



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:47 PM GMT

PDB ID : 3UXV
Title : Crystal Structure of 7-cyano-7-deazaguanine reductase, QueF from *Vibrio cholerae* complexed with NADP and PreQ
Authors : Kim, Y.; Zhou, M.; Gu, M.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2011-12-05
Resolution : 1.56 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

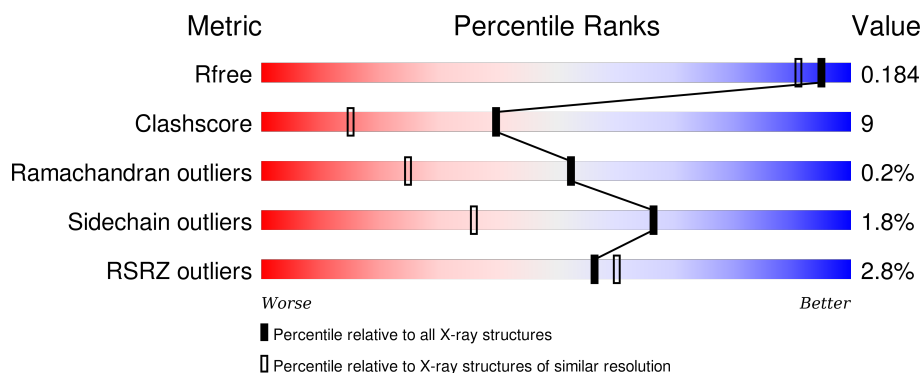
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.56 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}	91344	1665 (1.58-1.54)
Clashscore	102246	1014 (1.56-1.56)
Ramachandran outliers	100387	1704 (1.58-1.54)
Sidechain outliers	100360	1702 (1.58-1.54)
RSRZ outliers	91569	1668 (1.58-1.54)

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. 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	290	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>13%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	290	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>9%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	290	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>10%</div> <div>11%</div> </div> </div>
1	D	290	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>12%</div> <div>•</div> <div>12%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	302	-	-	X	X
2	EDO	D	302	-	-	X	X
3	GOL	A	303	-	-	-	X
3	GOL	B	302	-	-	-	X
3	GOL	D	303	-	-	-	X
3	GOL	D	304	-	-	-	X
3	GOL	D	305	-	-	-	X
4	NAP	B	301[A]	-	-	-	X
4	NAP	B	301[B]	-	-	-	X
4	NAP	D	301[A]	-	-	-	X
4	NAP	D	301[B]	-	-	-	X
5	GUN	C	300	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10034 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.

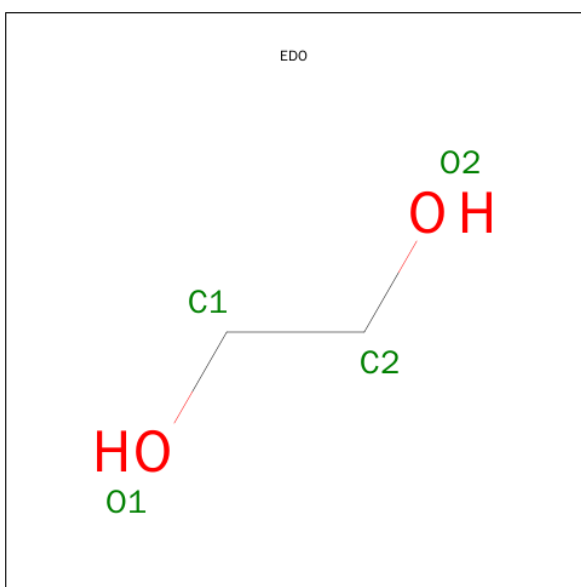
- Molecule 1 is a protein called NADPH-dependent 7-cyano-7-deazaguanine reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	Se	0	24	0
			2254	1396	403	443	6	6			
1	B	259	Total	C	N	O	S	Se	0	17	0
			2224	1380	394	437	6	7			
1	C	259	Total	C	N	O	S	Se	0	19	0
			2247	1395	400	439	6	7			
1	D	254	Total	C	N	O	S	Se	0	25	0
			2259	1403	400	444	6	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP C3LTF1
A	-1	ASN	-	EXPRESSION TAG	UNP C3LTF1
A	0	ALA	-	EXPRESSION TAG	UNP C3LTF1
A	194	ALA	CYS	engineered mutation	UNP C3LTF1
B	-2	SER	-	EXPRESSION TAG	UNP C3LTF1
B	-1	ASN	-	EXPRESSION TAG	UNP C3LTF1
B	0	ALA	-	EXPRESSION TAG	UNP C3LTF1
B	194	ALA	CYS	engineered mutation	UNP C3LTF1
C	-2	SER	-	EXPRESSION TAG	UNP C3LTF1
C	-1	ASN	-	EXPRESSION TAG	UNP C3LTF1
C	0	ALA	-	EXPRESSION TAG	UNP C3LTF1
C	194	ALA	CYS	engineered mutation	UNP C3LTF1
D	-2	SER	-	EXPRESSION TAG	UNP C3LTF1
D	-1	ASN	-	EXPRESSION TAG	UNP C3LTF1
D	0	ALA	-	EXPRESSION TAG	UNP C3LTF1
D	194	ALA	CYS	engineered mutation	UNP C3LTF1

