



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:44 AM GMT

PDB ID : 1F8V
Title : THE STRUCTURE OF PARIACOTO VIRUS REVEALS A DODECAHE-
DRAL CAGE OF DUPLEX RNA
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Deposited on : 2000-07-05
Resolution : 3.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

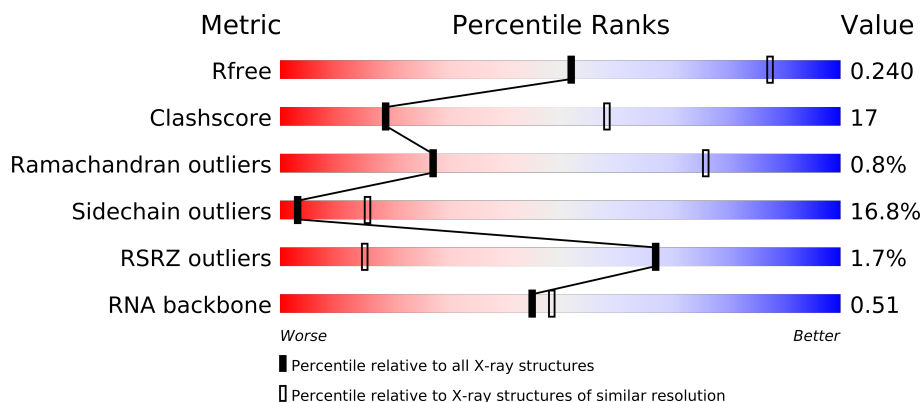
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.00 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}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)
RNA backbone	1838	1070 (3.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	R	25	
2	A	355	
2	B	355	
2	C	355	
3	D	40	
3	E	40	
3	F	40	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	SO4	C	500	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8719 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	25	Total	C	N	O	P	0	0	0
			509	229	62	193	25			

- Molecule 2 is a protein called MATURE CAPSID PROTEIN BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	355	Total	C	N	O	S	0	0	0
			2708	1721	474	501	12			
2	B	313	Total	C	N	O	S	0	0	0
			2378	1522	396	449	11			
2	C	311	Total	C	N	O	S	0	0	0
			2363	1513	393	446	11			

- Molecule 3 is a protein called MATURE CAPSID PROTEIN GAMMA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	26	Total	C	N	O	S	0	0	1
			204	130	36	36	2			
3	E	22	Total	C	N	O		0	0	1
			166	108	29	29				
3	F	22	Total	C	N	O		0	0	1
			166	108	29	29				

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		

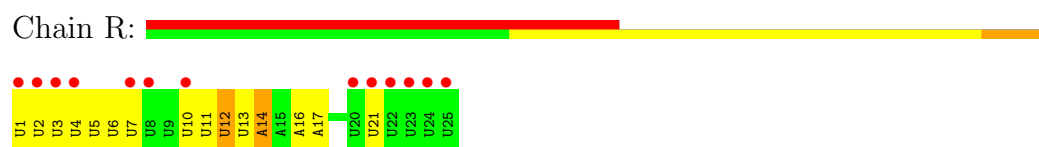
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	77	Total	O	0	0
			77	77		
6	B	60	Total	O	0	0
			60	60		
6	C	76	Total	O	0	0
			76	76		
6	D	2	Total	O	0	0
			2	2		
6	F	2	Total	O	0	0
			2	2		
6	R	2	Total	O	0	0
			2	2		

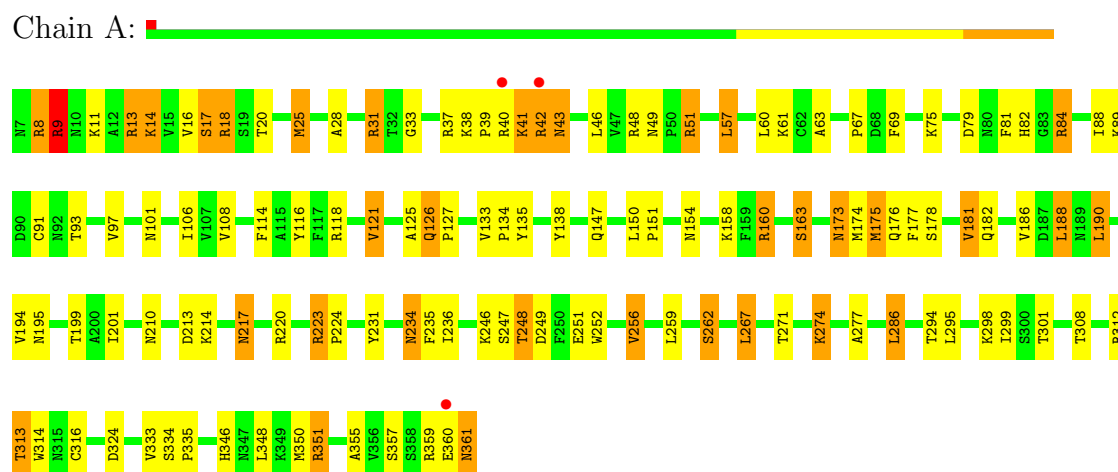
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: RNA



