



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 12:56 AM UTC

PDB ID : 5LIQ / pdb_00005liq
Title : The structure of C160S,C508S,C578S mutant of Nt.BspD6I nicking endonuclease at 0.185 nm resolution .
Authors : Kachalova, G.S.; Artyukh, R.I.; Perevyazova, T.A.; Yunusova, A.K.; Popov, A.N.; Bartunik, H.D.; Zheleznaya, L.A.
Deposited on : 2016-07-15
Resolution : 1.85 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

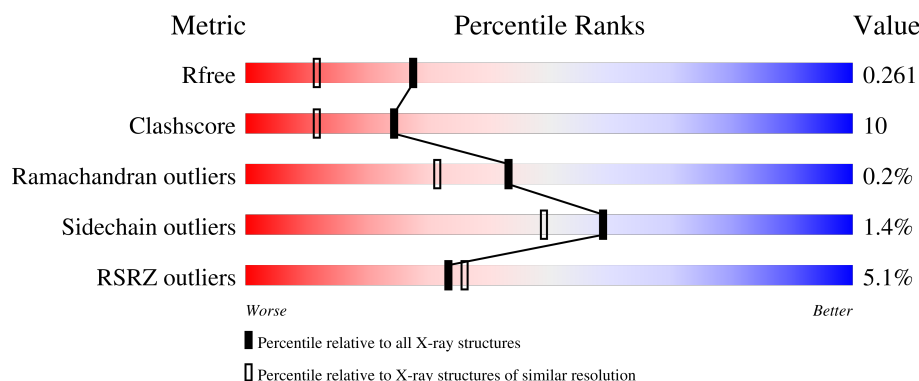
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	610	4% 75% 20% ..
1	B	610	6% 77% 17% ..

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	GOL	A	702	-	-	X	-
2	GOL	A	706	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10168 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 Nicking endonuclease N.BspD6I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	583	Total	C	N	O	S	0	13	0
			4920	3167	826	913	14			
1	B	583	Total	C	N	O	S	0	5	0
			4870	3133	822	902	13			

There are 18 discrepancies between the modelled and reference sequences:

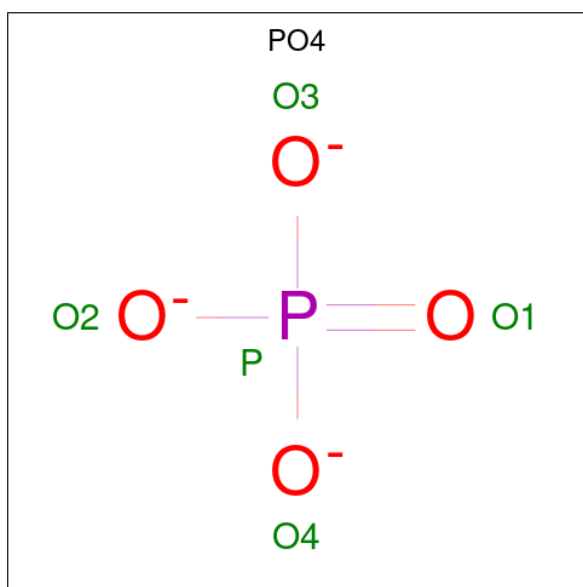
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q8GCA3
A	-4	HIS	-	expression tag	UNP Q8GCA3
A	-3	HIS	-	expression tag	UNP Q8GCA3
A	-2	HIS	-	expression tag	UNP Q8GCA3
A	-1	HIS	-	expression tag	UNP Q8GCA3
A	0	HIS	-	expression tag	UNP Q8GCA3
A	160	SER	CYS	engineered mutation	UNP Q8GCA3
A	508	SER	CYS	engineered mutation	UNP Q8GCA3
A	578	SER	CYS	engineered mutation	UNP Q8GCA3
B	-5	HIS	-	expression tag	UNP Q8GCA3
B	-4	HIS	-	expression tag	UNP Q8GCA3
B	-3	HIS	-	expression tag	UNP Q8GCA3
B	-2	HIS	-	expression tag	UNP Q8GCA3
B	-1	HIS	-	expression tag	UNP Q8GCA3
B	0	HIS	-	expression tag	UNP Q8GCA3
B	160	SER	CYS	engineered mutation	UNP Q8GCA3
B	508	SER	CYS	engineered mutation	UNP Q8GCA3
B	578	SER	CYS	engineered mutation	UNP Q8GCA3

