



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:42 PM UTC

PDB ID : 9CJM / pdb_00009cjm
Title : Red fluorescent protein mRuby3
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Deposited on : 2024-07-07
Resolution : 3.00 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

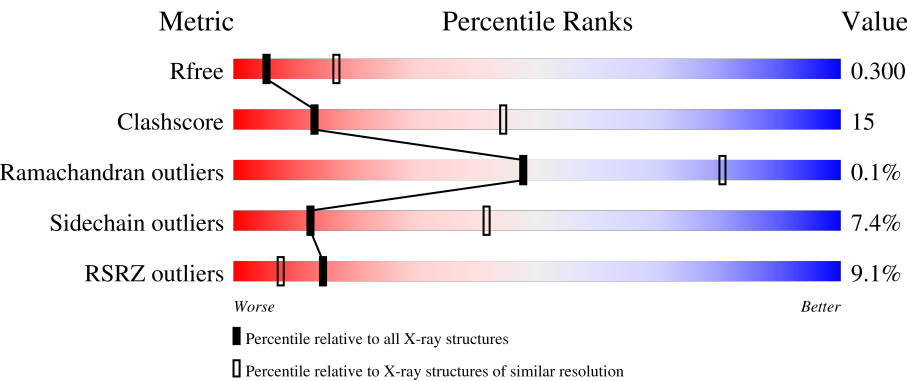
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 $\leq 5\%$. 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	235	<div><div>5%</div><div><div></div><div></div><div></div><div></div></div><div>63%26%5%6%</div></div>
1	B	235	<div><div>6%</div><div><div></div><div></div><div></div><div></div></div><div>71%19%•6%</div></div>
1	C	235	<div><div>12%</div><div><div></div><div></div><div></div><div></div></div><div>66%23%•7%</div></div>
1	D	235	<div><div>10%</div><div><div></div><div></div><div></div><div></div></div><div>67%23%•8%</div></div>

2 Entry composition [i](#)

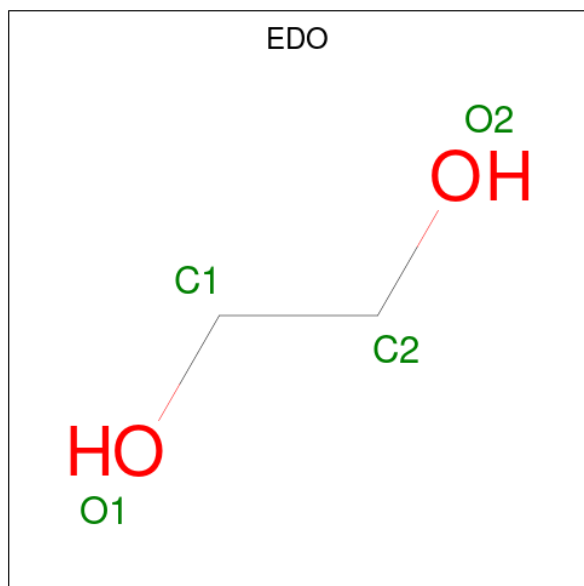
There are 3 unique types of molecules in this entry. The entry contains 7082 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Red fluorescent protein mRuby3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	2	0
			1773	1119	308	335	11			
1	B	220	Total	C	N	O	S	0	2	0
			1773	1119	308	335	11			
1	C	219	Total	C	N	O	S	0	2	0
			1767	1116	307	333	11			
1	D	217	Total	C	N	O	S	0	1	0
			1743	1102	300	330	11			

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



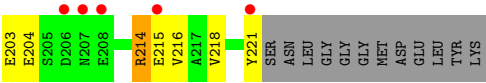
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is water.

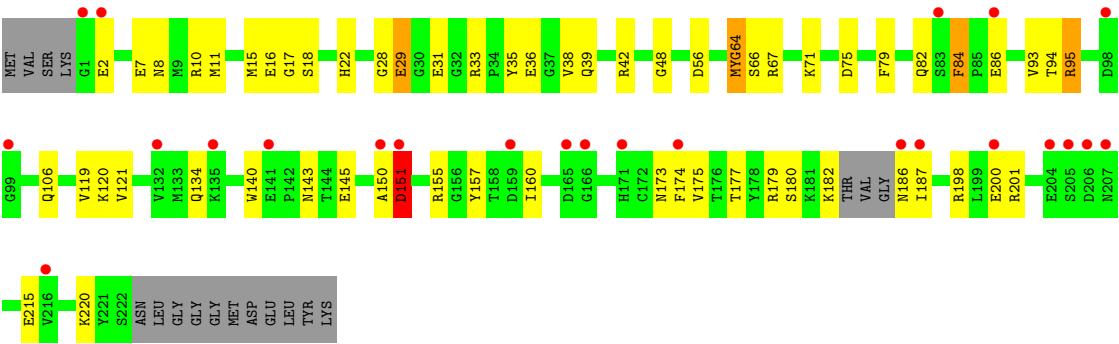
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total 8	O 8	0	0
3	B	8	Total 8	O 8	0	0
3	C	1	Total 1	O 1	0	0
3	D	5	Total 5	O 5	0	0