- Molecule 2: MATURE CAPSID PROTEIN BETA

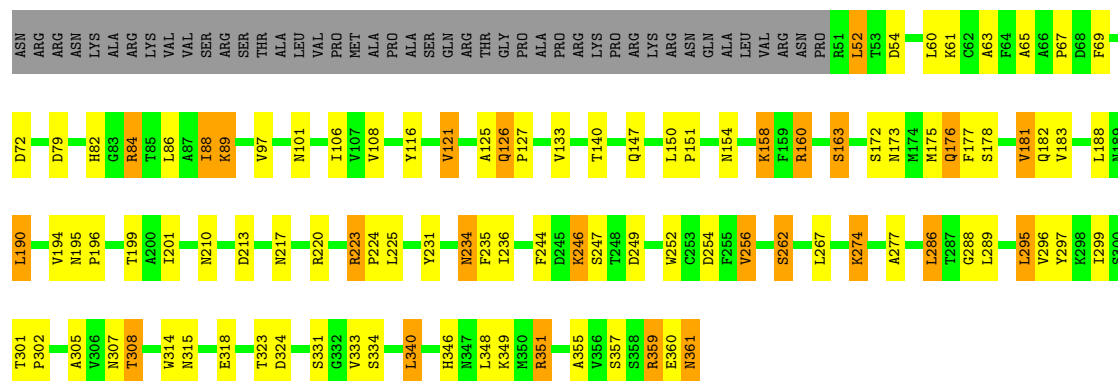


- Molecule 2: MATURE CAPSID PROTEIN BETA



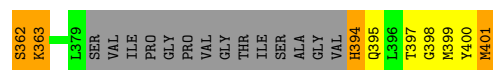
- Molecule 2: MATURE CAPSID PROTEIN BETA

Chain C:



- Molecule 3: MATURE CAPSID PROTEIN GAMMA

Chain D:



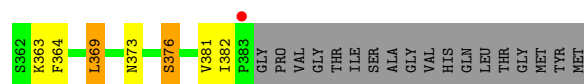
- Molecule 3: MATURE CAPSID PROTEIN GAMMA

Chain E:



- Molecule 3: MATURE CAPSID PROTEIN GAMMA

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	329.33Å 346.94Å 424.89Å 90.00° 90.83° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 207.27 – 3.02	Depositor EDS
% Data completeness (in resolution range)	65.6 (20.00-3.00) 80.7 (207.27-3.02)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.21 (at 3.01Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.219 , 0.221 0.240 , 0.240	Depositor DCC
R_{free} test set	150647 reflections (11.12%)	DCC
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.579	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 11.1	EDS
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 1505799 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	8719	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, SO4

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	R	0.46	1/562 (0.2%)	0.69	0/866
2	A	0.44	0/2779	0.68	1/3792 (0.0%)
2	B	0.45	0/2444	0.69	1/3342 (0.0%)
2	C	0.44	0/2428	0.69	1/3319 (0.0%)
3	D	0.54	0/207	0.55	0/275
3	E	0.55	0/168	0.59	0/227
3	F	0.55	0/168	0.60	0/227
All	All	0.45	1/8756 (0.0%)	0.68	3/12048 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	1	U	OP3-P	-7.16	1.52	1.61

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	247	SER	N-CA-C	-5.41	96.39	111.00
2	B	86	LEU	N-CA-C	-5.21	96.92	111.00
2	C	247	SER	N-CA-C	-5.07	97.32	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

