



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:19 AM UTC

PDB ID : 2GJE / pdb_00002gje
Title : Structure of a guideRNA-binding protein complex bound to a gRNA
Authors : Schumacher, M.A.; Karamooz, E.; Zikova, A.; Trantirek, L.; Lukes, J.
Deposited on : 2006-03-30
Resolution : 3.37 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

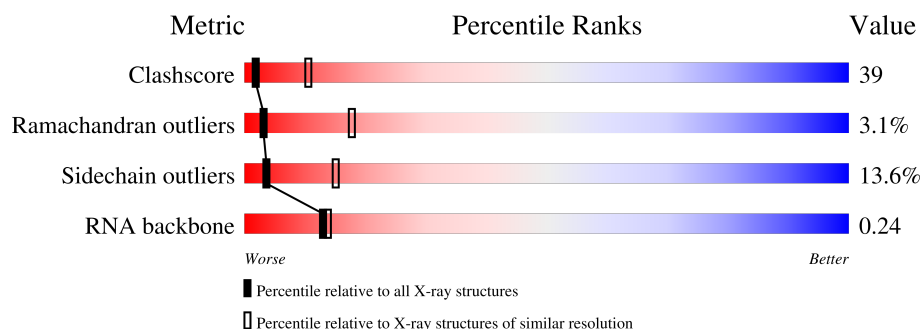
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.37 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1067 (3.42-3.34)
Ramachandran outliers	187476	1056 (3.42-3.34)
Sidechain outliers	187428	1056 (3.42-3.34)
RNA backbone	3983	1122 (3.76-3.00)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	R	39	8% 15% 5% 5% 67%
2	S	5	40% 60%
3	A	195	24% 38% 10% • 26%
4	D	187	34% 35% 10% 21%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2769 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 RNA chain called guide RNA 40-mer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	13	Total	C	N	O	P	0	0	0
			272	124	49	87	12			

- Molecule 2 is a RNA chain called RNA tetramer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	5	Total	C	N	O	P	0	0	0
			105	48	19	34	4			

- Molecule 3 is a protein called mitochondrial RNA-binding protein 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	A	145	Total	C	N	O	S	Se	0	0	0
			1187	752	216	215	1	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	MSE	MET	modified residue	UNP Q952G2
A	125	MSE	MET	modified residue	UNP Q952G2
A	204	MSE	MET	modified residue	UNP Q952G2

- Molecule 4 is a protein called mitochondrial RNA-binding protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	147	Total	C	N	O	S	Se	0	0	0
			1204	759	222	219	1	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	43	GLU	LEU	conflict	UNP P90629

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Chain	Residue	Modelled	Actual	Comment	Reference
D	46	MSE	MET	modified residue	UNP P90629
D	109	MSE	MET	modified residue	UNP P90629
D	139	MSE	MET	modified residue	UNP P90629

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total O 1 1	0	0

3 Residue-property plots

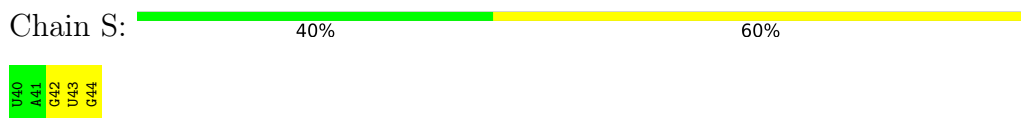
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