- Molecule 1: Red fluorescent protein mRuby3





● Molecule 1: Red fluorescent protein mRuby3



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	73.00Å 101.49Å 273.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.51 – 3.00 68.51 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.1 (68.51-3.00) 93.1 (68.51-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.76 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.278 , 0.306 0.271 , 0.300	Depositor DCC
R_{free} test set	958 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	14.6	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 13.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	7082	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.82% 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: NRQ, EDO

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	0.81	0/1788	1.22	6/2410 (0.2%)
1	B	0.81	0/1788	1.16	5/2410 (0.2%)
1	C	0.81	0/1782	1.17	5/2402 (0.2%)
1	D	0.79	0/1758	1.14	4/2369 (0.2%)
All	All	0.80	0/7116	1.17	20/9591 (0.2%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	ARG	CB-CA-C	6.76	117.23	110.33
1	C	196	ASP	CA-CB-CG	6.57	119.17	112.60
1	C	174	PHE	CA-CB-CG	6.44	120.24	113.80
1	C	62	PHE	CA-C-O	-6.31	110.08	120.80
1	B	84	PHE	CB-CA-C	6.20	118.41	109.11
1	B	165	ASP	CA-CB-CG	6.19	118.79	112.60
1	A	106	GLN	CB-CG-CD	6.08	122.94	112.60
1	A	52	PRO	CB-CA-C	-5.90	103.48	111.85
1	D	84	PHE	CB-CA-C	5.89	117.94	109.11
1	C	84	PHE	CB-CA-C	5.86	117.91	109.11
1	D	186	ASN	CA-C-N	5.79	130.72	123.14
1	D	186	ASN	C-N-CA	5.79	130.72	123.14
1	B	174	PHE	CA-CB-CG	5.65	119.45	113.80
1	A	84	PHE	CB-CA-C	5.64	117.57	109.11
1	D	151	ASP	CA-CB-CG	5.53	118.13	112.60
1	B	177	THR	CB-CA-C	5.49	119.20	110.19
1	A	107	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	171	HIS	CA-CB-CG	-5.24	108.56	113.80
1	C	159	ASP	CA-CB-CG	5.08	117.68	112.60
1	B	103	THR	CB-CA-C	5.02	118.42	109.38

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	1773	0	1724	58	0
1	B	1773	0	1724	36	0
1	C	1767	0	1719	66	0
1	D	1743	0	1686	52	0
2	A	4	0	6	0	0
3	A	8	0	0	0	0
3	B	8	0	0	0	0
3	C	1	0	0	0	0
3	D	5	0	0	0	0
All	All	7082	0	6859	206	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 15.

