



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:06 PM UTC

PDB ID : 6RO0 / pdb_00006ro0
Title : CRYSTAL STRUCTURE OF GENETICALLY DETOXIFIED PERTUSSIS TOXIN GDPT.
Authors : Bertrand, T.
Deposited on : 2019-05-10
Resolution : 2.13 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:

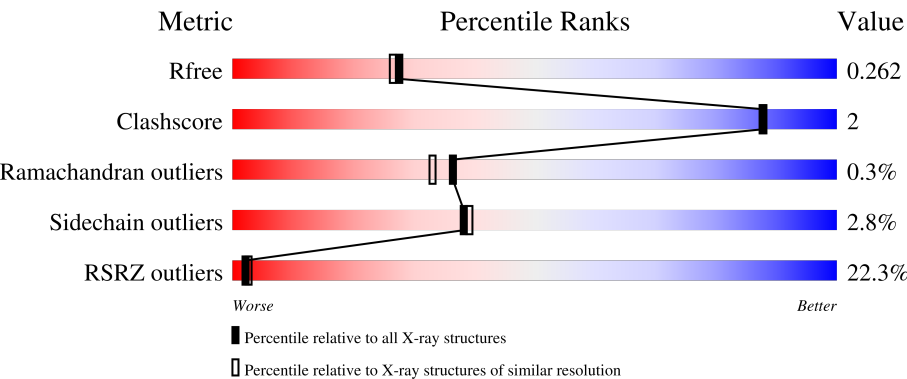
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.13 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	269	14% 78% 5% 17%
1	G	269	29% 76% 6% 17%
2	B	226	8% 81% 7% 13%
2	H	226	6% 80% 8% 12%
3	C	227	46% 80% 7% 13%

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Mol	Chain	Length	Quality of chain
3	I	227	15% 80% 6% 14%
4	D	152	13% 68% 28%
4	E	152	28% 66% 6% 28%
4	J	152	7% 66% 7% 28%
4	K	152	13% 67% 5% 28%
5	F	133	19% 61% 12% 26%
5	L	133	12% 61% 13% 26%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15156 atoms, of which 72 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 Pertussis toxin subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1762	1092	316	348	6			
1	G	222	Total	C	N	O	S	0	0	0
			1744	1082	314	342	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	LYS	ARG	engineered mutation	UNP T1SR96
A	129	GLY	GLU	engineered mutation	UNP T1SR96
G	9	LYS	ARG	engineered mutation	UNP T1SR96
G	129	GLY	GLU	engineered mutation	UNP T1SR96

- Molecule 2 is a protein called Islet-activating protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	197	Total	C	N	O	S	0	0	0
			1529	966	261	293	9			
2	H	199	Total	C	N	O	S	0	0	0
			1542	973	263	297	9			

- Molecule 3 is a protein called Islet-activating protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	197	Total	C	N	O	S	0	0	0
			1528	974	259	286	9			
3	I	196	Total	C	N	O	S	0	0	0
			1521	969	258	285	9			

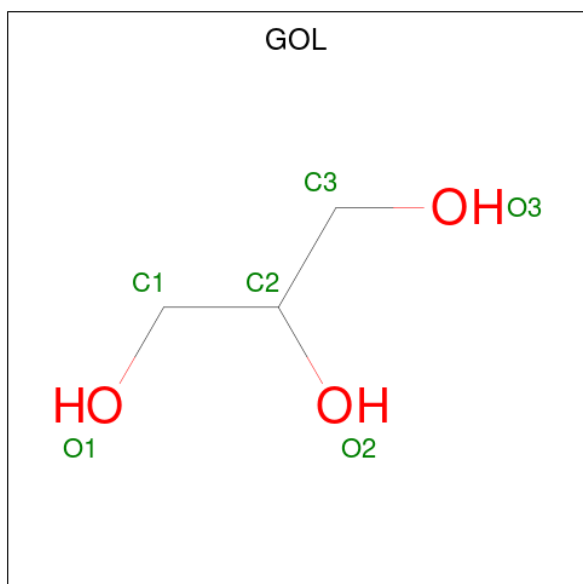
- Molecule 4 is a protein called Islet-activating protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	110	Total	C	N	O	S	0	0	0
			838	536	143	147	12			
4	E	110	Total	C	N	O	S	0	0	0
			838	536	143	147	12			
4	J	110	Total	C	N	O	S	0	0	0
			838	536	143	147	12			
4	K	110	Total	C	N	O	S	0	0	0
			838	536	143	147	12			