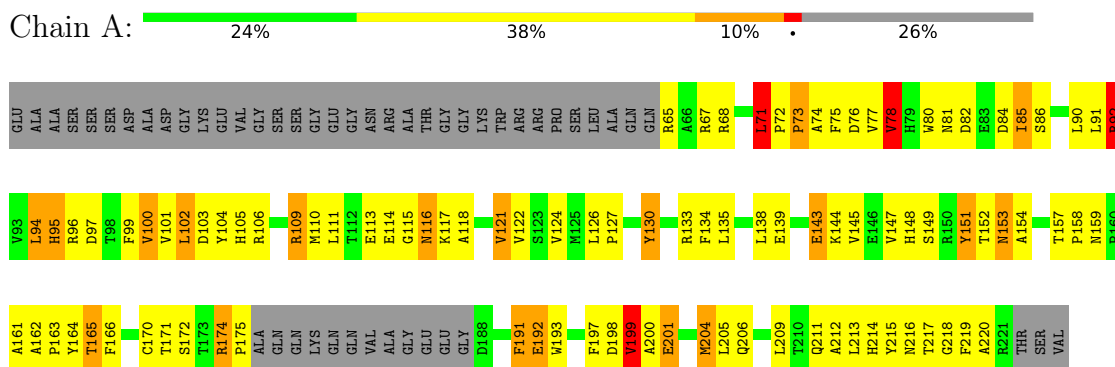
- Molecule 1: guide RNA 40-mer



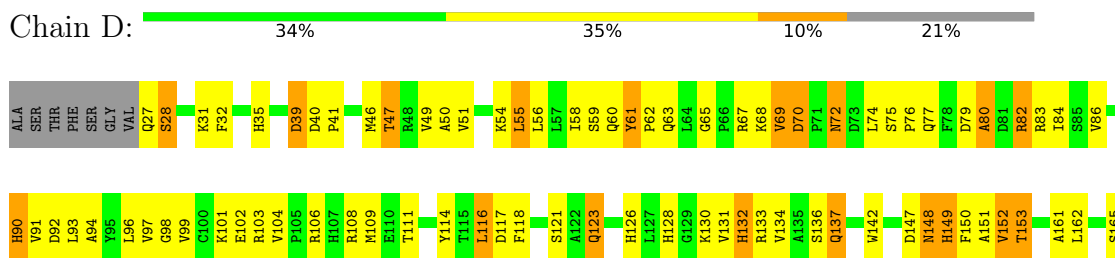
- Molecule 2: RNA tetramer



- Molecule 3: mitochondrial RNA-binding protein 2



- Molecule 4: mitochondrial RNA-binding protein 1



F168
H171
Y172
A173
THR
ARG
ALA
ALA
GLU
GLY
GLY
GLU
LYS
ILE
ALA
ALA
THR
THR
SER
SER
GLU
GLY
GLY
ALA
ARG
ARG
LYS
ARG
SER
SER
VAL
SER
ASP
THR
SER
ARG
THR
HIS

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	157.60Å 157.60Å 81.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	69.85 – 3.37	Depositor
% Data completeness (in resolution range)	91.8 (69.85-3.37)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.282 , 0.300	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2769	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

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	R	0.48	0/304	1.32	5/471 (1.1%)
2	S	0.69	0/117	1.05	0/181
3	A	0.79	1/1213 (0.1%)	1.30	17/1643 (1.0%)
4	D	0.66	0/1231	1.13	12/1657 (0.7%)
All	All	0.71	1/2865 (0.0%)	1.22	34/3952 (0.9%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	191	PHE	CA-C	-5.01	1.46	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	18	C	OP2-P-O3'	-14.26	65.21	108.00
1	R	18	C	OP1-P-O3'	-12.81	69.58	108.00
3	A	121	VAL	N-CA-C	11.88	122.95	111.67
1	R	18	C	O3'-P-O5'	9.65	118.48	104.00
4	D	28	SER	N-CA-C	-8.91	91.83	110.80
3	A	121	VAL	CB-CA-C	-8.20	102.12	111.80
3	A	130	TYR	N-CA-C	7.79	120.86	111.82
3	A	110	MSE	N-CA-C	7.48	120.65	110.55
3	A	71	LEU	N-CA-C	7.45	120.16	110.40
3	A	78	VAL	N-CA-C	7.28	118.36	108.17
4	D	137	GLN	N-CA-C	-7.27	103.03	113.21
1	R	19	C	O5'-P-OP2	-7.25	86.27	108.00
4	D	65	GLY	CA-C-N	7.09	128.70	119.84
4	D	65	GLY	C-N-CA	7.09	128.70	119.84
3	A	153	ASN	N-CA-C	-7.01	95.52	107.23
3	A	71	LEU	CA-C-N	6.95	127.54	120.38
3	A	71	LEU	C-N-CA	6.95	127.54	120.38
4	D	79	ASP	N-CA-C	6.78	119.92	107.99
3	A	191	PHE	CA-C-N	-6.63	111.69	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	191	PHE	C-N-CA	-6.63	111.69	122.82
3	A	191	PHE	N-CA-C	-6.51	98.12	108.73
3	A	100	VAL	N-CA-C	-6.12	98.74	107.98
3	A	192	GLU	N-CA-C	-5.83	100.55	109.41
4	D	82	ARG	N-CA-C	-5.66	106.27	112.72
4	D	55	LEU	N-CA-C	5.52	117.41	108.41
1	R	19	C	O5'-P-OP1	-5.43	91.69	108.00
4	D	61	TYR	N-CA-C	-5.41	102.66	110.40
4	D	116	LEU	N-CA-C	5.35	118.00	109.81
4	D	151	ALA	N-CA-C	-5.28	105.52	111.28
4	D	130	LYS	N-CA-C	-5.28	99.81	108.41
3	A	219	PHE	N-CA-C	-5.10	107.23	113.50
3	A	92	ARG	N-CA-C	-5.09	100.87	109.07
4	D	39	ASP	N-CA-C	-5.04	106.98	113.23
3	A	151	TYR	N-CA-C	5.00	120.22	113.72