All (206) 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:D:84:PHE:O	1:D:182:LYS:NZ	1.60	1.29
1:C:75:ASP:OD2	1:C:221:TYR:OH	1.70	1.09
1:C:29:GLU:OE2	1:C:42:ARG:NH2	1.86	1.08
1:A:198[A]:ARG:HH11	1:A:198[A]:ARG:HG2	0.88	1.01
1:A:198[A]:ARG:HG2	1:A:198[A]:ARG:NH1	1.66	0.97
1:A:198[A]:ARG:HH12	1:A:200:GLU:HB2	1.29	0.96
1:C:64:NRQ:O2	1:C:64:NRQ:HD1	1.65	0.96
1:B:7:GLU:CD	1:B:7:GLU:H	1.73	0.94
1:A:2:GLU:OE2	1:A:82:GLN:HG2	1.67	0.93
1:D:64:NRQ:HD1	1:D:64:NRQ:O2	1.67	0.93
1:D:84:PHE:C	1:D:182:LYS:HZ1	1.77	0.92
1:A:198[A]:ARG:HH11	1:A:198[A]:ARG:CG	1.80	0.91
1:C:172:CYS:HG	1:C:174:PHE:HE1	1.18	0.86
1:B:29:GLU:OE2	1:B:42:ARG:NE	2.08	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:NRQ:HD1	1:A:64:NRQ:O2	1.75	0.85
1:D:84:PHE:C	1:D:182:LYS:NZ	2.35	0.85
1:A:159:ASP:OD1	1:A:173:ASN:ND2	2.10	0.84
1:C:39:GLN:HG2	1:C:64:NRQ:HE3	1.59	0.84
1:C:91:GLU:HG2	1:C:105:THR:HG22	1.58	0.84
1:A:67:ARG:HD2	1:A:178:TYR:CE2	2.12	0.84
1:B:64:NRQ:HD1	1:B:64:NRQ:O2	1.78	0.82
1:C:91:GLU:CG	1:C:105:THR:HG22	2.10	0.81
1:A:64:NRQ:O3	1:A:106:GLN:NE2	2.13	0.80
1:C:140:TRP:CE3	1:C:160:ILE:HG21	2.17	0.80
1:D:155:ARG:HH21	1:D:179:ARG:HH21	1.28	0.79
1:B:214:ARG:HH12	1:B:216:VAL:CG2	1.97	0.77
1:C:140:TRP:CE3	1:C:160:ILE:CG2	2.69	0.76
1:A:86:GLU:HG3	1:A:182:LYS:HA	1.68	0.76
1:C:214:ARG:HH21	1:C:214:ARG:HB3	1.52	0.75
1:D:64:NRQ:CD1	1:D:67:ARG:HH12	2.00	0.74
1:B:214:ARG:HH12	1:B:216:VAL:HG21	1.52	0.73
1:C:172:CYS:SG	1:C:174:PHE:HE1	2.13	0.72
1:D:39:GLN:HE22	1:D:66:SER:HB3	1.52	0.72
1:D:33:ARG:HB3	1:D:36:GLU:HG3	1.73	0.71
1:C:140:TRP:HE3	1:C:160:ILE:CG2	2.03	0.71
1:B:86:GLU:O	1:B:181:LYS:HE2	1.91	0.71
1:B:198[A]:ARG:HG3	1:B:198[A]:ARG:HH11	1.57	0.70
1:C:16:GLU:HB3	1:C:120:LYS:HE3	1.75	0.69
1:A:11:MET:SD	1:A:41:MET:CE	2.81	0.69
1:B:214:ARG:NH1	1:B:216:VAL:CG2	2.56	0.68
1:A:67:ARG:HD2	1:A:178:TYR:HE2	1.58	0.67
1:B:39:GLN:HG3	1:B:64:NRQ:HE3	1.76	0.67
1:A:91:GLU:HG2	1:A:105:THR:HG22	1.76	0.66
1:A:158:THR:CG2	1:A:160:ILE:HG12	2.26	0.66
1:B:67:ARG:HD2	1:B:178:TYR:CE1	2.31	0.65
1:A:67:ARG:NH2	1:A:197:HIS:NE2	2.45	0.64
1:D:95:ARG:HB3	1:D:95:ARG:NH1	2.12	0.64
1:A:11:MET:SD	1:A:41:MET:HE3	2.38	0.64
1:D:95:ARG:HB3	1:D:95:ARG:HH11	1.62	0.64
1:C:98:ASP:OD1	1:C:170:LEU:HD11	1.97	0.64
1:B:158:THR:CG2	1:B:160:ILE:HG12	2.29	0.63
1:A:203:GLU:HB3	1:A:212:VAL:HB	1.82	0.62
1:C:199:LEU:HD13	1:C:215:GLU:HG2	1.80	0.62
1:A:158:THR:HG21	1:A:160:ILE:CG1	2.30	0.61
1:A:39:GLN:OE1	1:A:66:SER:OG	2.19	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:NRQ:SD	1:C:215:GLU:HG3	2.41	0.61
1:C:140:TRP:HE3	1:C:160:ILE:HG22	1.64	0.61
1:D:155:ARG:NH2	1:D:179:ARG:HH21	1.98	0.60
1:C:140:TRP:CE3	1:C:160:ILE:HG22	2.37	0.59
1:C:199:LEU:HD13	1:C:215:GLU:CG	2.32	0.59
1:A:94:THR:HA	1:A:174:PHE:HB3	1.85	0.59
1:B:214:ARG:NH1	1:B:216:VAL:HG23	2.18	0.59
1:C:16:GLU:OE1	1:C:120:LYS:NZ	2.36	0.58
1:D:106:GLN:HG3	1:D:119:VAL:HG22	1.85	0.58
1:C:11:MET:HE3	1:C:39:GLN:HB2	1.85	0.58
1:A:86:GLU:OE1	1:A:182:LYS:HG3	2.04	0.58
1:C:64:NRQ:HD1	1:C:64:NRQ:C2	2.33	0.58
1:A:198[A]:ARG:NH1	1:A:198[A]:ARG:CG	2.50	0.58
1:D:64:NRQ:CD1	1:D:67:ARG:NH1	2.67	0.57
