	361	ALA	3.4
1	C	82	LYS	3.3
2	E	373	ILE	3.3
2	E	371	LYS	3.3
1	C	58	ARG	3.2
1	C	265	ALA	3.2
1	A	83	GLY	3.2
1	A	363	ASN	3.2
1	C	163	VAL	3.2
1	A	335	ASP	3.1
1	B	362	GLN	3.1
1	B	58	ARG	3.1
2	D	368	GLU	3.0
1	B	75	ASP	3.0
2	F	379	ALA	3.0
1	B	73	PRO	3.0
1	C	363	ASN	3.0
1	B	334	HIS	2.9
2	E	372	SER	2.9
1	B	69	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	335	ASP	2.9
2	F	381	ALA	2.9
1	B	308	VAL	2.9
2	E	368	GLU	2.9
1	C	61	GLN	2.8
1	C	233	GLU	2.8
1	C	77	ASN	2.8
1	B	56	LEU	2.8
1	C	108	GLY	2.8
1	A	211	SER	2.8
1	C	281	GLY	2.8
1	A	185	ALA	2.7
2	D	369	ARG	2.7
2	D	371	LYS	2.7
2	D	366	MET	2.7
1	B	251	GLU	2.7
1	C	66	PHE	2.7
1	C	356	VAL	2.7
1	A	302	SER	2.7
1	B	212	SER	2.7
1	A	303	ALA	2.7
1	A	25	VAL	2.6
1	B	72	ALA	2.6
1	A	80	PRO	2.6
1	C	57	THR	2.6
1	A	306	GLY	2.6
1	B	135	THR	2.6
1	A	62	PRO	2.6
1	B	71	PHE	2.5
1	B	264	PRO	2.5
2	F	376	SER	2.5
1	C	83	GLY	2.5
1	A	74	PRO	2.5
1	C	76	PHE	2.5
1	B	172	ASN	2.4
1	B	336	SER	2.4
1	C	75	ASP	2.4
1	B	361	ALA	2.4
1	A	69	CYS	2.4
1	C	56	LEU	2.4
2	D	372	SER	2.4
1	A	79	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	186	GLY	2.4
1	C	234	SER	2.3
1	A	61	GLN	2.3
1	A	290	GLY	2.3
2	D	378	LEU	2.3
2	E	370	VAL	2.3
1	B	94	SER	2.3
1	C	67	LEU	2.3
1	C	261	THR	2.2
1	A	87	ARG	2.2
1	B	80	PRO	2.2
1	C	243	SER	2.2
1	B	219	GLY	2.2
1	A	59	LEU	2.2
1	C	193	CYS	2.2
2	F	368	GLU	2.2
1	A	241	SER	2.2
1	B	254	ASP	2.2
1	C	63	GLY	2.2
1	A	356	VAL	2.2
1	A	105	PHE	2.2
1	A	115	ILE	2.2
2	F	369	ARG	2.2
2	D	370	VAL	2.2
1	B	332	PHE	2.2
1	C	72	ALA	2.2
1	A	131	GLY	2.2
1	A	174	GLY	2.2
1	B	233	GLU	2.1
1	A	355	PRO	2.1
1	A	182	MET	2.1
1	A	98	VAL	2.1
1	A	240	PHE	2.1
1	C	251	GLU	2.1
1	A	78	THR	2.1
1	A	321	TYR	2.1
1	A	251	GLU	2.1
1	A	305	GLU	2.1
1	C	318	CYS	2.1
1	A	287	GLY	2.1
1	A	84	ILE	2.1
1	A	218	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	207	ASP	2.1
1	B	130	ALA	2.1
1	C	213	LEU	2.1
1	C	121	VAL	2.1
1	A	279	ASP	2.0
1	B	280	SER	2.0
1	C	209	ALA	2.0
1	A	77	ASN	2.0
1	A	238	GLY	2.0
1	C	360	ALA	2.0
1	B	104	SER	2.0
1	B	213	LEU	2.0
1	A	172	ASN	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CA	A	403	1/1	0.75	0.30	115,115,115,115	0
5	EPE	B	403	15/15	0.91	0.22	60,78,89,89	0
6	CL	B	402	1/1	0.92	0.12	81,81,81,81	0
5	EPE	A	404	15/15	0.93	0.20	64,81,93,93	0
5	EPE	C	401	15/15	0.94	0.18	60,83,92,93	0
4	CA	A	402	1/1	0.96	0.07	51,51,51,51	0
4	CA	A	401	1/1	0.97	0.12	56,56,56,56	0
4	CA	B	401	1/1	0.98	0.04	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.