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



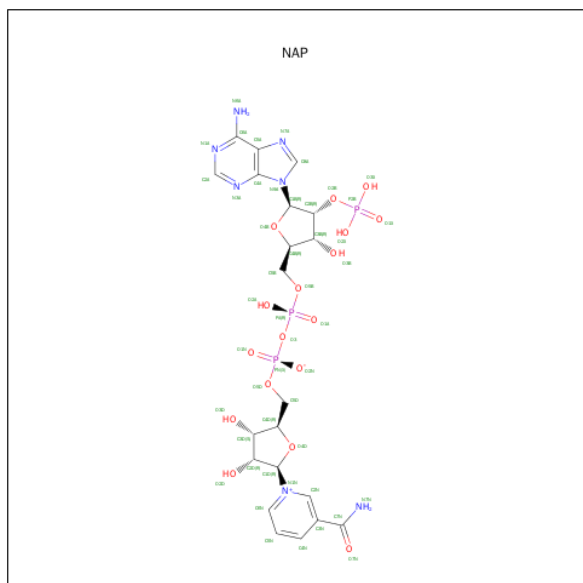
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

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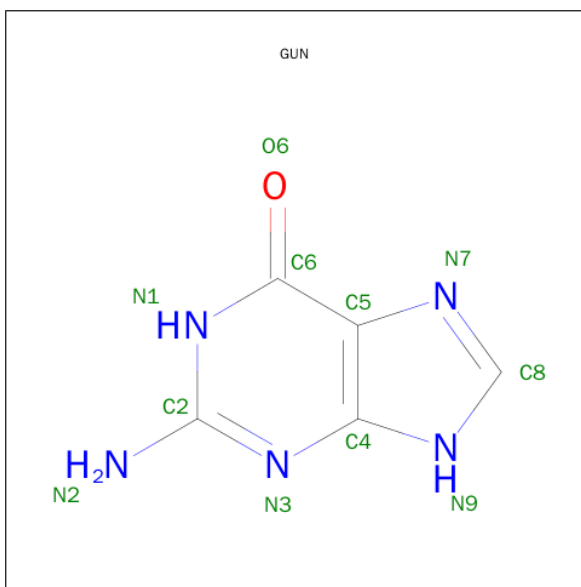
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	1
			78	30	10	32	6		
4	D	1	Total	C	N	O	P	0	1
			80	30	12	32	6		

- Molecule 5 is GUANINE (three-letter code: GUN) (formula: $C_5H_5N_5O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			11	5	5	1		
5	C	1	Total	C	N	O	0	0
			11	5	5	1		

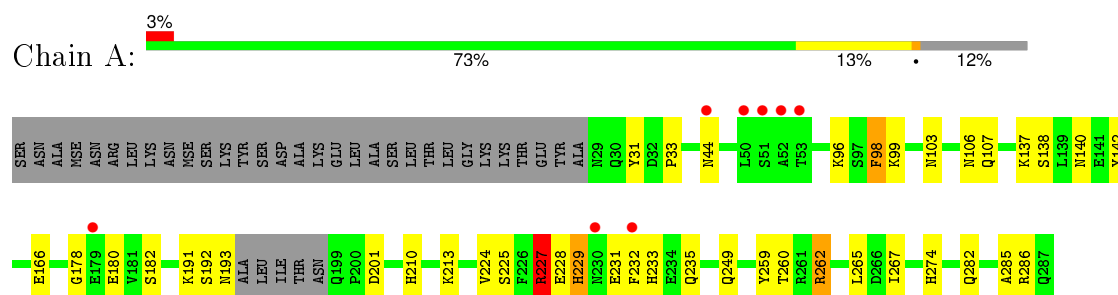
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	210	Total	O	0	0
			210	210		
6	B	194	Total	O	0	0
			194	194		
6	C	204	Total	O	0	0
			204	204		
6	D	224	Total	O	0	0
			224	224		

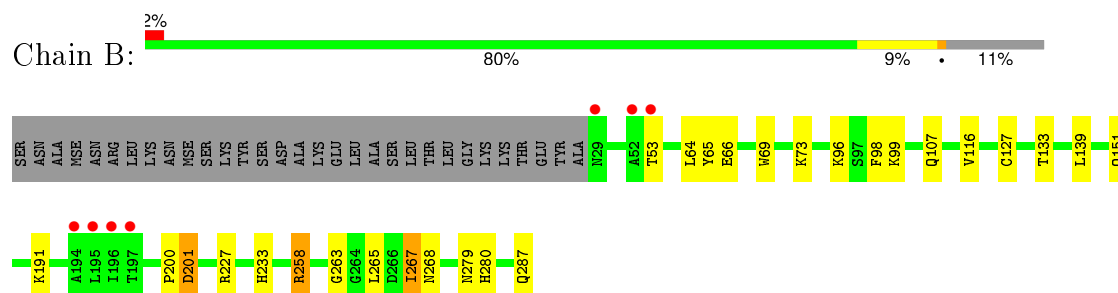
3 Residue-property plots [i](#)

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.