1:B:158:THR:HG21	1:B:160:ILE:HG12	1.87	0.57
1:C:98:ASP:OD1	1:C:98:ASP:N	2.28	0.57
1:A:12:LYS:HG3	1:A:114:GLU:OE2	2.05	0.57
1:C:157:TYR:CE1	1:C:175:VAL:HG13	2.39	0.57
1:C:67:ARG:NH2	1:C:145:GLU:OE1	2.38	0.57
1:C:11:MET:CE	1:C:39:GLN:HG3	2.35	0.57
1:B:94:THR:HA	1:B:174:PHE:HB3	1.87	0.56
1:C:16:GLU:CD	1:C:120:LYS:NZ	2.63	0.56
1:C:79:PHE:CZ	1:C:153:GLY:HA2	2.40	0.56
1:D:67:ARG:NH2	1:D:145:GLU:OE1	2.38	0.56
1:C:56:ASP:OD1	1:C:201:ARG:NH2	2.38	0.56
1:C:92:ARG:HD2	1:C:174:PHE:CD2	2.41	0.56
1:C:11:MET:CE	1:C:39:GLN:HB2	2.36	0.55
1:A:158:THR:CG2	1:A:160:ILE:CG1	2.85	0.55
1:D:11:MET:HE3	1:D:31:GLU:CA	2.36	0.55
1:B:158:THR:HG21	1:B:160:ILE:CG1	2.37	0.55
1:D:64:NRQ:O2	1:D:67:ARG:NH1	2.40	0.55
1:A:141:GLU:OE2	1:A:163:LYS:HG2	2.07	0.55
1:B:96:TYR:HB3	1:B:98:ASP:OD1	2.06	0.55
1:C:64:NRQ:N2	1:C:215:GLU:OE2	2.39	0.55
1:A:94:THR:CG2	1:A:172:CYS:SG	2.95	0.54
1:A:203:GLU:OE2	1:D:8:ASN:CG	2.50	0.54
1:C:39:GLN:N	1:C:39:GLN:OE1	2.40	0.54
1:D:79:PHE:CZ	1:D:180:SER:OG	2.59	0.54
1:A:34:PRO:HG3	1:A:69:PHE:CE2	2.43	0.54
1:A:11:MET:HE1	1:A:39:GLN:HE21	1.73	0.54
1:B:91:GLU:OE1	1:B:105:THR:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:TYR:HB3	1:C:98:ASP:OD1	2.08	0.54
1:A:64:NRQ:HE2	1:A:143:ASN:OD1	2.08	0.53
1:B:10[B]:ARG:NH2	1:C:203:GLU:OE2	2.42	0.53
1:C:91:GLU:HG3	1:C:105:THR:HG22	1.89	0.53
1:C:174:PHE:CD1	1:C:174:PHE:N	2.77	0.53
1:A:131:PRO:HG2	1:A:170:LEU:HD22	1.91	0.53
1:A:50:PRO:HB3	1:A:207:ASN:HB3	1.89	0.53
1:A:94:THR:HG23	1:A:172:CYS:SG	2.49	0.52
1:C:92:ARG:HD2	1:C:174:PHE:HD2	1.73	0.52
1:B:7:GLU:CD	1:B:7:GLU:N	2.53	0.52
1:C:138:LYS:HE3	1:C:165:ASP:OD1	2.10	0.52
1:D:94:THR:HA	1:D:174:PHE:HB3	1.91	0.52
1:B:158:THR:CG2	1:B:160:ILE:CG1	2.88	0.52
1:B:198[A]:ARG:HG3	1:B:198[A]:ARG:NH1	2.24	0.52
1:A:158:THR:HG21	1:A:160:ILE:HG12	1.89	0.52
1:A:7:GLU:HG2	1:A:8:ASN:N	2.25	0.52
1:B:64:NRQ:HE1	1:B:92:ARG:NH2	2.24	0.52
1:D:11:MET:HE3	1:D:31:GLU:N	2.25	0.52
1:A:155:ARG:NH1	1:A:157:TYR:OH	2.33	0.51
1:C:71:LYS:HD2	1:C:218:VAL:HG13	1.93	0.51
1:C:138:LYS:NZ	1:D:220:LYS:NZ	2.58	0.51
1:C:16:GLU:CD	1:C:120:LYS:HZ3	2.18	0.51
1:C:64:NRQ:HB12	1:C:215:GLU:OE2	2.10	0.51
1:D:150:ALA:O	1:D:151:ASP:OD1	2.29	0.50
1:B:64:NRQ:CZ	1:B:145:GLU:OE1	2.60	0.50
1:A:64:NRQ:OH	1:A:158:THR:OG1	2.28	0.50
1:C:15:MET:HE2	1:C:119:VAL:HG11	1.94	0.50
1:D:35:TYR:O	1:D:71:LYS:HG3	2.12	0.49
1:D:140:TRP:HE3	1:D:160:ILE:HG12	1.77	0.49
1:B:34:PRO:HB2	1:B:81:LYS:HE3	1.94	0.49
1:C:11:MET:HE2	1:C:39:GLN:HG3	1.94	0.49
1:D:140:TRP:CE3	1:D:160:ILE:HG12	2.48	0.49
1:B:64:NRQ:CZ	1:B:174:PHE:HE1	2.25	0.49
1:C:214:ARG:HH21	1:C:214:ARG:CB	2.22	0.49
1:D:33:ARG:NH2	1:D:36:GLU:OE2	2.45	0.49
1:D:177:THR:CG2	1:D:179:ARG:HE	2.26	0.49
1:A:64:NRQ:HD1	1:A:64:NRQ:C2	2.43	0.48
1:D:36:GLU:HB2	1:D:38:VAL:HG12	1.95	0.48
1:A:86:GLU:O	1:A:181:LYS:HE3	2.14	0.48
1:C:38:VAL:C	1:C:39:GLN:OE1	2.57	0.48
1:C:67:ARG:HD2	1:C:70:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:HIS:HE1	1:D:48:GLY:O	1.97	0.48
1:A:50:PRO:HB3	1:A:207:ASN:CB	2.44	0.47
1:D:15:MET:HE2	1:D:119:VAL:CG1	2.43	0.47
1:D:33:ARG:CB	1:D:36:GLU:HG3	2.41	0.47