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

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	509	0	255	13	0
2	A	2708	0	2672	111	0
2	B	2378	0	2305	86	0
2	C	2363	0	2292	72	0
3	D	204	0	200	9	0
3	E	166	0	174	18	0
3	F	166	0	174	6	0
4	C	5	0	0	0	0
5	A	1	0	0	0	0
6	A	77	0	0	2	0
6	B	60	0	0	4	0
6	C	76	0	0	3	0
6	D	2	0	0	0	0
6	F	2	0	0	0	0
6	R	2	0	0	0	0
All	All	8719	0	8072	275	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (275) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:R:11:U:H3'	1:R:12:U:H5''	1.30	1.11
2:B:173:ASN:HD22	2:B:175:MET:H	1.06	1.03
2:A:121:VAL:HG13	2:A:125:ALA:HB3	1.48	0.96
2:A:173:ASN:H	2:A:176:GLN:HE21	1.12	0.95
2:C:262:SER:HB2	2:C:274:LYS:HB3	1.51	0.93
2:B:176:GLN:HB2	2:B:306:VAL:HG13	1.50	0.93
2:B:262:SER:HB2	2:B:274:LYS:HB3	1.49	0.93
2:B:93:THR:HG23	2:B:312:ARG:HG2	1.49	0.93
2:A:8:ARG:HA	2:A:8:ARG:HH11	1.34	0.92
2:B:121:VAL:HG13	2:B:125:ALA:HB3	1.50	0.92
2:A:173:ASN:HD22	2:A:175:MET:H	1.16	0.91
2:A:361:ASN:HB3	3:D:363:LYS:HD3	1.52	0.89
2:B:173:ASN:ND2	2:B:175:MET:H	1.71	0.88
2:C:173:ASN:HD22	2:C:175:MET:H	1.21	0.88
2:C:121:VAL:HG13	2:C:125:ALA:HB3	1.58	0.85
2:B:49:ASN:HB3	2:B:50:PRO:HD3	1.59	0.85
2:A:49:ASN:HB3	3:F:382:ILE:HD11	1.59	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:68:ASP:HB3	3:E:363:LYS:HE2	1.62	0.81
2:C:181:VAL:HG22	2:C:235:PHE:HA	1.64	0.79
2:A:173:ASN:ND2	2:A:175:MET:H	1.81	0.79
2:B:234:ASN:HD22	2:B:236:ILE:H	1.32	0.78
2:A:93:THR:HG23	2:A:312:ARG:HG2	1.67	0.77
2:A:51:ARG:HD3	2:A:51:ARG:O	1.84	0.77
2:C:223:ARG:HD2	6:C:524:HOH:O	1.84	0.77
2:C:361:ASN:H	2:C:361:ASN:ND2	1.83	0.75
2:A:46:LEU:HG	3:F:381:VAL:HG11	1.66	0.75
2:B:223:ARG:HB2	2:B:224:PRO:HD2	1.71	0.73
2:B:248:THR:HB	2:B:249:ASP:OD2	1.89	0.73
2:A:262:SER:HB2	2:A:274:LYS:CB	2.18	0.73
1:R:11:U:H3'	1:R:12:U:C5'	2.15	0.72
1:R:11:U:C3'	1:R:12:U:H5''	2.16	0.72
2:B:182:GLN:OE1	2:B:298:LYS:HE2	1.89	0.72
2:A:181:VAL:CG2	2:A:235:PHE:HA	2.20	0.72
2:A:173:ASN:N	2:A:176:GLN:HE21	1.86	0.71
2:B:361:ASN:O	3:E:364:PHE:HB2	1.89	0.71
2:C:63:ALA:HA	2:C:163:SER:HB2	1.71	0.70
2:A:14:LYS:HE3	2:A:28:ALA:HB2	1.72	0.70
2:A:262:SER:HB2	2:A:274:LYS:HB2	1.73	0.70
2:C:361:ASN:HD22	2:C:361:ASN:H	1.37	0.70
3:D:399:MET:HG2	3:E:379:LEU:HB3	1.74	0.69
2:C:262:SER:HB2	2:C:274:LYS:CB	2.22	0.69
2:A:223:ARG:HD2	6:A:527:HOH:O	1.93	0.68
2:C:181:VAL:CG2	2:C:235:PHE:HA	2.23	0.68
2:B:63:ALA:HA	2:B:163:SER:HB2	1.76	0.67
2:A:182:GLN:OE1	2:A:298:LYS:HE2	1.95	0.67
2:A:181:VAL:HG22	2:A:235:PHE:HA	1.77	0.67
2:B:52:LEU:HD13	2:B:340:LEU:HD13	1.77	0.66
2:C:223:ARG:HB2	2:C:224:PRO:HD2	1.78	0.66
2:A:210:ASN:HD21	2:B:267:LEU:HD13	1.60	0.65
2:A:42:ARG:HG3	3:E:376:SER:HB2	1.78	0.65
1:R:6:U:H2'	1:R:7:U:O4'	1.96	0.64
1:R:4:U:H5'	2:A:13:ARG:NH1	2.13	0.64
2:A:248:THR:HG21	2:B:160:ARG:NH2	2.11	0.64
2:A:220:ARG:HD2	2:B:324:ASP:OD2	1.98	0.63
2:A:31:ARG:O	2:B:228:ARG:HD2	1.99	0.63
2:C:361:ASN:OXT	3:F:364:PHE:HB2	1.99	0.63
2:A:31:ARG:HD3	2:A:33:GLY:O	1.99	0.63
1:R:4:U:H5'	2:A:13:ARG:HH12	1.64	0.62
2:A:57:LEU:HD13	2:A:61:LYS:HE2	1.80	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:154:ASN:O	2:C:220:ARG:NH2	2.32	0.62
1:R:13:U:H2'	1:R:14:A:O4'	1.99	0.62
2:B:262:SER:HB2	2:B:274:LYS:CB	2.26	0.62