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	272	0	141	21	0
2	S	105	0	55	7	0
3	A	1187	0	1158	116	0
4	D	1204	0	1172	81	2
5	D	1	0	0	0	0
All	All	2769	0	2526	209	2

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 39.

All (209) 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:A:117:LYS:HD2	3:A:117:LYS:H	1.11	1.10
3:A:77:VAL:HG21	3:A:197:PHE:HE1	1.27	0.98
3:A:174:ARG:HH21	3:A:175:PRO:HG2	1.28	0.94
3:A:77:VAL:HG22	3:A:201:GLU:HG2	1.53	0.91
1:R:18:C:OP2	3:A:117:LYS:NZ	2.07	0.87
4:D:68:LYS:HE3	4:D:77:GLN:HB2	1.56	0.87
3:A:77:VAL:HG21	3:A:197:PHE:CE1	2.09	0.86
3:A:171:THR:HG23	3:A:192:GLU:HG2	1.58	0.86
3:A:127:PRO:HD2	3:A:130:TYR:CE2	2.15	0.82
3:A:96:ARG:O	3:A:99:PHE:HB2	1.79	0.82
3:A:100:VAL:O	3:A:126:LEU:HB2	1.80	0.81
1:R:12:A:H3'	1:R:13:A:C8	2.15	0.81
4:D:54:LYS:HB3	4:D:90:HIS:HB3	1.62	0.81
1:R:20:U:O2	2:S:44:G:O6	1.99	0.79
4:D:171:HIS:HD2	4:D:172:TYR:CE2	2.01	0.79
3:A:82:ASP:OD2	3:A:111:LEU:HB2	1.84	0.78
3:A:117:LYS:HD2	3:A:117:LYS:N	1.96	0.76
3:A:191:PHE:CE2	3:A:193:TRP:CD1	2.73	0.76
4:D:116:LEU:HD21	4:D:131:VAL:HG13	1.66	0.76
3:A:127:PRO:HD2	3:A:130:TYR:CD2	2.23	0.74
3:A:76:ASP:OD2	3:A:92:ARG:HG3	1.88	0.74
3:A:174:ARG:NH2	3:A:175:PRO:HG2	2.03	0.74
3:A:126:LEU:HD11	3:A:134:PHE:HE2	1.54	0.73
3:A:101:VAL:C	3:A:102:LEU:HD23	2.14	0.73
3:A:215:TYR:CD1	3:A:220:ALA:HB2	2.24	0.72
4:D:51:VAL:HB	4:D:56:LEU:HD23	1.69	0.72
3:A:124:VAL:HG22	3:A:152:THR:HG21	1.71	0.72
3:A:71:LEU:HG	3:A:72:PRO:HD2	1.73	0.69
4:D:35:HIS:CD2	4:D:46:MSE:HG2	2.28	0.69
3:A:80:TRP:HH2	3:A:118:ALA:HB2	1.57	0.69
3:A:211:GLN:O	3:A:214:HIS:HB3	1.93	0.68
3:A:78:VAL:HG13	3:A:90:LEU:HD13	1.74	0.68
3:A:116:ASN:N	3:A:116:ASN:HD22	1.89	0.68
3:A:90:LEU:O	3:A:105:HIS:HB2	1.95	0.67
4:D:126:HIS:ND1	4:D:128:HIS:HD2	1.93	0.67
3:A:117:LYS:H	3:A:117:LYS:CD	1.96	0.67
3:A:95:HIS:CD2	3:A:95:HIS:O	2.49	0.66
4:D:171:HIS:HD2	4:D:172:TYR:HE2	1.42	0.66
4:D:31:LYS:HB3	4:D:50:ALA:HB2	1.78	0.65
4:D:108:ARG:HH11	4:D:108:ARG:HG3	1.61	0.65
3:A:95:HIS:HA	3:A:99:PHE:O	1.97	0.65
3:A:143:GLU:O	3:A:144:LYS:HB2	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:109:ARG:NH1	3:A:115:GLY:HA3	2.12	0.64
3:A:102:LEU:HD23	3:A:102:LEU:N	2.11	0.64
4:D:31:LYS:HB3	4:D:50:ALA:CB	2.28	0.64
3:A:191:PHE:CD2	3:A:193:TRP:HD1	2.16	0.63
3:A:94:LEU:CD1	3:A:101:VAL:HB	2.29	0.62