1:C:160:ILE:HD12	1:C:174:PHE:CZ	2.49	0.47
1:B:147:MET:HE3	1:B:147:MET:HA	1.97	0.47
1:D:28:GLY:C	1:D:29:GLU:HG2	2.39	0.47
1:B:64:NRQ:HD1	1:B:64:NRQ:C2	2.44	0.47
1:A:11:MET:HE1	1:A:39:GLN:NE2	2.30	0.47
1:C:92:ARG:HD3	1:C:176:THR:OG1	2.15	0.47
1:A:13:VAL:HG23	1:A:117:TYR:HB2	1.97	0.47
1:D:157:TYR:CD1	1:D:175:VAL:HG12	2.50	0.46
1:D:106:GLN:CG	1:D:119:VAL:HG22	2.44	0.46
1:C:41:MET:HE3	1:C:62:PHE:HB3	1.96	0.46
1:C:138:LYS:HZ2	1:D:220:LYS:NZ	2.12	0.46
1:C:10[B]:ARG:HH21	1:C:114:GLU:HB2	1.80	0.46
1:C:97:GLU:HG2	1:C:171:HIS:O	2.15	0.46
1:A:86:GLU:HG3	1:A:182:LYS:CA	2.41	0.46
1:D:7:GLU:HG3	1:D:8:ASN:N	2.30	0.46
1:A:120:LYS:NZ	1:A:120:LYS:HB3	2.31	0.46
1:D:18:SER:HA	1:D:22:HIS:O	2.16	0.46
1:B:11:MET:HE2	1:B:69:PHE:CZ	2.52	0.45
1:B:29:GLU:OE1	1:C:29:GLU:CD	2.60	0.45
1:C:60:THR:O	1:C:92:ARG:NH2	2.49	0.45
1:A:214:ARG:HH21	1:A:216:VAL:HB	1.81	0.45
1:A:11:MET:HG3	1:A:41:MET:HE2	1.99	0.44
1:C:138:LYS:NZ	1:D:220:LYS:HZ3	2.14	0.44
1:B:151:ASP:O	1:B:179:ARG:NH2	2.51	0.44
1:C:16:GLU:HB3	1:C:120:LYS:CE	2.43	0.44
1:B:8:ASN:HB3	1:B:10[B]:ARG:NH2	2.32	0.44
1:D:64:NRQ:HD1	1:D:64:NRQ:C2	2.43	0.44
1:C:158:THR:HG23	1:C:158:THR:O	2.17	0.44
1:C:160:ILE:HG22	1:C:161:ALA:N	2.33	0.44
1:D:155:ARG:NH2	1:D:179:ARG:NH2	2.65	0.44
1:A:6:LYS:HB3	1:A:7:GLU:OE1	2.18	0.43
1:D:140:TRP:CZ3	1:D:160:ILE:HG23	2.53	0.43
1:C:10[B]:ARG:HE	1:C:10[B]:ARG:HB3	1.23	0.43
1:D:187:ILE:HG13	1:D:187:ILE:O	2.19	0.43
1:B:18:SER:HA	1:B:22:HIS:O	2.19	0.43
1:D:64:NRQ:HE2	1:D:143:ASN:OD1	2.17	0.43
1:A:18:SER:HA	1:A:22:HIS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:ARG:HH21	1:D:179:ARG:NH2	2.06	0.43
1:A:188:LYS:HD3	1:A:189:MET:N	2.34	0.43
1:D:15:MET:HE2	1:D:119:VAL:HG11	2.01	0.43
1:A:90:TRP:HE1	1:A:106:GLN:NE2	2.17	0.43
1:A:134:GLN:HA	1:A:134:GLN:OE1	2.19	0.42
1:C:18:SER:HA	1:C:22:HIS:O	2.19	0.42
1:D:16:GLU:O	1:D:120:LYS:HA	2.19	0.42
1:A:177:THR:HG22	1:A:179[B]:ARG:HD3	2.01	0.42
1:A:198[A]:ARG:NH1	1:A:200:GLU:HB2	2.13	0.42
1:C:11:MET:CE	1:C:39:GLN:CG	2.97	0.42
1:B:161:ALA:HB2	1:B:171:HIS:CE1	2.54	0.42
1:C:67:ARG:CD	1:C:70:ILE:HD11	2.50	0.42
1:A:141:GLU:OE2	1:A:163:LYS:HE2	2.19	0.42
1:B:84:PHE:O	1:B:182:LYS:NZ	2.52	0.41
1:C:142:PRO:CG	1:C:198:ARG:HE	2.33	0.41
1:D:134:GLN:HA	1:D:134:GLN:OE1	2.20	0.41
1:B:198[A]:ARG:HH11	1:B:198[A]:ARG:CG	2.31	0.41
1:D:198:ARG:NH1	1:D:200:GLU:HB2	2.35	0.41
1:D:56:ASP:OD1	1:D:201:ARG:NH2	2.54	0.41
1:C:179[A]:ARG:HE	1:C:179[A]:ARG:HB2	1.70	0.41
1:D:17:GLY:HA3	1:D:121:VAL:O	2.21	0.41
1:A:149:PRO:HG3	1:A:190:PRO:O	2.21	0.41
1:D:2:GLU:OE2	1:D:82:GLN:HG2	2.21	0.41
1:A:138:LYS:HE2	1:A:165:ASP:OD1	2.21	0.41
1:A:11:MET:SD	1:A:41:MET:HE2	2.59	0.40
1:A:79:PHE:CZ	1:A:153:GLY:HA2	2.56	0.40
1:B:15:MET:HE3	1:B:15:MET:HB2	2.01	0.40
1:D:15:MET:HE3	1:D:15:MET:HB2	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	217/235 (92%)	212 (98%)	5 (2%)	0	100	100
1	B	217/235 (92%)	213 (98%)	4 (2%)	0	100	100
1	C	216/235 (92%)	210 (97%)	6 (3%)	0	100	100
1	D	211/235 (90%)	207 (98%)	3 (1%)	1 (0%)	24	60
All	All	861/940 (92%)	842 (98%)	18 (2%)	1 (0%)	48	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	151	ASP