2:A:324:ASP:OD2	2:C:220:ARG:HD2	1.99	0.62
2:C:84:ARG:HG2	2:C:84:ARG:HH11	1.65	0.62
2:A:8:ARG:NH1	2:A:9:ARG:H	1.99	0.61
2:B:49:ASN:HB2	3:E:380:SER:HB3	1.81	0.61
2:B:173:ASN:HD22	2:B:173:ASN:C	2.04	0.61
2:A:79:ASP:OD2	2:A:160:ARG:NH2	2.33	0.61
2:C:79:ASP:OD2	2:C:160:ARG:NH2	2.33	0.61
1:R:11:U:H2'	1:R:12:U:O4'	2.02	0.60
2:A:93:THR:HG23	2:A:312:ARG:CG	2.32	0.60
2:A:217:ASN:HD22	2:A:217:ASN:N	1.99	0.60
2:B:121:VAL:CG1	2:B:125:ALA:HB3	2.29	0.60
2:A:223:ARG:HB2	2:A:224:PRO:HD2	1.84	0.60
2:C:84:ARG:CG	2:C:84:ARG:HH11	2.15	0.60
2:B:359:ARG:CZ	2:B:359:ARG:HB2	2.32	0.60
3:D:397:THR:O	3:D:399:MET:N	2.35	0.59
2:B:334:SER:HB2	2:B:335:PRO:HD2	1.85	0.59
2:A:234:ASN:HD22	2:A:236:ILE:H	1.51	0.59
2:C:277:ALA:HB2	2:C:286:LEU:HD13	1.85	0.59
2:A:63:ALA:HA	2:A:163:SER:HB2	1.83	0.59
2:C:173:ASN:ND2	2:C:175:MET:H	1.95	0.59
2:B:217:ASN:HD22	2:B:217:ASN:N	2.00	0.59
2:B:181:VAL:CG2	2:B:235:PHE:HA	2.33	0.58
2:B:239:ALA:N	2:B:358:SER:HB3	2.19	0.58
2:B:93:THR:HG23	2:B:312:ARG:CG	2.29	0.58
2:B:201:ILE:HG12	6:B:363:HOH:O	2.03	0.58
2:A:84:ARG:HG2	2:A:84:ARG:HH11	1.69	0.58
3:F:373:ASN:O	3:F:376:SER:HB2	2.04	0.58
2:A:173:ASN:ND2	2:A:176:GLN:H	2.02	0.57
2:A:201:ILE:HG12	6:B:362:HOH:O	2.04	0.57
2:A:262:SER:HB2	2:A:274:LYS:HB3	1.84	0.57
2:A:39:PRO:HG2	3:E:374:GLN:HE21	1.69	0.57
2:C:52:LEU:CD1	2:C:340:LEU:HD13	2.35	0.56
2:A:210:ASN:ND2	2:B:267:LEU:HD13	2.19	0.56
3:D:362:SER:N	3:D:363:LYS:HE3	2.20	0.56
3:D:363:LYS:H	3:D:363:LYS:CD	2.16	0.56
2:C:158:LYS:HD2	2:C:254:ASP:OD2	2.06	0.56
2:A:173:ASN:H	2:A:176:GLN:NE2	1.93	0.56
2:A:324:ASP:HB2	2:C:223:ARG:HE	1.70	0.56
2:C:361:ASN:C	3:F:364:PHE:HB2	2.26	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:121:VAL:CG1	2:A:125:ALA:HB3	2.31	0.56
2:B:220:ARG:NH2	2:C:154:ASN:O	2.39	0.56
2:A:177:PHE:CD1	2:A:178:SER:N	2.75	0.55
2:A:126:GLN:OE1	2:A:223:ARG:HB3	2.07	0.55
2:A:42:ARG:HG3	3:E:376:SER:CB	2.35	0.55
2:B:181:VAL:HG23	2:B:235:PHE:HA	1.89	0.55
2:B:194:VAL:HG12	2:B:210:ASN:HB3	1.89	0.55
2:A:67:PRO:HB3	2:A:314:TRP:CZ2	2.42	0.54
2:A:262:SER:CB	2:A:274:LYS:HB2	2.37	0.54
2:C:217:ASN:N	2:C:217:ASN:HD22	2.05	0.54
2:A:220:ARG:NH2	2:B:154:ASN:O	2.40	0.54
2:A:194:VAL:HG12	2:A:210:ASN:HB3	1.91	0.53
2:B:220:ARG:HD2	2:C:324:ASP:OD2	2.09	0.53
2:B:249:ASP:N	2:B:249:ASP:OD2	2.42	0.53
2:B:67:PRO:HB3	2:B:314:TRP:CZ2	2.43	0.53
2:B:306:VAL:O	2:B:306:VAL:HG22	2.09	0.53
2:C:84:ARG:HG2	2:C:84:ARG:NH1	2.19	0.53
1:R:16:A:O2'	1:R:17:A:H5'	2.09	0.53
2:C:61:LYS:HD3	2:C:69:PHE:CZ	2.44	0.53
2:C:195:ASN:ND2	2:C:213:ASP:OD1	2.39	0.52
6:A:502:HOH:O	2:C:201:ILE:HG12	2.09	0.52
2:A:49:ASN:HD22	2:A:51:ARG:HG3	1.75	0.52
2:C:299:ILE:HD12	2:C:299:ILE:N	2.24	0.52
2:C:256:VAL:HG22	2:C:256:VAL:O	2.09	0.52
2:A:299:ILE:HD12	2:A:299:ILE:N	2.25	0.52
2:A:231:TYR:CB	2:A:355:ALA:HB3	2.40	0.52
2:B:74:GLY:O	2:B:89:LYS:HD3	2.09	0.52
2:A:259:LEU:HD23	2:A:267:LEU:HD11	1.92	0.51
2:B:346:HIS:HA	2:B:349:LYS:HE2	1.91	0.51
2:A:8:ARG:NH1	2:A:9:ARG:N	2.59	0.51
2:A:195:ASN:ND2	2:A:213:ASP:OD2	2.42	0.51
2:A:361:ASN:N	2:A:361:ASN:HD22	2.10	0.50
2:B:249:ASP:O	2:B:250:PHE:HB2	2.10	0.50
2:C:249:ASP:OD1	2:C:249:ASP:N	2.45	0.50
2:A:48:ARG:NH1	3:D:400:TYR:O	2.39	0.50
2:B:160:ARG:HD2	2:B:252:TRP:CE2	2.47	0.49