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

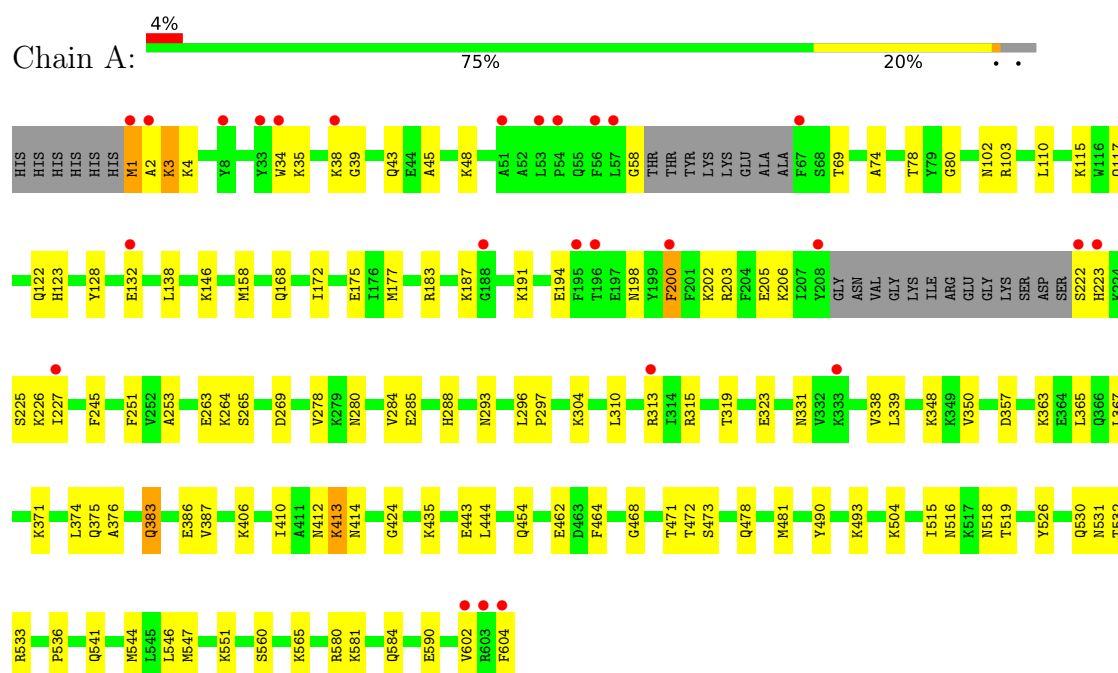
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	186	Total	O	0	0
			186	186		
4	B	109	Total	O	0	0
			109	109		

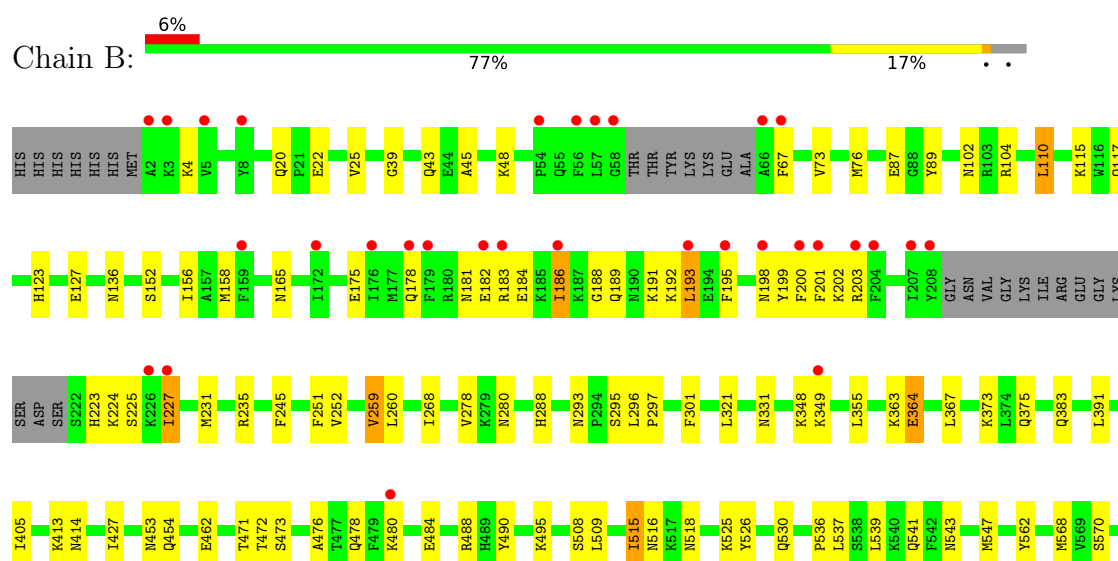
3 Residue-property plots

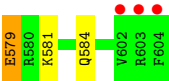
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Nicking endonuclease N.BspD6I



• Molecule 1: Nicking endonuclease N.BspD6I





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.20Å 92.48Å 113.81Å 90.00° 105.67° 90.00°	Depositor
Resolution (Å)	19.58 – 1.85 19.58 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.58-1.85) 99.5 (19.58-1.85)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.209 , 0.251 (Not available) , 0.261	Depositor DCC
R_{free} test set	6247 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10168	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 75.75 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1906e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PO4