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	189/199 (95%)	175 (93%)	14 (7%)	13	42
1	B	189/199 (95%)	172 (91%)	17 (9%)	9	34
1	C	188/199 (94%)	170 (90%)	18 (10%)	8	31
1	D	186/199 (94%)	177 (95%)	9 (5%)	23	57
All	All	752/796 (94%)	694 (92%)	58 (8%)	13	40

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	23	GLN
1	A	33	ARG
1	A	75	ASP
1	A	86	GLU
1	A	93	VAL
1	A	119	VAL
1	A	120	LYS
1	A	155	ARG
1	A	160	ILE

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Mol	Chain	Res	Type
1	A	171	HIS
1	A	188	LYS
1	A	198[A]	ARG
1	A	198[B]	ARG
1	B	6	LYS
1	B	7	GLU
1	B	29	GLU
1	B	93	VAL
1	B	111	GLU
1	B	112	ASP
1	B	114	GLU
1	B	119	VAL
1	B	120	LYS
1	B	129	ASN
1	B	147	MET
1	B	173	ASN
1	B	179	ARG
1	B	188	LYS
1	B	198[A]	ARG
1	B	198[B]	ARG
1	B	200	GLU
1	C	10[A]	ARG
1	C	10[B]	ARG
1	C	11	MET
1	C	29	GLU
1	C	75	ASP
1	C	91	GLU
1	C	93	VAL
1	C	98	ASP
1	C	103	THR
1	C	106	GLN
1	C	120	LYS
1	C	155	ARG
1	C	174	PHE
1	C	184	VAL
1	C	187	ILE
1	C	204	GLU
1	C	214	ARG
1	C	216	VAL
1	D	10	ARG
1	D	29	GLU
1	D	42	ARG