2:B:79:ASP:OD2	2:B:160:ARG:NH2	2.40	0.49
2:A:135:TYR:OH	2:A:313:THR:HG22	2.12	0.49
2:A:249:ASP:OD2	2:A:249:ASP:N	2.46	0.49
2:C:348:LEU:HA	2:C:351:ARG:HG3	1.95	0.49
2:A:234:ASN:ND2	2:A:236:ILE:HG22	2.28	0.48
2:C:357:SER:OG	2:C:359:ARG:HG3	2.12	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:49:ASN:HD22	2:A:51:ARG:CG	2.27	0.48
2:C:231:TYR:CB	2:C:355:ALA:HB3	2.44	0.48
2:B:277:ALA:HB2	2:B:286:LEU:HD13	1.95	0.48
2:A:361:ASN:CB	3:D:363:LYS:HD3	2.36	0.48
2:C:97:VAL:HG22	2:C:308:THR:CG2	2.43	0.48
2:B:350:MET:HG2	2:C:333:VAL:HG13	1.95	0.48
1:R:11:U:H2'	1:R:12:U:C4'	2.44	0.48
2:C:177:PHE:CZ	2:C:236:ILE:HB	2.49	0.48
2:C:160:ARG:NH1	2:C:318:GLU:OE1	2.44	0.48
2:C:177:PHE:CD1	2:C:178:SER:N	2.82	0.48
2:A:277:ALA:HB2	2:A:286:LEU:HD13	1.95	0.48
2:A:88:ILE:O	2:A:316:CYS:HA	2.14	0.47
2:A:173:ASN:CG	2:A:176:GLN:HG2	2.35	0.47
2:A:91:CYS:HB2	2:A:314:TRP:CD1	2.49	0.47
1:R:5:U:O2'	1:R:6:U:H5'	2.15	0.47
2:C:301:THR:HG23	2:C:307:ASN:ND2	2.29	0.47
2:A:194:VAL:CG1	2:A:210:ASN:HB3	2.44	0.47
2:B:126:GLN:NE2	2:B:127:PRO:O	2.48	0.47
3:D:394:HIS:HB3	3:D:395:GLN:H	1.47	0.47
1:R:11:U:C3'	1:R:12:U:C5'	2.86	0.47
1:R:2:U:O2'	1:R:3:U:H5'	2.14	0.47
2:B:49:ASN:HB3	2:B:50:PRO:CD	2.37	0.47
2:A:81:PHE:HE1	2:C:246:LYS:O	1.98	0.47
2:C:72:ASP:OD1	2:C:89:LYS:HE2	2.15	0.47
2:A:173:ASN:HD21	2:A:176:GLN:H	1.60	0.47
2:A:61:LYS:HB3	2:A:69:PHE:CE1	2.50	0.47
2:A:91:CYS:HA	2:A:313:THR:O	2.14	0.47
2:B:173:ASN:C	2:B:173:ASN:ND2	2.67	0.47
2:A:42:ARG:CZ	3:E:376:SER:HA	2.45	0.47
2:C:183:VAL:HA	2:C:296:VAL:O	2.15	0.47
2:A:160:ARG:HD2	2:A:252:TRP:CE2	2.50	0.46
3:E:381:VAL:HG12	3:E:382:ILE:H	1.79	0.46
2:B:359:ARG:HB2	2:B:359:ARG:NH1	2.31	0.46
2:B:86:LEU:HA	2:B:86:LEU:HD12	1.82	0.46
2:A:346:HIS:O	2:B:82:HIS:HD2	1.97	0.46
2:C:302:PRO:HG2	2:C:305:ALA:HB2	1.98	0.46
2:B:160:ARG:HD3	2:B:318:GLU:OE1	2.15	0.46
2:C:126:GLN:NE2	2:C:127:PRO:O	2.49	0.46
2:A:150:LEU:HB3	2:A:151:PRO:HD2	1.97	0.46
3:E:372:LEU:HD22	3:E:372:LEU:O	2.15	0.46
2:C:288:GLY:HA3	6:C:529:HOH:O	2.15	0.46
3:F:369:LEU:HA	3:F:369:LEU:HD12	1.82	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:141:ASN:ND2	2:B:156:TYR:OH	2.49	0.45
2:B:299:ILE:N	2:B:299:ILE:HD12	2.31	0.45
2:B:343:GLU:OE2	3:E:378:THR:HB	2.17	0.45
2:C:173:ASN:ND2	2:C:176:GLN:H	2.15	0.45
2:B:234:ASN:ND2	2:B:236:ILE:H	2.07	0.45
2:A:116:TYR:CZ	2:A:133:VAL:HG21	2.51	0.45
2:A:8:ARG:NH1	2:A:8:ARG:HA	2.17	0.45
2:A:256:VAL:O	2:A:256:VAL:HG22	2.16	0.45
2:A:8:ARG:HD2	2:A:8:ARG:HA	1.48	0.45
2:C:84:ARG:HA	2:C:84:ARG:HD3	1.77	0.45
2:A:108:VAL:O	2:A:294:THR:HG23	2.17	0.45
2:C:234:ASN:ND2	2:C:236:ILE:HG22	2.32	0.45
2:C:108:VAL:HB	2:C:295:LEU:HB2	1.98	0.45
2:B:88:ILE:HD12	2:B:319:LEU:HD11	1.99	0.45
2:A:234:ASN:ND2	2:A:236:ILE:H	2.13	0.44
2:C:194:VAL:CG1	2:C:210:ASN:HB3	2.47	0.44
3:D:401:MET:HE3	6:B:420:HOH:O	2.18	0.44
2:B:160:ARG:NH1	2:B:318:GLU:OE1	2.43	0.44
2:A:17:SER:O	2:A:18:ARG:O	2.35	0.44
2:B:348:LEU:HD11	3:E:372:LEU:HD23	1.99	0.44
2:B:101:ASN:HB2	2:B:303:THR:HG23	1.99	0.44
2:B:357:SER:OG	2:B:359:ARG:HD3	2.18	0.44
2:C:244:PHE:CD1	2:C:349:LYS:HD2	2.53	0.44
2:B:172:SER:HB3	2:B:176:GLN:HG3	2.00	0.44
2:C:82:HIS:HA	2:C:334:SER:HB3	1.99	0.44
2:C:84:ARG:HD2	2:C:331:SER:HB2	2.00	0.44