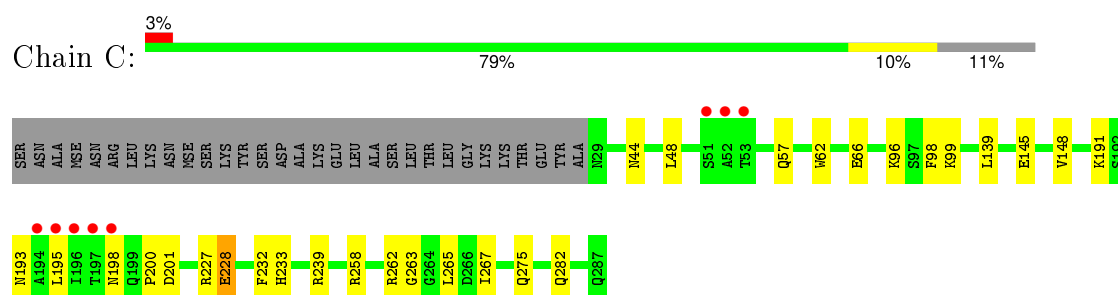
- Molecule 1: NADPH-dependent 7-cyano-7-deazaguanine reductase



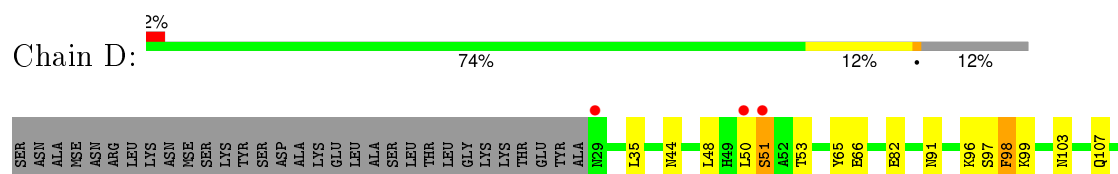
- Molecule 1: NADPH-dependent 7-cyano-7-deazaguanine reductase

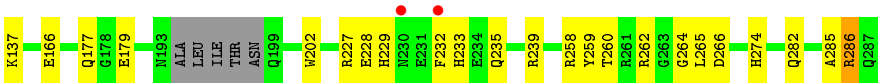


- Molecule 1: NADPH-dependent 7-cyano-7-deazaguanine reductase



- Molecule 1: NADPH-dependent 7-cyano-7-deazaguanine reductase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.37Å 71.39Å 71.36Å 109.89° 119.61° 99.46°	Depositor
Resolution (Å)	30.96 – 1.56 30.96 – 1.56	Depositor EDS
% Data completeness (in resolution range)	94.7 (30.96-1.56) 77.9 (30.96-1.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 1.56Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_920)	Depositor
R, R_{free}	0.161 , 0.189 0.157 , 0.184	Depositor DCC
R_{free} test set	7148 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.5	EDS
Estimated twinning fraction	0.478 for l,-h-k-l,h 0.015 for -h-k-l,l,k 0.016 for k,h,-h-k-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 141941 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10034	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.32% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAP, GUN, 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	0.79	0/2296	0.88	4/3107 (0.1%)
1	B	0.84	1/2266 (0.0%)	0.88	2/3070 (0.1%)
1	C	0.80	0/2289	0.86	1/3101 (0.0%)
1	D	0.78	0/2300	0.87	7/3114 (0.2%)
All	All	0.81	1/9151 (0.0%)	0.88	14/12392 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	65	TYR	CE2-CZ	-5.15	1.31	1.38

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	D	286	ARG	NE-CZ-NH1	-5.67	117.47	120.30
1	D	258	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	D	65	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	C	258	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	98	PHE	CB-CG-CD2	5.26	124.48	120.80
1	D	98	PHE	CB-CG-CD2	5.21	124.45	120.80
1	A	262[A]	ARG	NE-CZ-NH1	-5.15	117.73	120.30
1	A	262[B]	ARG	NE-CZ-NH1	-5.15	117.73	120.30
1	A	98	PHE	CB-CG-CD1	-5.13	117.21	120.80
1	D	65	TYR	CG-CD1-CE1	-5.11	117.22	121.30
1	B	65	TYR	CB-CG-CD2	-5.04	117.97	121.00
1	D	98	PHE	CB-CG-CD1	-5.02	117.29	120.80
1	D	266	ASP	CB-CG-OD1	5.00	122.80	118.30

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	2254	0	2127	53	0
1	B	2224	0	2109	36	0
1	C	2247	0	2139	25	0
1	D	2259	0	2140	52	0
2	A	4	0	6	11	0
2	D	4	0	6	11	0
3	A	6	0	8	1	0
3	B	6	0	8	1	0
3	D	18	0	24	6	0
4	B	78	0	36	6	0
4	D	80	0	38	7	0
5	B	11	0	5	0	0
5	C	11	0	5	0	0
6	A	210	0	0	12	0
6	B	194	0	0	3	0
6	C	204	0	0	4	0
6	D	224	0	0	5	0
All	All	10034	0	8651	159	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 9.