1:R:12:A:H3'	1:R:13:A:H8	1.64	0.62
3:A:198:ASP:OD1	3:A:201:GLU:HB2	2.01	0.61
3:A:191:PHE:CD2	3:A:193:TRP:CD1	2.88	0.61
4:D:116:LEU:HD21	4:D:131:VAL:CG1	2.31	0.61
4:D:32:PHE:CE1	4:D:49:VAL:HB	2.35	0.60
4:D:131:VAL:HG22	4:D:142:TRP:CB	2.31	0.60
3:A:191:PHE:CE2	3:A:193:TRP:HD1	2.20	0.59
3:A:215:TYR:CE2	4:D:168:PHE:HB3	2.37	0.59
4:D:97:VAL:O	4:D:98:GLY:C	2.45	0.59
3:A:162:ALA:O	3:A:165:THR:HG23	2.03	0.58
3:A:215:TYR:CE1	3:A:220:ALA:HB2	2.37	0.58
4:D:121:SER:OG	4:D:123:GLN:OE1	2.21	0.58
3:A:127:PRO:HD2	3:A:130:TYR:HE2	1.66	0.58
1:R:20:U:C2	2:S:44:G:O6	2.57	0.58
3:A:138:LEU:HD21	3:A:205:LEU:HD23	1.86	0.57
4:D:59:SER:HA	4:D:84:ILE:O	2.05	0.57
3:A:76:ASP:HB3	3:A:90:LEU:HD11	1.86	0.57
1:R:13:A:H2'	1:R:14:A:H8	1.68	0.57
3:A:122:VAL:HG11	3:A:193:TRP:HE1	1.68	0.56
4:D:108:ARG:HG3	4:D:108:ARG:NH1	2.20	0.56
4:D:62:PRO:HG2	4:D:82:ARG:HB3	1.87	0.56
3:A:135:LEU:O	3:A:139:GLU:HG3	2.05	0.56
4:D:58:ILE:HB	4:D:86:VAL:CG2	2.36	0.56
4:D:86:VAL:HG23	4:D:86:VAL:O	2.05	0.56
3:A:216:ASN:C	3:A:218:GLY:H	2.15	0.55
3:A:197:PHE:HD1	3:A:201:GLU:HB3	1.72	0.55
3:A:126:LEU:HD11	3:A:134:PHE:CE2	2.38	0.55
4:D:93:LEU:HD23	4:D:162:LEU:HD13	1.88	0.55
3:A:115:GLY:O	3:A:117:LYS:NZ	2.39	0.55
4:D:114:TYR:HD2	4:D:116:LEU:HG	1.72	0.55
3:A:135:LEU:HD21	3:A:209:LEU:HB2	1.89	0.54
3:A:157:THR:OG1	3:A:158:PRO:HD2	2.08	0.54
3:A:95:HIS:O	3:A:95:HIS:HD2	1.90	0.54
3:A:109:ARG:HH11	3:A:115:GLY:HA3	1.73	0.54
3:A:135:LEU:HA	3:A:138:LEU:HD12	1.89	0.54
3:A:148:HIS:HE1	3:A:153:ASN:ND2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:116:ASN:N	3:A:116:ASN:ND2	2.56	0.53
1:R:21:G:OP1	3:A:96:ARG:NH1	2.41	0.53
4:D:150:PHE:HA	4:D:153:THR:OG1	2.07	0.53
3:A:95:HIS:CD2	3:A:95:HIS:C	2.87	0.53
4:D:31:LYS:CB	4:D:50:ALA:HB2	2.38	0.53
4:D:98:GLY:O	4:D:101:LYS:N	2.39	0.53
3:A:84:ASP:C	3:A:86:SER:H	2.17	0.53
4:D:83:ARG:HE	4:D:134:VAL:HG11	1.73	0.52
3:A:122:VAL:HG11	3:A:193:TRP:NE1	2.24	0.52
3:A:174:ARG:HE	3:A:175:PRO:HD2	1.75	0.52
3:A:163:PRO:O	3:A:164:TYR:HB2	2.10	0.52
1:R:21:G:N1	2:S:43:U:N3	2.58	0.51
3:A:126:LEU:CD1	3:A:134:PHE:HE2	2.22	0.51
3:A:164:TYR:CE2	4:D:103:ARG:HG2	2.45	0.51
3:A:217:THR:HG22	3:A:217:THR:O	2.09	0.51
1:R:14:A:H2'	1:R:14:A:N3	2.26	0.51
3:A:172:SER:O	3:A:191:PHE:N	2.31	0.51
3:A:158:PRO:HA	3:A:166:PHE:CD1	2.46	0.51
3:A:135:LEU:HD23	3:A:138:LEU:HD13	1.93	0.51