2:A:267:LEU:HD22	2:C:210:ASN:OD1	2.18	0.43
2:C:182:GLN:HA	2:C:231:TYR:O	2.19	0.43
2:C:160:ARG:HD2	2:C:252:TRP:CE2	2.53	0.43
2:A:186:VAL:HG23	2:A:188:LEU:HD13	1.99	0.43
2:C:150:LEU:HB3	2:C:151:PRO:HD2	2.00	0.43
2:B:173:ASN:ND2	2:B:175:MET:N	2.53	0.43
2:C:121:VAL:CG1	2:C:125:ALA:HB3	2.39	0.43
2:B:214:LYS:C	2:B:215:ARG:HG2	2.39	0.43
2:A:158:LYS:HD3	2:A:252:TRP:HB3	2.01	0.43
2:A:106:ILE:HD13	2:A:118:ARG:HG3	2.01	0.43
3:E:363:LYS:HG3	3:E:363:LYS:H	1.38	0.43
2:B:256:VAL:O	2:B:256:VAL:HG22	2.19	0.43
2:B:238:GLY:HA3	2:B:358:SER:HB3	2.00	0.43
2:A:84:ARG:HG2	2:A:84:ARG:NH1	2.33	0.43
2:C:52:LEU:HD13	2:C:340:LEU:HD13	1.99	0.43
2:B:135:TYR:OH	2:B:313:THR:HG22	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:82:HIS:HD2	2:C:346:HIS:O	2.02	0.43
2:B:192:GLU:HG3	2:B:214:LYS:HE3	2.01	0.42
2:C:314:TRP:O	2:C:315:ASN:HB3	2.18	0.42
2:A:182:GLN:HA	2:A:231:TYR:O	2.18	0.42
2:A:334:SER:HB2	2:A:335:PRO:CD	2.50	0.42
2:B:234:ASN:ND2	2:B:236:ILE:HG22	2.34	0.42
2:A:41:LYS:HB2	2:A:43:ASN:ND2	2.34	0.42
2:A:234:ASN:HD22	2:A:236:ILE:N	2.17	0.42
2:B:91:CYS:HB2	2:B:314:TRP:CD1	2.54	0.42
2:C:106:ILE:HB	2:C:297:TYR:HB2	2.02	0.42
2:B:150:LEU:HB3	2:B:151:PRO:HD2	2.02	0.42
3:E:369:LEU:HD23	3:E:369:LEU:HA	1.82	0.42
2:B:234:ASN:HD22	2:B:236:ILE:N	2.09	0.42
2:A:126:GLN:NE2	2:A:127:PRO:O	2.53	0.42
2:B:91:CYS:HA	2:B:313:THR:O	2.19	0.42
2:A:267:LEU:HA	2:A:267:LEU:HD12	1.90	0.42
2:B:108:VAL:HB	2:B:295:LEU:HB2	2.01	0.42
2:A:348:LEU:HA	2:A:351:ARG:HG3	2.01	0.42
2:A:42:ARG:NH2	3:E:375:ILE:O	2.53	0.42
2:A:42:ARG:HE	3:E:376:SER:HB3	1.83	0.42
2:B:256:VAL:HG13	2:B:288:GLY:HA2	2.02	0.42
2:B:60:LEU:HD12	2:B:60:LEU:HA	1.93	0.42
2:A:334:SER:HB2	2:A:335:PRO:HD2	2.02	0.41
2:A:61:LYS:HD2	2:A:69:PHE:CZ	2.54	0.41
2:C:86:LEU:HG	2:C:88:ILE:HD13	2.03	0.41
2:C:223:ARG:HB2	2:C:223:ARG:HH11	1.84	0.41
2:A:177:PHE:CZ	2:A:236:ILE:HB	2.54	0.41
2:A:25:MET:HG3	2:A:25:MET:O	2.16	0.41
2:C:65:ALA:C	2:C:67:PRO:HD2	2.40	0.41
2:C:190:LEU:HD13	2:C:289:LEU:HD22	2.03	0.41
2:A:42:ARG:NE	3:E:376:SER:HB3	2.36	0.41
2:A:138:TYR:CD2	2:A:138:TYR:C	2.94	0.41
2:C:116:TYR:CZ	2:C:133:VAL:HG21	2.56	0.41
2:A:217:ASN:ND2	2:A:217:ASN:N	2.67	0.41
2:A:101:ASN:N	2:A:301:THR:O	2.54	0.41
2:B:343:GLU:HG3	6:B:420:HOH:O	2.21	0.41
2:A:114:PHE:HA	2:A:134:PRO:HA	2.03	0.41
2:A:190:LEU:HA	2:A:190:LEU:HD12	1.89	0.41
2:B:257:ARG:HA	2:B:286:LEU:O	2.21	0.40
2:C:82:HIS:HB2	6:C:512:HOH:O	2.21	0.40
2:B:183:VAL:HA	2:B:296:VAL:O	2.22	0.40
2:A:97:VAL:HG13	2:A:308:THR:HG22	2.02	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:189:ASN:CG	2:C:158:LYS:HD3	2.42	0.40
2:B:217:ASN:N	2:B:217:ASN:ND2	2.68	0.40
2:B:176:GLN:HB2	2:B:306:VAL:CG1	2.37	0.40
2:B:361:ASN:C	3:E:364:PHE:HB2	2.42	0.40
2:B:361:ASN:HA	2:B:361:ASN:HD22	1.60	0.40
2:B:190:LEU:HA	2:B:190:LEU:HD12	1.87	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	
2	A	353/355 (99%)	332 (94%)	17 (5%)	4 (1%)	21	67
2	B	311/355 (88%)	292 (94%)	17 (6%)	2 (1%)	33	81
2	C	309/355 (87%)	295 (96%)	13 (4%)	1 (0%)	50	90
3	D	22/40 (55%)	20 (91%)	1 (4%)	1 (4%)	4	22
3	E	20/40 (50%)	19 (95%)	1 (5%)	0	100	100
3	F	20/40 (50%)	19 (95%)	1 (5%)	0	100	100
All	All	1035/1185 (87%)	977 (94%)	50 (5%)	8 (1%)	27	76