All (159) 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:B:64:LEU:HD22	1:B:265:LEU:HD23	1.35	1.07
6:A:727:HOH:O	1:B:66[B]:GLU:HG2	1.73	0.86
1:B:64:LEU:HD22	1:B:265:LEU:CD2	2.05	0.85
1:D:91:ASN:HD21	3:D:304:GOL:H12	1.42	0.85
1:D:232:PHE:HD2	1:D:235[A]:GLN:NE2	1.77	0.83
1:C:66[B]:GLU:HG2	6:C:689:HOH:O	1.80	0.81
1:D:66[B]:GLU:HG3	6:D:289:HOH:O	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:ASN:HD21	1:B:287:GLN:HE22	1.30	0.75
1:D:232:PHE:HD2	1:D:235[A]:GLN:HE22	1.32	0.74
1:D:232:PHE:CD2	1:D:235[A]:GLN:NE2	2.55	0.74
1:B:191:LYS:HE2	1:B:200:PRO:HB3	1.71	0.72
1:A:286:ARG:HB2	2:A:302:EDO:H21	1.70	0.72
1:C:191:LYS:HE2	1:C:200:PRO:HB3	1.72	0.71
6:C:689:HOH:O	1:D:260[A]:THR:HG21	1.91	0.70
1:D:286:ARG:HB2	2:D:302:EDO:H12	1.73	0.70
1:B:133[B]:THR:HG22	6:B:379:HOH:O	1.91	0.70
1:A:107:GLN:NE2	6:A:728:HOH:O	2.23	0.69
1:D:262:ARG:HG3	4:D:301[B]:NAP:H1D	1.74	0.69
1:A:260[A]:THR:HG21	6:A:727:HOH:O	1.93	0.68
1:C:227[B]:ARG:HG3	6:C:354:HOH:O	1.93	0.68
4:B:301[B]:NAP:H52N	4:B:301[B]:NAP:O3X	1.93	0.67
1:D:285:ALA:N	2:D:302:EDO:H21	2.09	0.67
1:A:285:ALA:N	2:A:302:EDO:H12	2.10	0.66
1:A:228[B]:GLU:O	1:A:229[B]:HIS:HB2	1.96	0.66
1:C:227[B]:ARG:NH1	1:D:107:GLN:OE1	2.30	0.65
1:D:91:ASN:HD21	3:D:304:GOL:C1	2.07	0.65
1:D:202:TRP:HB2	1:D:260[B]:THR:CG2	2.28	0.63
1:A:274:HIS:HB3	3:A:303:GOL:O2	1.98	0.63
1:B:99:LYS:HZ3	4:B:301[A]:NAP:H51N	1.64	0.63
1:B:191:LYS:HD3	1:B:227[B]:ARG:CG	2.30	0.62
1:B:258:ARG:HA	1:B:268:ASN:HD22	1.63	0.61
1:C:233:HIS:HD2	1:C:267[B]:ILE:HG22	1.63	0.61
1:C:96:LYS:HB2	4:D:301[A]:NAP:H2D	1.81	0.61
1:D:48:LEU:HD11	1:D:235[B]:GLN:HE22	1.65	0.61
1:D:66[B]:GLU:HG2	1:D:264:GLY:HA3	1.83	0.61
1:A:232:PHE:HB2	1:A:235:GLN:CD	2.21	0.61
1:A:286:ARG:CB	2:A:302:EDO:H21	2.30	0.60
1:A:201:ASP:OD2	1:A:262[A]:ARG:HD2	2.02	0.60
1:B:96:LYS:HB2	4:B:301[A]:NAP:H2D	1.83	0.60
1:C:191:LYS:HD3	1:C:227[A]:ARG:HG2	1.84	0.59
1:D:285:ALA:H	2:D:302:EDO:H21	1.67	0.59
1:A:107:GLN:OE1	1:B:227[B]:ARG:NH1	2.36	0.58
1:D:286:ARG:CB	2:D:302:EDO:H12	2.32	0.58
1:D:91:ASN:ND2	3:D:304:GOL:H12	2.17	0.58
1:A:182:SER:OG	1:A:210:HIS:HD2	1.86	0.58
1:A:227[B]:ARG:NH2	1:B:107:GLN:OE1	2.37	0.58
1:D:44:ASN:CB	1:D:235[B]:GLN:HG3	2.34	0.58
1:D:202:TRP:HB2	1:D:260[B]:THR:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:LEU:HD13	2:D:302:EDO:H22	1.86	0.57
1:D:227:ARG:NH2	6:D:817:HOH:O	2.10	0.57
1:A:232:PHE:HB2	1:A:235:GLN:OE1	2.04	0.57
1:B:191:LYS:HD3	1:B:227[A]:ARG:CG	2.35	0.57
1:D:260[B]:THR:HG23	6:D:339:HOH:O	2.05	0.56