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	1.27	13/5041 (0.3%)	1.18	11/6782 (0.2%)
1	B	1.28	14/4973 (0.3%)	1.20	16/6692 (0.2%)
All	All	1.27	27/10014 (0.3%)	1.19	27/13474 (0.2%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	387	VAL	N-CA	6.92	1.54	1.46
1	B	104	ARG	C-O	-6.77	1.20	1.23
1	B	25	VAL	N-CA	6.74	1.54	1.46
1	B	20	GLN	CA-C	6.23	1.59	1.52
1	A	547	MET	N-CA	6.22	1.53	1.46
1	A	546	LEU	CA-C	6.19	1.60	1.52
1	A	532	THR	N-CA	6.06	1.53	1.45
1	B	110	LEU	N-CA	5.74	1.53	1.46
1	B	165	ASN	N-CA	-5.56	1.39	1.46
1	A	74	ALA	C-O	-5.53	1.19	1.24
1	A	424	GLY	N-CA	5.51	1.52	1.45
1	B	355	LEU	C-O	-5.49	1.17	1.24
1	A	454	GLN	N-CA	5.44	1.52	1.45
1	B	252	VAL	N-CA	5.40	1.52	1.46
1	A	315	ARG	N-CA	5.32	1.52	1.46
1	A	560	SER	N-CA	-5.25	1.39	1.45
1	B	427	ILE	C-O	-5.24	1.18	1.24
1	A	468	GLY	N-CA	5.22	1.52	1.45
1	B	295	SER	N-CA	5.19	1.53	1.46
1	A	80	GLY	N-CA	5.18	1.52	1.45
1	A	413	LYS	CA-C	5.16	1.59	1.52
1	A	376	ALA	N-CA	5.14	1.52	1.46
1	B	568	MET	CA-C	5.13	1.59	1.52
1	B	508	SER	N-CA	5.10	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	259[A]	VAL	C-O	5.04	1.29	1.23
1	B	259[B]	VAL	C-O	5.04	1.29	1.23
1	B	136	ASN	C-O	-5.03	1.18	1.24

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	484	GLU	CA-C-N	-6.29	112.07	119.05
1	B	484	GLU	C-N-CA	-6.29	112.07	119.05
1	B	364	GLU	N-CA-C	-6.10	104.71	111.36
1	A	265	SER	N-CA-C	6.08	118.41	111.11
1	B	152	SER	N-CA-C	-6.03	101.84	110.59
1	A	580	ARG	N-CA-C	5.91	119.75	112.54
1	B	181	ASN	N-CA-C	5.84	117.72	111.36
1	A	3	LYS	N-CA-C	5.81	118.13	109.59
1	A	200	PHE	N-CA-C	-5.80	104.56	111.69
1	B	472	THR	CA-C-N	5.73	129.84	121.31
1	B	472	THR	C-N-CA	5.73	129.84	121.31
1	B	570	SER	N-CA-C	5.72	117.52	111.28
1	A	183	ARG	CA-C-N	5.65	127.85	120.28
1	A	183	ARG	C-N-CA	5.65	127.85	120.28
1	A	168	GLN	N-CA-C	5.63	120.01	113.20
1	B	193	LEU	N-CA-C	5.57	117.35	111.28
1	B	515	ILE	N-CA-C	5.56	116.23	108.89
1	B	454	GLN	CA-C-N	-5.52	114.91	120.21
1	B	454	GLN	C-N-CA	-5.52	114.91	120.21
1	B	224	LYS	N-CA-C	-5.51	104.96	110.97
1	A	194	GLU	CA-C-N	5.44	127.51	120.44
1	A	194	GLU	C-N-CA	5.44	127.51	120.44
1	A	383	GLN	N-CA-C	-5.42	105.45	111.36
1	A	472	THR	N-CA-C	-5.36	106.78	113.38
1	B	156	ILE	N-CA-C	-5.30	105.23	111.00
1	B	223	HIS	N-CA-C	-5.09	106.42	113.18
1	B	22	GLU	CB-CA-C	-5.03	102.29	110.85

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	4920	0	4986	103	0
1	B	4870	0	4921	90	0
2	A	36	0	48	18	0
2	B	12	0	16	3	0
3	A	20	0	0	0	0
3	B	15	0	0	0	0
4	A	186	0	0	16	0
4	B	109	0	0	10	0
All	All	10168	0	9971	196	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 10.