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	16	VAL
2	A	18	ARG
3	D	398	GLY
2	A	9	ARG
2	A	360	GLU
2	B	178	SER
2	B	50	PRO
2	C	360	GLU

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	
2	A	290/290 (100%)	236 (81%)	54 (19%)	2	13
2	B	255/290 (88%)	216 (85%)	39 (15%)	4	19
2	C	253/290 (87%)	216 (85%)	37 (15%)	5	21
3	D	22/33 (67%)	18 (82%)	4 (18%)	2	13
3	E	19/33 (58%)	12 (63%)	7 (37%)	0	1
3	F	19/33 (58%)	16 (84%)	3 (16%)	4	18
All	All	858/969 (88%)	714 (83%)	144 (17%)	3	15

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	8	ARG
2	A	9	ARG
2	A	11	LYS
2	A	13	ARG
2	A	14	LYS
2	A	17	SER
2	A	20	THR
2	A	25	MET
2	A	31	ARG
2	A	37	ARG
2	A	38	LYS
2	A	40	ARG
2	A	41	LYS
2	A	42	ARG
2	A	43	ASN
2	A	51	ARG
2	A	57	LEU
2	A	60	LEU
2	A	75	LYS
2	A	84	ARG
2	A	89	LYS
2	A	121	VAL
2	A	126	GLN

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Mol	Chain	Res	Type
2	A	147	GLN
2	A	160	ARG
2	A	163	SER
2	A	173	ASN
2	A	174	MET
2	A	175	MET
2	A	181	VAL
2	A	188	LEU
2	A	190	LEU
2	A	199	THR
2	A	214	LYS
2	A	217	ASN
2	A	223	ARG
2	A	234	ASN
2	A	246	LYS
2	A	248	THR
2	A	251	GLU
2	A	256	VAL
2	A	262	SER
2	A	267	LEU
2	A	271	THR
2	A	274	LYS
2	A	286	LEU
2	A	295	LEU
2	A	313	THR
2	A	333	VAL
2	A	350	MET
2	A	351	ARG
2	A	357	SER
2	A	359	ARG
2	A	361	ASN
3	D	362	SER
3	D	363	LYS
3	D	394	HIS
3	D	401	MET
2	B	51	ARG
2	B	52	LEU
2	B	60	LEU
2	B	75	LYS
2	B	93	THR
2	B	126	GLN
2	B	128	THR