1:A:229[A]:HIS:HB3	6:A:827:HOH:O	2.06	0.56
1:A:285:ALA:H	2:A:302:EDO:H12	1.70	0.56
1:D:232:PHE:HB2	1:D:235[A]:GLN:CD	2.26	0.56
1:D:274:HIS:HB3	3:D:303:GOL:H11	1.87	0.56
1:B:64:LEU:CD2	1:B:265:LEU:HD23	2.22	0.55
2:A:302:EDO:H11	1:B:139:LEU:HD13	1.87	0.55
1:A:229[A]:HIS:ND1	1:A:231[A]:GLU:OE2	2.39	0.54
1:A:228[B]:GLU:O	1:A:229[B]:HIS:CB	2.55	0.54
1:D:274:HIS:HB3	3:D:303:GOL:C1	2.37	0.54
1:B:191:LYS:HD3	1:B:227[B]:ARG:HG2	1.89	0.54
1:B:191:LYS:HD3	1:B:227[B]:ARG:HG3	1.89	0.54
1:A:180[A]:GLU:OE1	1:A:210:HIS:HE1	1.90	0.54
1:D:286:ARG:HE	2:D:302:EDO:H12	1.73	0.54
1:C:263:GLY:HA3	4:D:301[B]:NAP:N3A	2.23	0.54
1:D:51:SER:OG	1:D:53:THR:HG23	2.08	0.54
1:C:193:ASN:HB3	1:C:198:ASN:HA	1.89	0.53
1:A:106:ASN:O	1:B:227[B]:ARG:NH1	2.38	0.53
1:C:233:HIS:HD2	1:C:267[B]:ILE:CG2	2.19	0.53
1:D:262:ARG:CG	4:D:301[B]:NAP:H1D	2.39	0.53
1:A:99:LYS:NZ	1:A:103:ASN:HD21	2.07	0.52
1:B:263:GLY:HA3	4:B:301[B]:NAP:N3A	2.25	0.52
1:A:178:GLY:HA3	1:A:213:LYS:HB3	1.92	0.52
1:D:286:ARG:HE	2:D:302:EDO:C1	2.23	0.52
6:A:455:HOH:O	1:B:73:LYS:HE3	2.10	0.51
1:D:82[A]:GLU:HG2	6:D:476:HOH:O	2.10	0.51
1:D:96:LYS:HB2	4:D:301[B]:NAP:H2D	1.93	0.51
1:A:286:ARG:H	2:A:302:EDO:C2	2.24	0.51
1:D:286:ARG:H	2:D:302:EDO:C1	2.24	0.51
1:C:228:GLU:HG3	6:C:787:HOH:O	2.10	0.51
1:D:99[B]:LYS:NZ	1:D:103:ASN:HD21	2.09	0.51
1:D:66[B]:GLU:CG	1:D:264:GLY:HA3	2.41	0.50
1:A:233:HIS:HB3	1:A:259:TYR:CE2	2.46	0.50
1:A:166[A]:GLU:O	1:A:225:SER:HB2	2.12	0.50
1:B:268:ASN:ND2	1:B:287:GLN:HE22	2.06	0.49
1:B:191:LYS:HD3	1:B:227[A]:ARG:HG2	1.94	0.49
1:D:44:ASN:OD1	1:D:235[A]:GLN:NE2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:TRP:CE2	1:C:267[B]:ILE:HG13	2.48	0.49
1:D:44:ASN:HB3	1:D:235[B]:GLN:HG3	1.95	0.48
1:B:267[A]:ILE:HG13	1:B:268:ASN:N	2.28	0.48
1:D:51:SER:OG	1:D:53:THR:CG2	2.62	0.48
1:A:286:ARG:HE	2:A:302:EDO:C2	2.26	0.48
1:D:233:HIS:HB3	1:D:259:TYR:CE2	2.48	0.48
1:D:202:TRP:HB2	1:D:260[B]:THR:HG22	1.95	0.48
1:D:262:ARG:HD3	4:D:301[B]:NAP:O1X	2.14	0.47
1:C:99:LYS:HZ3	4:D:301[A]:NAP:H51N	1.80	0.47
1:A:99:LYS:HZ3	1:A:103:ASN:HD21	1.62	0.47
1:A:224:VAL:O	1:A:227[B]:ARG:HB2	2.15	0.47
1:C:48:LEU:HD21	1:C:239[B]:ARG:HD2	1.97	0.47
1:D:229:HIS:NE2	1:D:239[B]:ARG:NE	2.63	0.46
1:C:195:LEU:HD12	1:C:232:PHE:CE1	2.50	0.46
1:A:31:TYR:CZ	1:A:33:PRO:HG3	2.50	0.46
1:C:191:LYS:HD3	1:C:227[A]:ARG:CG	2.44	0.46
1:A:180[A]:GLU:OE1	1:A:210:HIS:CE1	2.68	0.46
1:B:191:LYS:HD3	1:B:227[A]:ARG:HG3	1.93	0.45
1:D:166:GLU:HA	1:D:228:GLU:HB2	1.98	0.45
1:A:262[A]:ARG:HG3	6:A:741:HOH:O	2.16	0.45