All (196) 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:A:175:GLU:OE2	1:A:203:ARG:NH1	1.64	1.28
1:B:175:GLU:OE2	1:B:203[A]:ARG:NH1	1.73	1.21
1:A:531:ASN:ND2	2:A:706:GOL:H11	1.56	1.19
1:B:581:LYS:HG2	1:B:584:GLN:NE2	1.58	1.19
1:A:310:LEU:CD1	1:A:313:ARG:HH21	1.54	1.19
1:A:285[B]:GLU:HG2	4:A:932:HOH:O	1.51	1.10
1:A:339:LEU:HD13	1:A:365:LEU:CD2	1.81	1.09
1:B:203[B]:ARG:HH11	1:B:203[B]:ARG:CG	1.67	1.05
1:A:310:LEU:HD13	1:A:313:ARG:HH21	1.20	1.05
1:B:581:LYS:CG	1:B:584:GLN:NE2	2.22	1.03
1:A:310:LEU:CD1	1:A:313:ARG:NH2	2.22	1.02
1:B:203[B]:ARG:HH11	1:B:203[B]:ARG:HG3	0.86	1.01
1:B:203[B]:ARG:HG3	1:B:203[B]:ARG:NH1	1.69	1.01
1:A:531:ASN:HD21	2:A:706:GOL:C1	1.73	1.00
1:B:117:GLN:HE22	1:B:278:VAL:H	1.09	0.99
1:A:531:ASN:HD21	2:A:706:GOL:H11	0.83	0.99
1:A:177:MET:HA	1:A:177:MET:HE2	1.44	0.99
1:A:339:LEU:HD13	1:A:365:LEU:HD23	1.45	0.97
1:B:201:PHE:CD2	1:B:227:ILE:HD11	2.00	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:ARG:HH21	2:A:706:GOL:H31	1.31	0.95
1:A:175:GLU:CD	1:A:203:ARG:HH12	1.74	0.93
2:A:706:GOL:H32	4:A:804:HOH:O	1.69	0.92
1:A:533:ARG:NH2	2:A:706:GOL:H31	1.86	0.90
1:B:175:GLU:CD	1:B:203[A]:ARG:HH12	1.80	0.90
1:A:117:GLN:HE22	1:A:278:VAL:H	1.15	0.89
1:A:339:LEU:HD13	1:A:365:LEU:HD22	1.52	0.89
1:A:331:ASN:HD21	1:A:375:GLN:HE22	1.16	0.89
1:B:462[B]:GLU:HG3	4:B:903:HOH:O	1.74	0.87
1:B:462[B]:GLU:H	1:B:462[B]:GLU:CD	1.81	0.86
1:B:581:LYS:H	1:B:584:GLN:HE22	1.26	0.83
1:A:435:LYS:HA	2:A:702:GOL:H11	1.60	0.82
1:B:331:ASN:HD21	1:B:375:GLN:HE22	1.26	0.82
1:B:364:GLU:HG2	4:B:894:HOH:O	1.79	0.82
1:A:78:THR:OG1	1:A:122[B]:GLN:OE1	1.98	0.81
1:A:533:ARG:HH21	2:A:706:GOL:C3	1.92	0.81
1:A:310:LEU:HD11	1:A:313:ARG:NH2	1.96	0.80
1:A:205:GLU:HA	1:A:227:ILE:HD13	1.63	0.79
1:A:339:LEU:CD1	1:A:365:LEU:HD22	2.15	0.76
1:B:581:LYS:HG2	1:B:584:GLN:HE22	1.48	0.76
1:A:383:GLN:OE1	4:A:801:HOH:O	2.05	0.75
1:A:205:GLU:HA	1:A:227:ILE:CD1	2.17	0.74
1:B:201:PHE:CG	1:B:227:ILE:HD11	2.22	0.73
1:B:581:LYS:HG2	1:B:584:GLN:CD	2.13	0.73
1:B:478:GLN:HE22	1:B:516:ASN:H	1.34	0.72
1:B:476:ALA:O	1:B:480:LYS:HG3	1.88	0.72
1:A:478:GLN:HE22	1:A:516:ASN:H	1.39	0.71
1:A:435:LYS:HG3	2:A:702:GOL:C1	2.19	0.71
1:A:2:ALA:HB1	4:A:939:HOH:O	1.89	0.71
1:A:3:LYS:HD2	1:A:132:GLU:OE1	1.90	0.70
1:B:321:LEU:HD11	1:B:373:LYS:HD2	1.74	0.69
1:A:45:ALA:HA	1:A:48:LYS:HE2	1.75	0.69
1:A:177:MET:HA	1:A:177:MET:CE	2.21	0.69
1:A:435:LYS:HG3	2:A:702:GOL:H12	1.72	0.69
1:B:581:LYS:H	1:B:584:GLN:NE2	1.91	0.68
2:A:703:GOL:H31	4:A:855:HOH:O	1.94	0.67
1:B:526:TYR:CD2	1:B:530:GLN:HG3	2.30	0.66
1:A:253:ALA:HB2	1:A:410:ILE:HD12	1.77	0.66
1:B:87:GLU:HG3	1:B:89:TYR:CD2	2.32	0.64
1:B:203[B]:ARG:CG	1:B:203[B]:ARG:NH1	2.35	0.63
1:A:478:GLN:NE2	1:A:516:ASN:H	1.95	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:LYS:NZ	1:B:293:ASN:O	2.33	0.62
1:B:183:ARG:O	1:B:192:LYS:HE3	1.98	0.62
1:A:319:THR:O	1:A:323[B]:GLU:HG2	2.00	0.62
1:B:203[B]:ARG:N	1:B:203[B]:ARG:HD2	2.14	0.62
1:B:462[B]:GLU:CD	1:B:462[B]:GLU:N	2.56	0.62