- Molecule 5 is a protein called Pertussis toxin subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	98	Total	C	N	O	S	0	0	0
			764	489	125	144	6			
5	L	98	Total	C	N	O	S	0	0	0
			764	489	125	144	6			

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	B	1	Total	C	H	O	0	0
			14	3	8	3		
6	B	1	Total	C	H	O	0	0
			14	3	8	3		
6	B	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	H	O	0	0
			14	3	8	3		
6	F	1	Total	C	H	O	0	0
			14	3	8	3		
6	H	1	Total	C	H	O	0	0
			14	3	8	3		
6	H	1	Total	C	H	O	0	0
			14	3	8	3		
6	J	1	Total	C	H	O	0	0
			14	3	8	3		

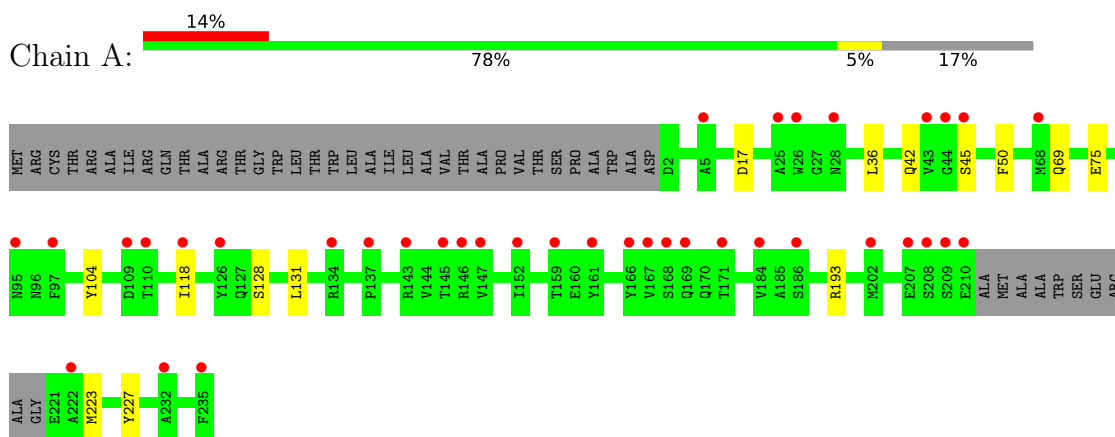
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	74	Total	O	0	0
			74	74		
7	B	101	Total	O	0	0
			101	101		
7	C	32	Total	O	0	0
			32	32		
7	D	30	Total	O	0	0
			30	30		
7	E	25	Total	O	0	0
			25	25		
7	F	40	Total	O	0	0
			40	40		
7	G	22	Total	O	0	0
			22	22		
7	H	86	Total	O	0	0
			86	86		
7	I	52	Total	O	0	0
			52	52		
7	J	25	Total	O	0	0
			25	25		
7	K	18	Total	O	0	0
			18	18		
7	L	19	Total	O	0	0
			19	19		

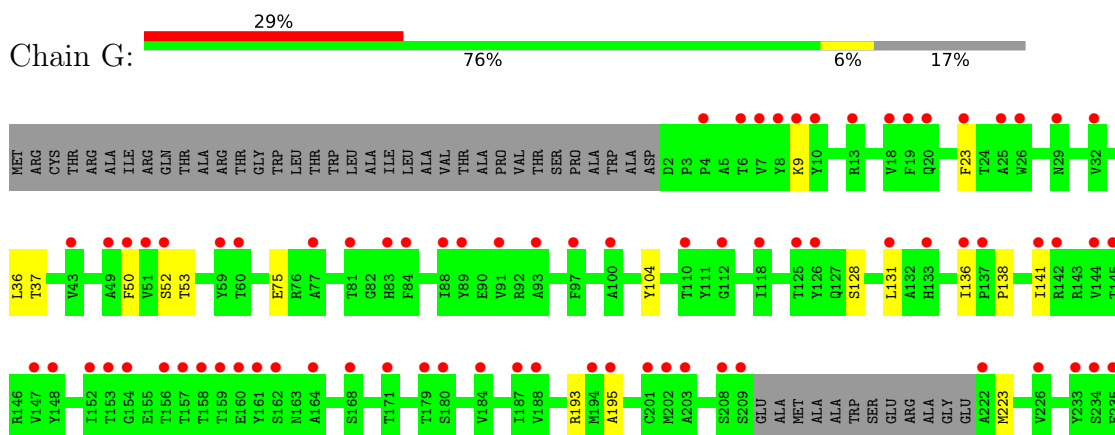
3 Residue-property plots [i](#)

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.