3:A:216:ASN:C	3:A:218:GLY:N	2.68	0.50
4:D:75:SER:HB2	4:D:76:PRO:HD2	1.93	0.50
4:D:132:HIS:ND1	4:D:132:HIS:C	2.69	0.50
4:D:93:LEU:HD11	4:D:161:ALA:HB3	1.93	0.50
4:D:114:TYR:CD1	4:D:114:TYR:N	2.77	0.50
1:R:22:U:O2	2:S:42:G:N2	2.45	0.50
4:D:106:ARG:NH1	4:D:117:ASP:OD1	2.45	0.50
4:D:61:TYR:HD1	4:D:83:ARG:HB3	1.76	0.50
4:D:152:VAL:O	4:D:153:THR:C	2.53	0.49
3:A:94:LEU:HD12	3:A:101:VAL:HB	1.92	0.49
3:A:144:LYS:HG3	3:A:157:THR:HB	1.95	0.49
3:A:159:ASN:HB3	3:A:165:THR:OG1	2.13	0.49
3:A:171:THR:HG23	3:A:192:GLU:CG	2.35	0.49
4:D:99:VAL:HG22	4:D:104:VAL:HG23	1.93	0.49
1:R:21:G:C2'	1:R:22:U:H5'	2.43	0.49
3:A:199:VAL:HG21	4:D:103:ARG:O	2.12	0.49
4:D:111:THR:OG1	4:D:114:TYR:CE1	2.65	0.48
3:A:85:ILE:O	3:A:85:ILE:HG22	2.13	0.48
3:A:126:LEU:HD22	3:A:130:TYR:CD2	2.48	0.48
3:A:212:ALA:O	3:A:213:LEU:C	2.56	0.48
3:A:152:THR:HG22	3:A:172:SER:OG	2.14	0.48
3:A:65:ARG:HA	3:A:68:ARG:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:77:VAL:CG2	3:A:201:GLU:HG2	2.33	0.48
4:D:123:GLN:OE1	4:D:123:GLN:N	2.46	0.47
4:D:152:VAL:HG12	4:D:153:THR:N	2.28	0.47
3:A:77:VAL:HG13	3:A:201:GLU:CD	2.39	0.47
4:D:61:TYR:CD1	4:D:83:ARG:HB3	2.48	0.47
4:D:171:HIS:HD2	4:D:172:TYR:CD2	2.32	0.47
1:R:19:C:O2'	3:A:67:ARG:NH2	2.47	0.47
3:A:75:PHE:O	3:A:75:PHE:CG	2.67	0.47
3:A:75:PHE:CD1	3:A:75:PHE:C	2.92	0.47
3:A:172:SER:N	3:A:191:PHE:O	2.48	0.47
3:A:75:PHE:O	3:A:75:PHE:CD1	2.68	0.47
3:A:147:VAL:HG12	3:A:148:HIS:N	2.29	0.47
3:A:134:PHE:C	3:A:138:LEU:HD12	2.40	0.46
4:D:41:PRO:HA	4:D:63:GLN:NE2	2.30	0.46
3:A:198:ASP:O	3:A:200:ALA:N	2.48	0.46
3:A:76:ASP:CG	3:A:92:ARG:HG3	2.40	0.46
4:D:82:ARG:O	4:D:133:ARG:NH1	2.39	0.46
4:D:104:VAL:HG23	4:D:104:VAL:O	2.16	0.45
1:R:13:A:H2'	1:R:14:A:C8	2.50	0.45
4:D:51:VAL:HG23	4:D:55:LEU:C	2.42	0.45
3:A:106:ARG:HB3	3:A:121:VAL:HG21	1.98	0.45
4:D:58:ILE:HB	4:D:86:VAL:HG23	1.97	0.45
4:D:147:ASP:O	4:D:148:ASN:C	2.59	0.45
1:R:12:A:C3'	1:R:13:A:C8	2.94	0.45
4:D:126:HIS:ND1	4:D:128:HIS:CD2	2.80	0.45
4:D:108:ARG:O	4:D:108:ARG:HG2	2.16	0.45
3:A:104:TYR:C	3:A:104:TYR:CD1	2.94	0.45
3:A:72:PRO:O	3:A:73:PRO:C	2.55	0.45
4:D:172:TYR:HD2	4:D:172:TYR:N	2.15	0.45
3:A:134:PHE:O	3:A:138:LEU:HD12	2.17	0.44
4:D:67:ARG:HG2	4:D:68:LYS:O	2.18	0.44
4:D:126:HIS:CE1	4:D:128:HIS:HD2	2.35	0.44
1:R:12:A:OP1	4:D:80:ALA:HB2	2.17	0.44
1:R:20:U:H2'	1:R:21:G:O4'	2.18	0.44