1:B:280:HIS:CE1	6:B:465:HOH:O	2.69	0.45
6:A:690:HOH:O	1:B:99:LYS:HD2	2.15	0.45
1:A:286:ARG:H	2:A:302:EDO:C1	2.30	0.45
2:A:302:EDO:C1	1:B:139:LEU:HD13	2.46	0.44
1:C:57:GLN:HG3	1:C:275:GLN:O	2.18	0.44
1:B:133[B]:THR:HG23	6:B:384:HOH:O	2.17	0.44
1:C:233:HIS:CD2	1:C:267[B]:ILE:CG2	3.01	0.44
1:A:44[A]:ASN:ND2	1:A:235:GLN:HE21	2.16	0.44
1:A:44[A]:ASN:CB	1:A:235:GLN:HG2	2.47	0.44
1:A:282:GLN:HG2	6:A:644:HOH:O	2.17	0.44
1:B:201[B]:ASP:CG	1:B:233:HIS:HE2	2.20	0.44
1:A:192:SER:HB3	6:A:827:HOH:O	2.18	0.44
1:A:233:HIS:HD2	1:A:267[B]:ILE:HD12	1.83	0.44
1:C:201:ASP:CG	1:C:233:HIS:HE1	2.21	0.44
1:D:35:LEU:O	1:D:97:SER:HB2	2.18	0.43
1:A:44[A]:ASN:CG	1:A:235:GLN:HE21	2.22	0.43
1:A:44[B]:ASN:CB	1:A:235:GLN:HG2	2.49	0.43
1:A:138:SER:OG	1:A:140[B]:ASN:ND2	2.51	0.43
1:D:107:GLN:NE2	6:D:789:HOH:O	2.51	0.43
1:D:202:TRP:O	1:D:260[B]:THR:HG22	2.18	0.43
1:B:69:TRP:CE2	1:B:116:VAL:HG21	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:LYS:HE2	1:A:142:TYR:OH	2.18	0.43
1:A:232:PHE:HD2	1:A:235:GLN:HE22	1.66	0.43
1:B:279:ASN:HD21	1:C:145[B]:GLU:CD	2.22	0.43
1:A:286:ARG:HE	2:A:302:EDO:H21	1.84	0.43
1:D:232:PHE:HD2	1:D:235[A]:GLN:CD	2.21	0.42
1:B:151:GLN:HE22	1:C:282[A]:GLN:NE2	2.17	0.42
1:D:179[B]:GLU:H	1:D:179[B]:GLU:CD	2.22	0.42
1:C:195:LEU:HD23	1:C:195:LEU:HA	1.78	0.42
1:D:50:LEU:HD23	1:D:50:LEU:HA	1.72	0.42
1:A:262[B]:ARG:HD3	4:B:301[B]:NAP:O1X	2.19	0.42
1:D:82[B]:GLU:HG3	1:D:137:LYS:NZ	2.34	0.42
1:A:140[B]:ASN:N	1:A:140[B]:ASN:HD22	2.18	0.42
1:D:44:ASN:HB2	1:D:235[B]:GLN:HG3	2.01	0.42
1:D:286:ARG:CG	2:D:302:EDO:H12	2.50	0.42
1:A:44[B]:ASN:CG	1:A:235:GLN:HG2	2.40	0.41
1:A:286:ARG:HG3	2:A:302:EDO:H11	2.03	0.41
1:B:151:GLN:HE21	1:C:148:VAL:HG12	1.85	0.41
1:D:282:GLN:HG2	3:D:305:GOL:O3	2.20	0.41
1:B:268:ASN:HD21	1:B:287:GLN:NE2	2.05	0.41
1:A:191:LYS:O	1:A:227[B]:ARG:HA	2.21	0.41
1:B:127:CYS:HA	3:B:302:GOL:H2	2.03	0.41
1:A:265:LEU:N	1:A:265:LEU:HD23	2.35	0.41
1:D:286:ARG:H	2:D:302:EDO:C2	2.33	0.41
1:A:274:HIS:CE1	6:A:351:HOH:O	2.74	0.41
1:C:139:LEU:HD13	2:D:302:EDO:C2	2.50	0.41
1:A:249:GLN:HG2	6:A:708:HOH:O	2.21	0.41
1:A:274:HIS:HE1	6:A:351:HOH:O	2.04	0.40
1:A:262[A]:ARG:NH1	1:B:66[A]:GLU:OE2	2.48	0.40
1:A:96:LYS:HB2	4:B:301[B]:NAP:H2D	2.03	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	275/290 (95%)	263 (96%)	8 (3%)	4 (2%)	13	1
1	B	274/290 (94%)	272 (99%)	2 (1%)	0	100	100
1	C	277/290 (96%)	271 (98%)	6 (2%)	0	100	100
1	D	275/290 (95%)	269 (98%)	6 (2%)	0	100	100
All	All	1101/1160 (95%)	1075 (98%)	22 (2%)	4 (0%)	52	14