1:B:203[B]:ARG:N	1:B:203[B]:ARG:CD	2.63	0.61
1:B:581:LYS:N	1:B:584:GLN:NE2	2.48	0.61
1:B:288:HIS:HE1	4:B:842:HOH:O	1.84	0.61
1:B:123:HIS:HD2	4:B:874:HOH:O	1.85	0.59
1:A:288:HIS:HE1	4:A:845:HOH:O	1.85	0.59
1:A:357:ASP:HB3	2:A:701:GOL:H2	1.85	0.58
1:B:280:ASN:ND2	1:B:280:ASN:H	2.02	0.58
1:A:110:LEU:C	1:A:110:LEU:HD23	2.29	0.58
1:B:515:ILE:HD13	1:B:536:PRO:HB2	1.86	0.58
1:B:581:LYS:HG3	1:B:584:GLN:NE2	2.18	0.58
1:B:87:GLU:HG3	1:B:89:TYR:HD2	1.69	0.57
1:B:259[B]:VAL:HG13	4:B:853:HOH:O	2.04	0.57
1:A:4:LYS:HG3	1:A:128:TYR:CZ	2.39	0.57
1:B:227:ILE:O	1:B:231:MET:HG3	2.04	0.57
1:A:338:VAL:CG1	1:A:365:LEU:HD13	2.35	0.56
1:B:117:GLN:NE2	1:B:278:VAL:H	1.92	0.56
1:A:551:LYS:HE3	1:A:604:PHE:CE1	2.41	0.56
1:A:146:LYS:NZ	1:A:269:ASP:OD1	2.22	0.55
1:A:435:LYS:HG3	2:A:702:GOL:H11	1.88	0.55
1:B:579:GLU:HG2	1:B:584:GLN:OE1	2.07	0.55
1:A:284:VAL:O	1:A:288:HIS:HD2	1.88	0.55
1:A:223:HIS:HA	1:A:226:LYS:HG3	1.88	0.55
1:B:117:GLN:HE22	1:B:278:VAL:N	1.92	0.55
1:B:198:ASN:HD21	1:B:202:LYS:HE3	1.71	0.55
1:A:581:LYS:HB2	1:A:584:GLN:OE1	2.07	0.54
1:B:39:GLY:O	1:B:43:GLN:HG3	2.08	0.54
1:B:478:GLN:NE2	1:B:516:ASN:H	2.02	0.54
1:A:516:ASN:HD22	1:A:519:THR:H	1.56	0.54
1:B:245:PHE:HB3	1:B:251:PHE:CD1	2.42	0.53
1:B:189:GLN:O	1:B:193:LEU:HD23	2.08	0.53
1:A:223:HIS:HA	1:A:226:LYS:HE2	1.91	0.53
1:A:253:ALA:CB	1:A:410:ILE:HD12	2.38	0.53
1:A:338:VAL:HG11	1:A:365:LEU:HD13	1.90	0.52
1:A:34:TRP:O	1:A:43:GLN:NE2	2.39	0.52
1:A:296:LEU:HA	1:A:297:PRO:C	2.34	0.52
1:A:205:GLU:CA	1:A:227:ILE:HD13	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:TYR:C	1:B:199:TYR:CD1	2.87	0.52
1:B:201:PHE:CE2	1:B:227:ILE:HD11	2.44	0.52
1:B:490:TYR:CD1	1:B:490:TYR:C	2.87	0.52
1:B:543:ASN:HB3	1:B:547:MET:HE3	1.93	0.51
1:B:182:GLU:HG3	1:B:195:PHE:HZ	1.74	0.51
1:A:177:MET:HE2	1:A:177:MET:CA	2.30	0.50
1:A:58:GLY:HA3	4:A:963:HOH:O	2.12	0.50
1:A:551:LYS:HE3	1:A:604:PHE:CD1	2.46	0.50
1:A:367:LEU:HD11	1:A:444:LEU:HD12	1.94	0.50
1:A:123:HIS:HD2	4:A:881:HOH:O	1.94	0.49
1:A:222:SER:O	1:A:226:LYS:HG3	2.13	0.49
1:B:259[B]:VAL:CG1	4:B:838:HOH:O	2.59	0.49
1:A:526:TYR:CD2	1:A:530:GLN:HG3	2.48	0.49
1:A:304:LYS:HD2	1:A:350:VAL:O	2.13	0.48
1:B:288:HIS:CE1	4:B:842:HOH:O	2.62	0.48
1:A:1:MET:HB3	1:A:3:LYS:H	1.78	0.48
1:A:348:LYS:N	1:A:348:LYS:HD2	2.27	0.48
1:B:363[A]:LYS:NZ	4:B:802:HOH:O	2.46	0.48
1:B:391:LEU:HB3	1:B:539:LEU:HD11	1.96	0.48
1:A:187:LYS:HD3	1:A:187:LYS:HA	1.51	0.48
1:B:110:LEU:C	1:B:110:LEU:HD23	2.38	0.48
1:A:590:GLU:HG3	4:A:921:HOH:O	2.13	0.48
1:B:158:MET:HG2	1:B:200:PHE:CD1	2.49	0.48
1:B:280:ASN:H	1:B:280:ASN:HD22	1.61	0.48
1:A:481:MET:CE	4:A:885:HOH:O	2.61	0.48
1:A:490:TYR:C	1:A:490:TYR:CD1	2.92	0.48
2:A:704:GOL:H31	4:A:801:HOH:O	2.13	0.48
1:A:35:LYS:HB3	1:A:35:LYS:HE2	1.41	0.47
1:A:263:GLU:HG2	4:A:977:HOH:O	2.14	0.47
1:B:73:VAL:HA	1:B:76:MET:HE3	1.96	0.47
1:B:581:LYS:CG	1:B:584:GLN:CD	2.82	0.47
1:A:2:ALA:CB	4:A:939:HOH:O	2.57	0.46
1:A:175:GLU:CD	1:A:203:ARG:NH1	2.46	0.46