4:D:126:HIS:CE1	4:D:128:HIS:CD2	3.06	0.44
4:D:39:ASP:OD2	4:D:39:ASP:N	2.51	0.44
4:D:92:ASP:C	4:D:94:ALA:N	2.74	0.44
4:D:133:ARG:O	4:D:136:SER:HB3	2.17	0.44
3:A:82:ASP:OD2	3:A:111:LEU:CB	2.62	0.44
3:A:205:LEU:O	3:A:206:GLN:C	2.60	0.44
3:A:80:TRP:CH2	3:A:118:ALA:HB2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:58:ILE:N	4:D:58:ILE:HD12	2.33	0.43
4:D:47:THR:HG23	4:D:60:GLN:HE21	1.83	0.43
4:D:171:HIS:CD2	4:D:172:TYR:CE2	2.93	0.43
4:D:172:TYR:CD2	4:D:172:TYR:N	2.85	0.43
3:A:154:ALA:HB2	3:A:170:CYS:CB	2.49	0.43
4:D:51:VAL:HG23	4:D:55:LEU:O	2.19	0.43
3:A:149:SER:C	3:A:151:TYR:N	2.74	0.43
4:D:47:THR:HG23	4:D:60:GLN:NE2	2.34	0.43
4:D:70:ASP:C	4:D:72:ASN:N	2.76	0.43
4:D:99:VAL:N	4:D:104:VAL:HG22	2.34	0.43
4:D:118:PHE:CD1	4:D:118:PHE:C	2.97	0.43
1:R:19:C:H1'	3:A:67:ARG:NH2	2.33	0.43
3:A:164:TYR:HD2	4:D:103:ARG:HD3	1.83	0.43
3:A:166:PHE:O	3:A:197:PHE:HB2	2.19	0.43
3:A:126:LEU:HD23	3:A:126:LEU:HA	1.88	0.42
4:D:70:ASP:O	4:D:72:ASN:N	2.52	0.42
4:D:96:LEU:HD22	4:D:118:PHE:CD2	2.53	0.42
4:D:92:ASP:O	4:D:93:LEU:C	2.60	0.42
3:A:148:HIS:CE1	3:A:153:ASN:ND2	2.86	0.42
3:A:215:TYR:HD1	3:A:220:ALA:HB2	1.78	0.42
3:A:84:ASP:C	3:A:86:SER:N	2.78	0.42
4:D:131:VAL:HG22	4:D:142:TRP:HB3	1.99	0.42
3:A:74:ALA:HB2	3:A:94:LEU:HB3	2.01	0.41
4:D:41:PRO:O	4:D:63:GLN:HB3	2.20	0.41
4:D:69:VAL:O	4:D:69:VAL:HG23	2.20	0.41
3:A:144:LYS:HG2	3:A:145:VAL:N	2.35	0.41
3:A:201:GLU:O	3:A:204:MSE:HB2	2.20	0.41
3:A:78:VAL:HG22	3:A:90:LEU:CD1	2.51	0.41
1:R:21:G:O6	2:S:43:U:O4	2.39	0.41
4:D:161:ALA:O	4:D:165:SER:HB3	2.20	0.41
1:R:13:A:H2'	1:R:14:A:O4'	2.21	0.41
3:A:143:GLU:O	3:A:158:PRO:HD2	2.21	0.41
1:R:14:A:N7	4:D:83:ARG:NH2	2.69	0.41
1:R:21:G:N2	2:S:43:U:C2	2.88	0.41
3:A:164:TYR:O	3:A:199:VAL:HA	2.21	0.41
4:D:51:VAL:O	4:D:51:VAL:HG13	2.19	0.41
4:D:82:ARG:O	4:D:133:ARG:HD3	2.21	0.41
4:D:106:ARG:HH22	4:D:108:ARG:HE	1.69	0.41
2:S:43:U:H2'	2:S:44:G:H8	1.85	0.40
3:A:154:ALA:HA	3:A:170:CYS:HA	2.03	0.40
3:A:216:ASN:HD22	3:A:216:ASN:HA	1.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:91:LEU:HD12	3:A:103:ASP:O	2.22	0.40
3:A:126:LEU:HA	3:A:127:PRO:HD3	1.75	0.40
4:D:93:LEU:HD21	4:D:162:LEU:N	2.36	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:67:ARG:NH2	4:D:67:ARG:NH2[8_556]	1.89	0.31
4:D:67:ARG:NH1	4:D:67:ARG:NH1[8_556]	1.91	0.29