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Mol	Chain	Res	Type
1	D	75	ASP
1	D	86	GLU
1	D	93	VAL
1	D	95	ARG
1	D	173	ASN
1	D	215	GLU

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

Mol	Chain	Res	Type
1	A	8	ASN
1	A	171	HIS
1	A	173	ASN
1	A	207	ASN
1	B	134	GLN
1	C	106	GLN
1	C	213	GLN
1	D	22	HIS
1	D	39	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
1	NRQ	D	64	1	24,24,25	1.43	4 (16%)	24,32,34	3.20	6 (25%)
1	NRQ	B	64	1	24,24,25	1.26	4 (16%)	24,32,34	3.42	6 (25%)
1	NRQ	C	64	1	24,24,25	1.29	3 (12%)	24,32,34	3.49	6 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	NRQ	A	64	1	24,24,25	1.31	3 (12%)	24,32,34	3.10	5 (20%)

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
1	NRQ	D	64	1	-	4/9/31/32	0/2/2/2
1	NRQ	B	64	1	-	4/9/31/32	0/2/2/2
1	NRQ	C	64	1	-	4/9/31/32	0/2/2/2
1	NRQ	A	64	1	-	5/9/31/32	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	NRQ	C2-N3	-4.03	1.30	1.40
1	D	64	NRQ	C2-N3	-3.69	1.31	1.40
1	B	64	NRQ	C2-N3	-3.46	1.32	1.40
1	C	64	NRQ	C2-N3	-3.22	1.32	1.40
1	C	64	NRQ	O2-C2	3.12	1.29	1.23
1	D	64	NRQ	O2-C2	2.99	1.29	1.23
1	D	64	NRQ	CA2-C2	-2.97	1.45	1.48
1	B	64	NRQ	O2-C2	2.85	1.28	1.23
1	C	64	NRQ	CA2-N2	-2.74	1.32	1.38
1	A	64	NRQ	O2-C2	2.57	1.28	1.23
1	B	64	NRQ	CA2-N2	-2.54	1.33	1.38
1	A	64	NRQ	CA2-N2	-2.45	1.33	1.38
1	D	64	NRQ	CA2-N2	-2.45	1.33	1.38
1	B	64	NRQ	C1-N2	2.22	1.38	1.33

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	64	NRQ	CB2-CA2-C2	11.40	136.18	122.36
1	B	64	NRQ	CB2-CA2-C2	10.82	135.47	122.36
1	A	64	NRQ	CB2-CA2-C2	9.79	134.22	122.36
1	D	64	NRQ	CB2-CA2-C2	9.27	133.60	122.36
1	C	64	NRQ	CB2-CA2-N2	-8.56	117.14	128.76
1	B	64	NRQ	CB2-CA2-N2	-8.32	117.47	128.76
1	A	64	NRQ	CB2-CA2-N2	-7.61	118.43	128.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	64	NRQ	CB2-CA2-N2	-7.19	118.99	128.76
1	D	64	NRQ	CA2-C2-N3	6.85	109.25	103.50
1	B	64	NRQ	CA2-C2-N3	6.79	109.20	103.50
1	A	64	NRQ	CA2-C2-N3	6.42	108.89	103.50
1	C	64	NRQ	CA2-C2-N3	5.65	108.25	103.50
1	D	64	NRQ	O2-C2-CA2	-5.64	127.42	131.02
1	B	64	NRQ	CG2-CB2-CA2	-4.28	124.78	129.87
1	C	64	NRQ	CG2-CB2-CA2	-4.28	124.78	129.87
1	C	64	NRQ	O2-C2-CA2	-3.92	128.52	131.02
1	C	64	NRQ	C2-CA2-N2	-3.19	106.67	108.95
1	D	64	NRQ	CG2-CB2-CA2	-3.14	126.13	129.87
1	B	64	NRQ	C2-CA2-N2	-2.70	107.02	108.95
1	A	64	NRQ	CG2-CB2-CA2	-2.64	126.72	129.87
1	D	64	NRQ	C2-CA2-N2	-2.37	107.26	108.95
1	A	64	NRQ	C2-CA2-N2	-2.24	107.34	108.95
1	B	64	NRQ	O2-C2-CA2	-2.24	129.59	131.02

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	64	NRQ	CA1-CB1-CG1-SD
1	B	64	NRQ	CA1-CB1-CG1-SD
1	A	64	NRQ	C2-CA2-CB2-CG2
1	B	64	NRQ	C2-CA2-CB2-CG2
1	C	64	NRQ	C2-CA2-CB2-CG2
1	D	64	NRQ	C2-CA2-CB2-CG2
1	B	64	NRQ	N2-CA2-CB2-CG2
1	A	64	NRQ	N2-CA2-CB2-CG2
1	C	64	NRQ	N2-CA2-CB2-CG2
1	D	64	NRQ	N2-CA2-CB2-CG2
1	A	64	NRQ	CB1-CG1-SD-CE
1	D	64	NRQ	C3-CA3-N3-C1
1	C	64	NRQ	CB1-CG1-SD-CE
1	D	64	NRQ	CB1-CG1-SD-CE
1	B	64	NRQ	CB1-CG1-SD-CE
1	A	64	NRQ	C3-CA3-N3-C1
1	C	64	NRQ	C3-CA3-N3-C1

There are no ring outliers.