1:A:443:GLU:O	1:A:444:LEU:HB2	2.16	0.46
1:B:363[A]:LYS:CE	4:B:802:HOH:O	2.63	0.46
1:B:413:LYS:HG3	1:B:414:ASN:N	2.31	0.45
1:B:296:LEU:HA	1:B:297:PRO:C	2.41	0.45
1:A:515:ILE:HD13	1:A:536:PRO:HB2	1.99	0.45
1:B:525:LYS:HE3	1:B:525:LYS:HB2	1.63	0.45
1:A:264:LYS:NZ	2:A:703:GOL:H32	2.33	0.44
1:B:301:PHE:CE1	2:B:702:GOL:H12	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:LYS:HZ2	2:A:702:GOL:H2	1.82	0.44
1:B:579:GLU:HB3	1:B:584:GLN:CD	2.42	0.44
1:A:158:MET:HG2	1:A:200:PHE:CD1	2.53	0.44
1:A:412:ASN:OD1	1:A:412:ASN:C	2.61	0.44
1:A:115:LYS:NZ	1:A:293:ASN:O	2.51	0.44
1:A:138:LEU:C	1:A:138:LEU:HD23	2.43	0.44
1:B:45:ALA:HA	1:B:48:LYS:HE2	1.99	0.44
1:B:301:PHE:CZ	2:B:702:GOL:H12	2.52	0.44
1:A:516:ASN:HD21	1:A:518:ASN:HB2	1.83	0.44
1:B:259[B]:VAL:HG12	4:B:838:HOH:O	2.17	0.44
1:B:260:LEU:HD22	1:B:268:ILE:HD13	2.00	0.44
1:A:198:ASN:HD21	1:A:202:LYS:HE3	1.83	0.44
1:A:464:PHE:CE1	1:A:565:LYS:HB2	2.53	0.43
1:B:537:LEU:HD22	1:B:541:GLN:HB3	2.00	0.43
1:A:280:ASN:ND2	1:A:280:ASN:H	2.16	0.43
1:A:288:HIS:CE1	4:A:845:HOH:O	2.66	0.43
1:B:201:PHE:CE2	1:B:227:ILE:CG1	3.02	0.43
1:A:39:GLY:O	1:A:43:GLN:HG3	2.19	0.43
1:A:462:GLU:O	1:A:504:LYS:HE2	2.19	0.43
1:A:103:ARG:HD2	4:A:886:HOH:O	2.19	0.42
1:A:374:LEU:HD11	1:A:444:LEU:HD23	2.01	0.42
1:A:413:LYS:HG3	1:A:414:ASN:N	2.34	0.42
1:B:87:GLU:HG3	1:B:89:TYR:CE2	2.53	0.42
1:B:188:GLY:O	1:B:191:LYS:N	2.52	0.42
1:B:188:GLY:O	1:B:191:LYS:HB2	2.19	0.42
1:A:245:PHE:HB3	1:A:251:PHE:CD2	2.55	0.42
1:B:201:PHE:CE2	1:B:227:ILE:HG13	2.54	0.42
1:B:4:LYS:HD3	1:B:127:GLU:OE2	2.20	0.42
1:A:533:ARG:CZ	2:A:706:GOL:H31	2.47	0.42
1:B:348:LYS:O	1:B:349:LYS:HD3	2.18	0.42
1:A:172[B]:ILE:HD13	1:A:172[B]:ILE:HA	1.88	0.42
1:B:201:PHE:N	1:B:231:MET:HE3	2.35	0.42
1:B:235:ARG:HD2	2:B:701:GOL:O3	2.20	0.42
1:B:184:GLU:HG2	1:B:184:GLU:O	2.20	0.41
1:B:473:SER:OG	1:B:478:GLN:HA	2.20	0.41
1:A:202:LYS:O	1:A:206:LYS:HD2	2.20	0.41
1:B:405:ILE:HD13	1:B:405:ILE:HA	1.83	0.41
1:A:493:LYS:HA	1:A:493:LYS:HD2	1.95	0.41
1:B:67:PHE:CD1	1:B:67:PHE:C	2.99	0.41
1:B:509:LEU:HD11	1:B:537:LEU:HD12	2.02	0.41
1:A:541:GLN:HA	1:A:544:MET:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:ASN:HD21	1:B:518:ASN:HB2	1.85	0.41
1:A:222:SER:O	1:A:226:LYS:CG	2.68	0.41
1:B:562:TYR:CD2	1:B:562:TYR:C	2.96	0.41
1:A:222:SER:O	1:A:225:SER:HB3	2.21	0.41
1:A:363:LYS:HE3	4:A:887:HOH:O	2.21	0.41
1:A:471:THR:OG1	1:A:473[A]:SER:HB2	2.21	0.41
1:B:259[B]:VAL:HG12	1:B:260:LEU:N	2.36	0.41
1:B:471:THR:OG1	1:B:473:SER:HB3	2.21	0.41
1:A:158:MET:HG2	1:A:200:PHE:CG	2.56	0.40
1:A:435:LYS:CG	2:A:702:GOL:H11	2.51	0.40
1:B:453:ASN:HA	1:B:488:ARG:HH12	1.86	0.40
1:A:191:LYS:HD3	1:A:191:LYS:HA	1.82	0.40
1:A:205:GLU:HA	1:A:227:ILE:HD11	2.02	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	590/610 (97%)	578 (98%)	12 (2%)	0	100	100
1	B	582/610 (95%)	565 (97%)	15 (3%)	2 (0%)	36	25
All	All	1172/1220 (96%)	1143 (98%)	27 (2%)	2 (0%)	43	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	186	ILE
1	B	225	SER