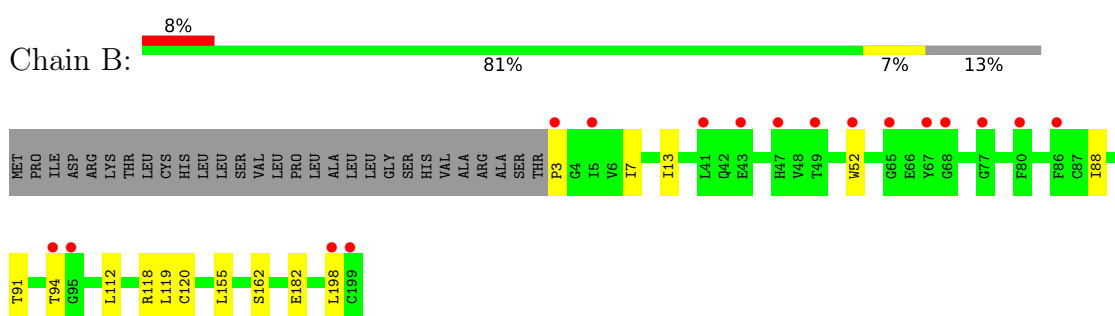
- Molecule 1: Pertussis toxin subunit 1



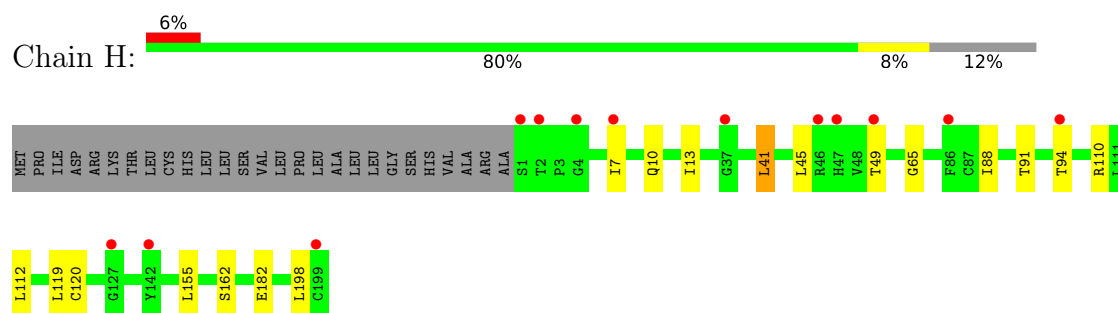
- Molecule 1: Pertussis toxin subunit 1



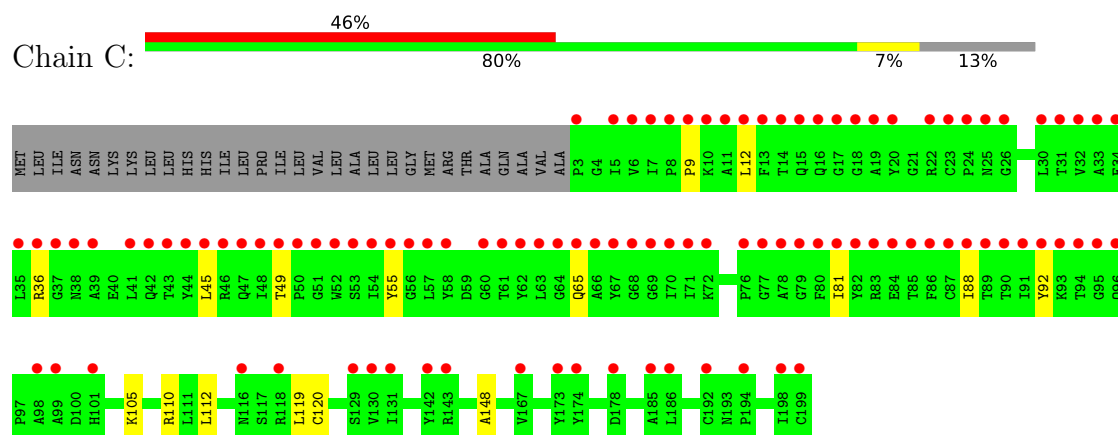
- Molecule 2: Islet-activating protein S2