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229[A]	HIS
1	A	229[B]	HIS
1	A	227[A]	ARG
1	A	227[B]	ARG

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	250/249 (100%)	246 (98%)	4 (2%)	70	41
1	B	247/249 (99%)	241 (98%)	6 (2%)	57	23
1	C	249/249 (100%)	244 (98%)	5 (2%)	63	31
1	D	251/249 (101%)	246 (98%)	5 (2%)	63	31
All	All	997/996 (100%)	977 (98%)	20 (2%)	66	31

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	PHE
1	A	193	ASN
1	A	227[A]	ARG
1	A	227[B]	ARG
1	B	53	THR
1	B	98	PHE
1	B	201[A]	ASP

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Mol	Chain	Res	Type
1	B	201[B]	ASP
1	B	267[A]	ILE
1	B	267[B]	ILE
1	C	44	ASN
1	C	98	PHE
1	C	228	GLU
1	C	262	ARG
1	C	265	LEU
1	D	51	SER
1	D	98	PHE
1	D	177	GLN
1	D	265[A]	LEU
1	D	265[B]	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	106	ASN
1	A	199	GLN
1	A	210	HIS
1	A	235	GLN
1	B	30	GLN
1	B	57	GLN
1	B	103	ASN
1	B	151	GLN
1	B	268	ASN
1	B	280	HIS
1	C	30	GLN
1	C	57	GLN
1	C	103	ASN
1	C	198	ASN
1	C	230	ASN
1	C	233	HIS
1	C	274	HIS
1	C	275	GLN
1	D	103	ASN
1	D	106	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 ⓘ

13 ligands 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	$\# Z > 2$
2	EDO	A	302	-	3,3,3	0.92	0	2,2,2	1.27	0
3	GOL	A	303	-	5,5,5	0.66	0	5,5,5	1.05	0
5	GUN	B	300	-	9,12,12	0.60	0	7,17,17	2.60	4 (57%)
4	NAP	B	301[A]	-	35,42,52	1.13	1 (2%)	46,65,80	2.32	6 (13%)
4	NAP	B	301[B]	-	35,42,52	0.88	1 (2%)	46,65,80	2.29	5 (10%)
3	GOL	B	302	-	5,5,5	0.42	0	5,5,5	0.69	0
5	GUN	C	300	-	9,12,12	0.68	0	7,17,17	2.51	4 (57%)
4	NAP	D	301[A]	-	36,43,52	0.82	1 (2%)	44,67,80	2.28	6 (13%)
4	NAP	D	301[B]	-	36,43,52	0.92	1 (2%)	44,67,80	2.21	2 (4%)
2	EDO	D	302	-	3,3,3	0.83	0	2,2,2	1.23	0
3	GOL	D	303	-	5,5,5	0.34	0	5,5,5	0.93	0
3	GOL	D	304	-	5,5,5	0.61	0	5,5,5	1.41	0
3	GOL	D	305	-	5,5,5	0.35	0	5,5,5	0.78	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	302	-	-	0/1/1/1	0/0/0/0
3	GOL	A	303	-	-	0/4/4/4	0/0/0/0
5	GUN	B	300	-	-	0/0/0/0	0/2/2/2
4	NAP	B	301[A]	-	-	0/23/56/67	0/4/4/5
4	NAP	B	301[B]	-	-	0/23/56/67	0/4/4/5
3	GOL	B	302	-	-	0/4/4/4	0/0/0/0
5	GUN	C	300	-	-	0/0/0/0	0/2/2/2
4	NAP	D	301[A]	-	-	0/23/59/67	0/4/4/5
4	NAP	D	301[B]	-	-	0/23/59/67	0/4/4/5
2	EDO	D	302	-	-	0/1/1/1	0/0/0/0
3	GOL	D	303	-	-	0/4/4/4	0/0/0/0
3	GOL	D	304	-	-	0/4/4/4	0/0/0/0
3	GOL	D	305	-	-	0/4/4/4	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	301[B]	NAP	P2B-O2X	2.04	1.62	1.54
4	D	301[A]	NAP	O4B-C1B	2.17	1.43	1.41
4	D	301[B]	NAP	O4B-C1B	2.68	1.44	1.41
4	B	301[A]	NAP	O4B-C1B	4.39	1.46	1.41