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	545/554 (98%)	538 (99%)	7 (1%)	61	51
1	B	536/554 (97%)	528 (98%)	8 (2%)	57	47
All	All	1081/1108 (98%)	1066 (99%)	15 (1%)	59	49

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	38	LYS
1	A	69	THR
1	A	102	ASN
1	A	386	GLU
1	A	406	LYS
1	A	602	VAL
1	B	102	ASN
1	B	178	GLN
1	B	186	ILE
1	B	227	ILE
1	B	367	LEU
1	B	383	GLN
1	B	495	LYS
1	B	579	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	102	ASN
1	A	117	GLN
1	A	123	HIS
1	A	136	ASN
1	A	181	ASN
1	A	223	HIS

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Mol	Chain	Res	Type
1	A	280	ASN
1	A	288	HIS
1	A	328	HIS
1	A	331	ASN
1	A	344	ASN
1	A	361	HIS
1	A	366	GLN
1	A	395	HIS
1	A	430	ASN
1	A	478	GLN
1	A	516	ASN
1	A	531	ASN
1	B	102	ASN
1	B	117	GLN
1	B	123	HIS
1	B	136	ASN
1	B	190	ASN
1	B	198	ASN
1	B	280	ASN
1	B	288	HIS
1	B	344	ASN
1	B	375	GLN
1	B	399	ASN
1	B	430	ASN
1	B	478	GLN
1	B	516	ASN
1	B	584	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

15 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	GOL	A	705	-	5,5,5	0.52	0	5,5,5	0.27	0
2	GOL	A	703	-	5,5,5	0.64	0	5,5,5	0.65	0
3	PO4	B	704	-	4,4,4	1.41	1 (25%)	6,6,6	0.97	0
2	GOL	A	706	-	5,5,5	0.61	0	5,5,5	0.90	0
2	GOL	B	702	-	5,5,5	0.49	0	5,5,5	0.98	0
2	GOL	A	701	-	5,5,5	0.37	0	5,5,5	0.86	0
2	GOL	B	701	-	5,5,5	0.46	0	5,5,5	1.48	1 (20%)
3	PO4	A	707	-	4,4,4	1.34	1 (25%)	6,6,6	1.17	0
3	PO4	B	705	-	4,4,4	0.99	0	6,6,6	1.36	1 (16%)
3	PO4	A	709	-	4,4,4	0.87	0	6,6,6	0.93	0
3	PO4	A	710	-	4,4,4	1.05	0	6,6,6	0.37	0
3	PO4	B	703	-	4,4,4	1.39	1 (25%)	6,6,6	1.42	1 (16%)
2	GOL	A	704	-	5,5,5	0.43	0	5,5,5	0.83	0
3	PO4	A	708	-	4,4,4	1.03	0	6,6,6	1.06	0
2	GOL	A	702	-	5,5,5	0.45	0	5,5,5	1.40	1 (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
2	GOL	A	705	-	-	4/4/4/4	-
2	GOL	A	703	-	-	0/4/4/4	-
2	GOL	A	706	-	-	1/4/4/4	-
2	GOL	B	702	-	-	3/4/4/4	-
2	GOL	A	701	-	-	2/4/4/4	-
2	GOL	B	701	-	-	2/4/4/4	-
2	GOL	A	704	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	702	-	-	4/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	704	PO4	P-O1	2.43	1.56	1.50
3	B	703	PO4	P-O1	2.39	1.56	1.50
3	A	707	PO4	P-O3	-2.21	1.48	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	703	PO4	O4-P-O1	-2.47	102.22	110.95
2	B	701	GOL	O3-C3-C2	-2.45	99.35	110.38
2	A	702	GOL	C3-C2-C1	-2.16	103.87	111.80
3	B	705	PO4	O4-P-O1	-2.07	103.62	110.95