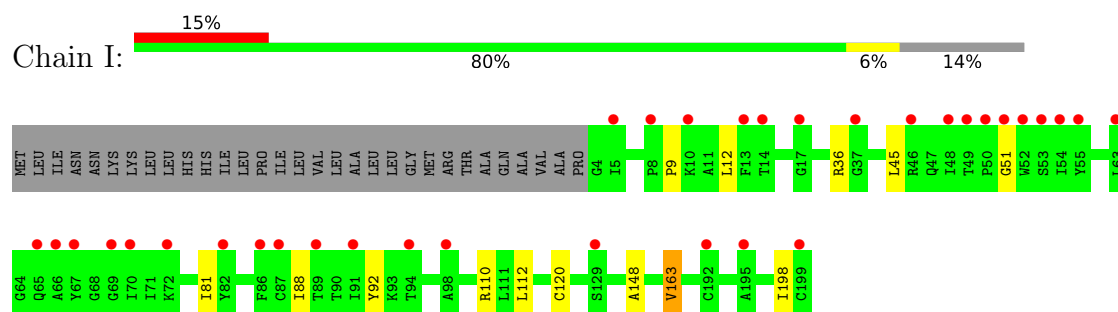
- Molecule 2: Islet-activating protein S2



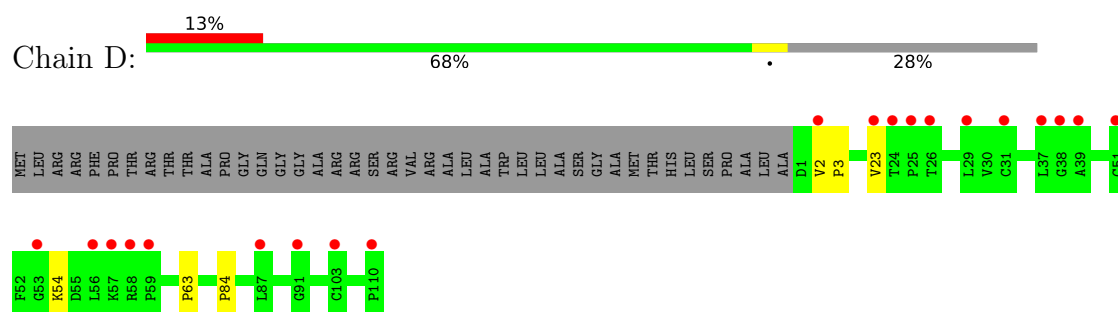
- Molecule 3: Islet-activating protein S3