4 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	64	NRQ	6	0
1	B	64	NRQ	6	0
1	C	64	NRQ	6	0
1	A	64	NRQ	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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	$\# Z > 2$
2	EDO	A	301	-	3,3,3	0.17	0	2,2,2	0.13	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
2	EDO	A	301	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	A	219/235 (93%)	0.87	12 (5%) 30 15	0, 4, 14, 25	2 (0%)
1	B	219/235 (93%)	0.89	15 (6%) 23 12	0, 5, 18, 39	2 (0%)
1	C	218/235 (92%)	1.16	28 (12%) 7 5	4, 15, 31, 42	2 (0%)
1	D	216/235 (91%)	1.10	24 (11%) 10 6	3, 15, 29, 59	1 (0%)
All	All	872/940 (92%)	1.00	79 (9%) 15 8	0, 10, 27, 59	7 (0%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	GLY	5.3
1	A	206	ASP	4.0
1	D	1	GLY	3.7
1	D	187	ILE	3.7
1	D	165	ASP	3.7
1	D	166	GLY	3.6
1	C	151	ASP	3.6
1	C	150	ALA	3.5
1	C	215	GLU	3.4
1	C	66	SER	3.4
1	B	2	GLU	3.4
1	C	165	ASP	3.3
1	D	186	ASN	3.3
1	C	86	GLU	3.2
1	D	98	ASP	3.2
1	C	3	GLU	3.1
1	A	151	ASP	3.1
1	D	151	ASP	3.0
1	B	66	SER	3.0
1	C	113	GLY	3.0
1	B	1	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	208	GLU	2.9
1	B	206	ASP	2.9
1	B	158	THR	2.9
1	B	62	PHE	2.9
1	C	16	GLU	2.8
1	A	204	GLU	2.7
1	B	215	GLU	2.7
1	C	166	GLY	2.7
1	D	205	SER	2.7
1	C	149	PRO	2.7
1	D	159	ASP	2.7
1	D	200	GLU	2.6
1	D	207	ASN	2.6
1	A	172	CYS	2.6
1	C	221	TYR	2.6
1	C	39	GLN	2.6
1	D	2	GLU	2.6
1	D	206	ASP	2.6
1	D	86	GLU	2.6
1	A	175	VAL	2.6
1	C	99	GLY	2.5
1	C	180	SER	2.5
1	C	179[A]	ARG	2.5
1	C	77	PRO	2.5
1	B	200	GLU	2.5
1	A	150	ALA	2.4
1	C	4	LEU	2.4
1	D	141	GLU	2.4
1	D	204	GLU	2.4
1	C	10[A]	ARG	2.4
1	C	105	THR	2.4
1	C	207	ASN	2.4
1	B	36	GLU	2.4
1	A	78	ASP	2.4
1	D	132	VAL	2.4
1	C	141	GLU	2.4
1	D	135	LYS	2.3
1	B	198[A]	ARG	2.3
1	C	125	ASN	2.3
1	A	111	GLU	2.3
1	D	150	ALA	2.3
1	A	165	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	216	VAL	2.2
1	B	167	GLY	2.2
1	A	149	PRO	2.2
1	C	190	PRO	2.2
1	B	75	ASP	2.2
1	C	75	ASP	2.2
1	C	206	ASP	2.2
1	D	99	GLY	2.1
1	D	171[A]	HIS	2.1
1	B	111	GLU	2.1
1	D	83	SER	2.1
1	A	207	ASN	2.1
1	D	174	PHE	2.1
1	B	156	GLY	2.1
1	C	41	MET	2.0
1	D	216	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	NRQ	C	64	23/24	0.74	0.24	38,43,47,47	0
1	NRQ	D	64	23/24	0.78	0.22	23,26,39,42	0
1	NRQ	B	64	23/24	0.80	0.24	16,23,26,27	0
1	NRQ	A	64	23/24	0.87	0.18	7,9,11,12	0

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(\AA^2)	Q<0.9
2	EDO	A	301	4/4	0.84	0.13	0,0,0,0	0

6.5 Other polymers [i](#)

There are no such residues in this entry.