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	301[B]	NAP	N3A-C2A-N1A	-13.27	118.74	128.89
4	B	301[B]	NAP	N3A-C2A-N1A	-13.21	118.78	128.89
4	D	301[A]	NAP	N3A-C2A-N1A	-12.83	119.07	128.89
4	B	301[A]	NAP	N3A-C2A-N1A	-12.67	119.19	128.89
5	B	300	GUN	C4-C5-N7	-3.75	106.03	109.48
5	C	300	GUN	C4-C5-N7	-3.71	106.07	109.48
5	C	300	GUN	N3-C2-N1	-3.70	121.82	127.44
5	B	300	GUN	N3-C2-N1	-3.59	121.98	127.44
4	B	301[A]	NAP	PN-O3-PA	-3.38	123.25	132.73
4	B	301[A]	NAP	O2B-P2B-O1X	-3.10	99.38	107.11
5	B	300	GUN	C5-C6-N1	-2.70	119.90	123.59
5	C	300	GUN	C5-C6-N1	-2.69	119.91	123.59
4	D	301[A]	NAP	O3-PA-O5B	-2.49	96.33	102.94
4	B	301[A]	NAP	O3-PA-O5B	-2.38	96.63	102.94
4	B	301[A]	NAP	C1B-N9A-C4A	-2.36	123.38	126.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	301[A]	NAP	PN-O3-PA	-2.33	126.19	132.73
4	D	301[A]	NAP	O2B-P2B-O1X	-2.28	101.41	107.11
4	D	301[B]	NAP	PN-O3-PA	-2.12	126.79	132.73
4	D	301[A]	NAP	O3B-C3B-C2B	-2.04	105.27	111.16
4	B	301[B]	NAP	C2A-N1A-C6A	2.06	122.44	118.77
4	B	301[A]	NAP	C1D-C2D-C3D	2.21	105.21	101.64
4	B	301[B]	NAP	C5D-C4D-C3D	2.31	124.37	115.21
5	C	300	GUN	C6-N1-C2	2.50	119.41	115.94
4	D	301[A]	NAP	C2A-N1A-C6A	2.64	123.48	118.77
4	B	301[B]	NAP	C1D-C2D-C3D	2.77	106.11	101.64
5	B	300	GUN	C6-N1-C2	2.97	120.06	115.94
4	B	301[B]	NAP	O5D-C5D-C4D	3.90	123.51	109.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	302	EDO	11	0
3	A	303	GOL	1	0
4	B	301[A]	NAP	2	0
4	B	301[B]	NAP	4	0
3	B	302	GOL	1	0
4	D	301[A]	NAP	2	0
4	D	301[B]	NAP	5	0
2	D	302	EDO	11	0
3	D	303	GOL	2	0
3	D	304	GOL	3	0
3	D	305	GOL	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	250/290 (86%)	-0.25	8 (3%)	51	55	12, 19, 42, 69	6 (2%)
1	B	255/290 (87%)	-0.33	7 (2%)	58	62	11, 18, 41, 62	9 (3%)
1	C	255/290 (87%)	-0.27	8 (3%)	52	56	11, 18, 42, 57	14 (5%)
1	D	250/290 (86%)	-0.28	5 (2%)	68	71	12, 19, 43, 69	6 (2%)
All	All	1010/1160 (87%)	-0.28	28 (2%)	56	60	11, 18, 43, 69	35 (3%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	195	LEU	6.8
1	C	195	LEU	6.6
1	C	194	ALA	5.8
1	B	196	ILE	5.6
1	C	196	ILE	5.1
1	A	50	LEU	4.6
1	A	51	SER	4.3
1	C	197	THR	4.2
1	C	52	ALA	4.1
1	D	51	SER	3.8
1	B	197	THR	3.7
1	B	52	ALA	3.6
1	A	230[A]	ASN	3.5
1	A	232	PHE	3.5
1	D	29[A]	ASN	3.3
1	A	52	ALA	3.3
1	B	194	ALA	3.1
1	D	50	LEU	3.1
1	A	44[A]	ASN	3.0
1	A	53	THR	2.8
1	A	179	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	51	SER	2.5
1	D	232	PHE	2.4
1	D	230	ASN	2.3
1	C	198	ASN	2.2
1	B	29[A]	ASN	2.2
1	C	53	THR	2.0
1	B	53	THR	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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	GOL	D	304	6/6	0.83	0.30	26.65	27,40,41,42	0
2	EDO	D	302	4/4	0.94	0.26	15.80	16,21,25,30	0
3	GOL	B	302	6/6	0.87	0.16	12.37	45,49,51,55	0
2	EDO	A	302	4/4	0.96	0.12	6.89	17,19,24,29	0
3	GOL	A	303	6/6	0.84	0.25	6.35	47,48,55,61	0
3	GOL	D	305	6/6	0.81	0.20	5.03	38,47,48,50	0
3	GOL	D	303	6/6	0.76	0.25	5.00	41,43,44,52	0
4	NAP	D	301[A]	40/48	0.87	0.20	3.00	18,31,47,49	40
4	NAP	D	301[B]	40/48	0.87	0.20	2.88	18,32,46,48	40
4	NAP	B	301[A]	39/48	0.86	0.19	2.78	22,30,46,51	39
4	NAP	B	301[B]	39/48	0.86	0.19	2.64	21,30,46,46	39
5	GUN	C	300	11/11	0.90	0.14	2.53	9,18,23,24	11
5	GUN	B	300	11/11	0.86	0.16	1.78	9,20,24,24	11

6.5 Other polymers ⓘ

There are no such residues in this entry.