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Mol	Chain	Res	Type
2	B	160	ARG
2	B	163	SER
2	B	173	ASN
2	B	178	SER
2	B	188	LEU
2	B	190	LEU
2	B	199	THR
2	B	212	VAL
2	B	214	LYS
2	B	217	ASN
2	B	228	ARG
2	B	230	ASN
2	B	231	TYR
2	B	232	SER
2	B	246	LYS
2	B	248	THR
2	B	256	VAL
2	B	257	ARG
2	B	262	SER
2	B	271	THR
2	B	274	LYS
2	B	286	LEU
2	B	295	LEU
2	B	300	SER
2	B	303	THR
2	B	306	VAL
2	B	333	VAL
2	B	340	LEU
2	B	350	MET
2	B	357	SER
2	B	359	ARG
2	B	361	ASN
3	E	362	SER
3	E	363	LYS
3	E	372	LEU
3	E	376	SER
3	E	378	THR
3	E	380	SER
3	E	382	ILE
2	C	52	LEU
2	C	54	ASP
2	C	60	LEU

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Mol	Chain	Res	Type
2	C	84	ARG
2	C	88	ILE
2	C	89	LYS
2	C	101	ASN
2	C	121	VAL
2	C	126	GLN
2	C	140	THR
2	C	147	GLN
2	C	158	LYS
2	C	160	ARG
2	C	163	SER
2	C	172	SER
2	C	176	GLN
2	C	181	VAL
2	C	188	LEU
2	C	190	LEU
2	C	196	PRO
2	C	199	THR
2	C	223	ARG
2	C	225	LEU
2	C	234	ASN
2	C	246	LYS
2	C	256	VAL
2	C	262	SER
2	C	267	LEU
2	C	274	LYS
2	C	286	LEU
2	C	295	LEU
2	C	308	THR
2	C	323	THR
2	C	340	LEU
2	C	351	ARG
2	C	359	ARG
2	C	361	ASN
3	F	363	LYS
3	F	369	LEU
3	F	376	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	43	ASN

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Mol	Chain	Res	Type
2	A	82	HIS
2	A	101	ASN
2	A	141	ASN
2	A	173	ASN
2	A	176	GLN
2	A	210	ASN
2	A	217	ASN
2	A	234	ASN
2	A	329	GLN
2	A	361	ASN
3	D	373	ASN
2	B	49	ASN
2	B	82	HIS
2	B	141	ASN
2	B	173	ASN
2	B	217	ASN
2	B	234	ASN
2	B	329	GLN
2	B	361	ASN
3	E	374	GLN
2	C	82	HIS
2	C	101	ASN
2	C	126	GLN
2	C	141	ASN
2	C	173	ASN
2	C	217	ASN
2	C	234	ASN
2	C	361	ASN
3	F	373	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	24/25 (96%)	4 (16%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	10	U
1	R	12	U
1	R	14	A

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Mol	Chain	Res	Type
1	R	21	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z > 2$
4	SO4	C	500	-	4,4,4	0.24	0	6,6,6	0.09	0

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
4	SO4	C	500	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	R	25/25 (100%)	2.48	13 (52%) 0 0	89, 182, 229, 229	0
2	A	355/355 (100%)	-0.03	3 (0%) 83 26	11, 19, 70, 117	0
2	B	313/355 (88%)	-0.12	0 100 100	11, 19, 36, 90	0
2	C	311/355 (87%)	-0.13	0 100 100	10, 19, 32, 82	0
3	D	26/40 (65%)	0.40	0 100 100	27, 61, 89, 96	0
3	E	22/40 (55%)	0.47	0 100 100	31, 58, 84, 86	0
3	F	22/40 (55%)	0.34	1 (4%) 32 7	18, 45, 61, 72	0
All	All	1074/1210 (88%)	0.00	17 (1%) 67 16	10, 19, 78, 229	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	21	U	5.8
1	R	25	U	5.7
1	R	1	U	5.3
1	R	2	U	5.2
1	R	24	U	4.8
1	R	23	U	4.5
1	R	3	U	4.0
1	R	20	U	3.6
1	R	22	U	2.9
1	R	4	U	2.8
3	F	383	PRO	2.7
2	A	360	GLU	2.5
1	R	7	U	2.4
2	A	42	ARG	2.2
1	R	10	U	2.2
2	A	40	ARG	2.2
1	R	8	U	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	SO4	C	500	5/5	0.82	5.01	189,189,189,189	5
5	CA	A	501	1/1	0.08	-5.13	39,39,39,39	0

6.5 Other polymers ⓘ

There are no such residues in this entry.