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	GOL	O1-C1-C2-C3
2	A	702	GOL	O1-C1-C2-C3
2	A	702	GOL	C1-C2-C3-O3
2	A	704	GOL	C1-C2-C3-O3
2	A	705	GOL	O1-C1-C2-C3
2	B	702	GOL	O1-C1-C2-C3
2	A	702	GOL	O2-C2-C3-O3
2	A	705	GOL	C1-C2-C3-O3
2	A	706	GOL	C1-C2-C3-O3
2	B	701	GOL	C1-C2-C3-O3
2	A	702	GOL	O1-C1-C2-O2
2	A	705	GOL	O1-C1-C2-O2
2	B	702	GOL	O1-C1-C2-O2
2	A	701	GOL	O1-C1-C2-O2
2	A	704	GOL	O1-C1-C2-O2
2	A	704	GOL	O2-C2-C3-O3
2	A	705	GOL	O2-C2-C3-O3
2	B	701	GOL	O2-C2-C3-O3
2	B	702	GOL	O2-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	703	GOL	2	0
2	A	706	GOL	8	0
2	B	702	GOL	2	0
2	A	701	GOL	1	0
2	B	701	GOL	1	0
2	A	704	GOL	1	0
2	A	702	GOL	6	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	583/610 (95%)	0.10	26 (4%) 38 41	17, 40, 78, 130	20 (3%)
1	B	583/610 (95%)	0.35	34 (5%) 29 31	17, 46, 81, 151	11 (1%)
All	All	1166/1220 (95%)	0.22	60 (5%) 33 36	17, 44, 81, 151	31 (2%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	604	PHE	9.3
1	B	604	PHE	9.3
1	A	2	ALA	6.9
1	B	2	ALA	6.2
1	A	1	MET	5.7
1	B	67	PHE	5.7
1	B	3	LYS	5.4
1	A	67	PHE	4.9
1	B	186	ILE	4.9
1	B	603	ARG	4.4
1	B	66	ALA	4.3
1	B	602	VAL	3.9
1	B	8	TYR	3.8
1	B	57	LEU	3.7
1	B	195	PHE	3.4
1	A	333[A]	LYS	3.4
1	B	58	GLY	3.2
1	A	51	ALA	3.2
1	A	57	LEU	3.2
1	B	480	LYS	3.2
1	B	56	PHE	3.2
1	B	204	PHE	3.2
1	A	56	PHE	3.1
1	A	603	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	8	TYR	3.0
1	B	182	GLU	2.9
1	B	193	LEU	2.9
1	B	203[A]	ARG	2.8
1	B	201	PHE	2.8
1	B	178	GLN	2.7
1	A	53	LEU	2.7
1	A	227	ILE	2.7
1	A	602	VAL	2.6
1	A	195	PHE	2.6
1	B	159	PHE	2.6
1	B	172	ILE	2.5
1	A	54	PRO	2.5
1	A	313	ARG	2.4
1	B	183	ARG	2.4
1	A	196	THR	2.3
1	B	198	ASN	2.3
1	A	132	GLU	2.2
1	A	200	PHE	2.2
1	B	208	TYR	2.2
1	B	227	ILE	2.2
1	B	200	PHE	2.2
1	A	223	HIS	2.2
1	B	349	LYS	2.2
1	B	226	LYS	2.2
1	A	33	TYR	2.1
1	A	222	SER	2.1
1	B	54	PRO	2.1
1	B	176	ILE	2.1
1	B	5	VAL	2.1
1	A	38	LYS	2.1
1	A	34	TRP	2.1
1	A	208	TYR	2.0
1	B	179	PHE	2.0
1	B	207	ILE	2.0
1	A	188	GLY	2.0

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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PO4	B	704	5/5	0.76	0.26	47,50,54,56	5
2	GOL	A	706	6/6	0.78	0.18	41,61,65,70	6
2	GOL	A	703	6/6	0.79	0.21	47,57,64,72	6
3	PO4	B	705	5/5	0.79	0.19	40,40,56,59	5
2	GOL	A	705	6/6	0.84	0.13	66,69,81,84	0
3	PO4	A	709	5/5	0.85	0.09	73,73,75,83	5
2	GOL	A	704	6/6	0.86	0.13	42,54,56,63	6
3	PO4	A	710	5/5	0.86	0.11	77,81,84,88	5
2	GOL	B	701	6/6	0.87	0.14	45,52,54,60	6
2	GOL	A	702	6/6	0.88	0.10	39,60,62,65	0
2	GOL	B	702	6/6	0.88	0.11	50,67,71,76	0
3	PO4	A	707	5/5	0.90	0.09	39,52,64,71	0
3	PO4	A	708	5/5	0.90	0.14	56,57,59,62	5
2	GOL	A	701	6/6	0.91	0.13	50,56,58,63	6
3	PO4	B	703	5/5	0.92	0.08	40,51,59,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.