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	
3	A	141/195 (72%)	121 (86%)	16 (11%)	4 (3%)	4	19
4	D	145/187 (78%)	124 (86%)	16 (11%)	5 (3%)	3	16
All	All	286/382 (75%)	245 (86%)	32 (11%)	9 (3%)	3	18

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	161	ALA
4	D	28	SER
3	A	85	ILE
3	A	199	VAL
4	D	148	ASN
3	A	97	ASP
4	D	80	ALA
4	D	149	HIS
4	D	152	VAL

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	
3	A	127/159 (80%)	108 (85%)	19 (15%)	3	12
4	D	130/155 (84%)	114 (88%)	16 (12%)	4	19
All	All	257/314 (82%)	222 (86%)	35 (14%)	3	15

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	71	LEU
3	A	73	PRO
3	A	78	VAL
3	A	81	ASN
3	A	92	ARG
3	A	94	LEU
3	A	95	HIS
3	A	102	LEU
3	A	109	ARG
3	A	113	GLU
3	A	114	GLU
3	A	116	ASN
3	A	133	ARG
3	A	143	GLU
3	A	165	THR
3	A	174	ARG
3	A	199	VAL
3	A	201	GLU
3	A	204	MSE
4	D	27	GLN
4	D	40	ASP
4	D	47	THR
4	D	69	VAL
4	D	70	ASP
4	D	72	ASN
4	D	74	LEU
4	D	90	HIS

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Mol	Chain	Res	Type
4	D	91	VAL
4	D	102	GLU
4	D	109	MSE
4	D	123	GLN
4	D	132	HIS
4	D	137	GLN
4	D	149	HIS
4	D	153	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	116	ASN
3	A	148	HIS
3	A	153	ASN
3	A	211	GLN
3	A	216	ASN
4	D	60	GLN
4	D	128	HIS
4	D	149	HIS
4	D	171	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	12/39 (30%)	6 (50%)	0
2	S	4/5 (80%)	0	0
All	All	16/44 (36%)	6 (37%)	0

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	12	A
1	R	15	U
1	R	17	A
1	R	18	C
1	R	19	C
1	R	21	G

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](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.