- Molecule 3: Islet-activating protein S3

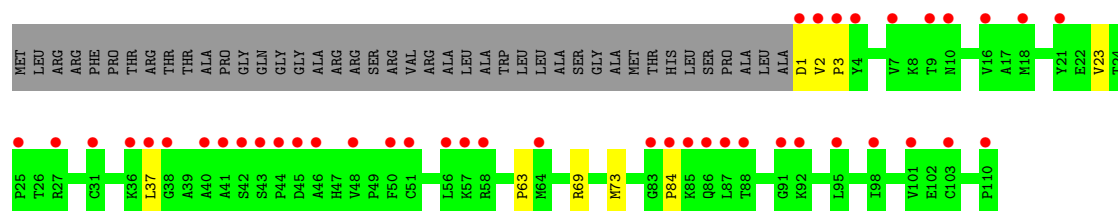


- Molecule 4: Islet-activating protein S4

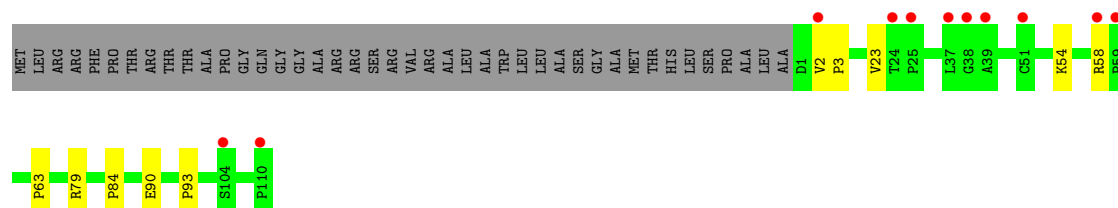


- Molecule 4: Islet-activating protein S4

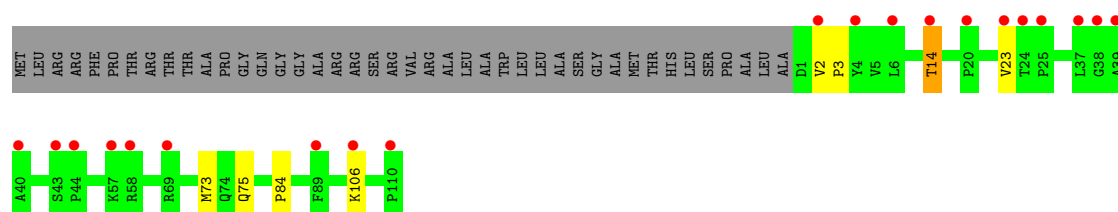




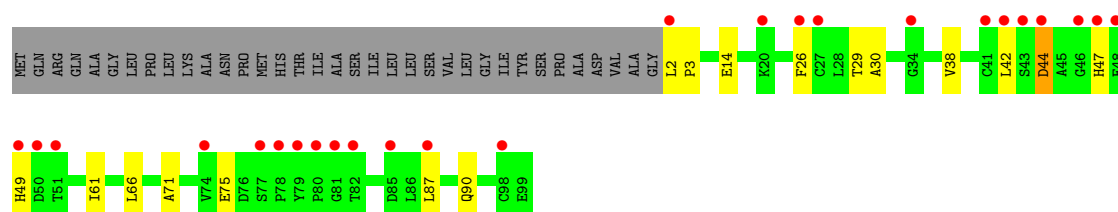
• Molecule 4: Islet-activating protein S4



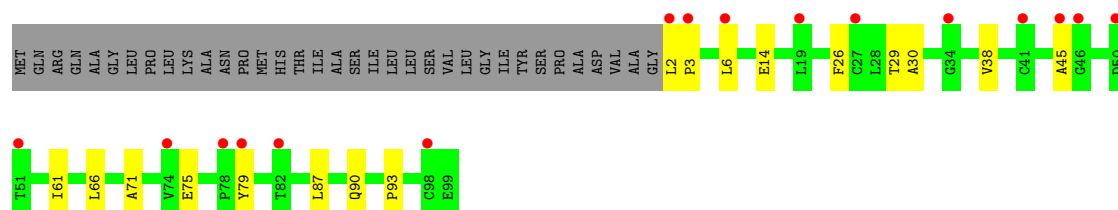
• Molecule 4: Islet-activating protein S4



• Molecule 5: Pertussis toxin subunit 5



• Molecule 5: Pertussis toxin subunit 5



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.46Å 160.80Å 194.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.62 – 2.13 46.62 – 2.13	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.62-2.13) 99.5 (46.62-2.13)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.14Å)	Xtriage
Refinement program	autoBUSTER 2.11.7	Depositor
R, R_{free}	0.240 , 0.260 (Not available) , 0.262	Depositor DCC
R_{free} test set	8309 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.633	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.0	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	0.95	EDS
Total number of atoms	15156	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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: GOL

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	0.66	0/1802	1.21	5/2447 (0.2%)
1	G	0.68	0/1784	1.22	2/2423 (0.1%)
2	B	0.66	0/1566	1.14	2/2126 (0.1%)
2	H	0.67	0/1579	1.14	0/2145
3	C	0.68	0/1565	1.18	2/2126 (0.1%)
3	I	0.67	0/1557	1.16	3/2115 (0.1%)
4	D	0.70	0/856	1.12	0/1155
4	E	0.68	0/856	1.09	0/1155
4	J	0.71	0/856	1.12	0/1155
4	K	0.68	0/856	1.11	0/1155
5	F	0.63	0/782	1.17	2/1059 (0.2%)
5	L	0.64	0/782	1.12	1/1059 (0.1%)
All	All	0.67	0/14841	1.16	17/20120 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	128	SER	CA-C-N	5.87	125.56	119.92
1	G	128	SER	C-N-CA	5.87	125.56	119.92
3	I	9	PRO	CA-C-N	5.54	127.97	120.38
3	I	9	PRO	C-N-CA	5.54	127.97	120.38
3	C	9	PRO	CA-C-N	5.43	127.82	120.38
3	C	9	PRO	C-N-CA	5.43	127.82	120.38
5	F	26	PHE	CA-CB-CG	5.27	119.07	113.80
1	A	17	ASP	CA-CB-CG	5.26	117.86	112.60
3	I	163	VAL	N-CA-CB	-5.26	105.16	112.52
2	B	3	PRO	CA-C-N	5.24	125.08	120.10
2	B	3	PRO	C-N-CA	5.24	125.08	120.10
5	L	26	PHE	CA-CB-CG	5.20	119.00	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	SER	CA-C-N	5.09	125.50	120.31
1	A	128	SER	C-N-CA	5.09	125.50	120.31
1	A	227	TYR	CA-C-N	5.04	127.03	120.28
1	A	227	TYR	C-N-CA	5.04	127.03	120.28
5	F	44	ASP	CA-CB-CG	5.02	117.62	112.60

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	A	1762	0	1652	5	0
1	G	1744	0	1640	7	0
2	B	1529	0	1481	4	0
2	H	1542	0	1495	8	0
3	C	1528	0	1492	5	0
3	I	1521	0	1484	4	0
4	D	838	0	874	4	0
4	E	838	0	874	6	0
4	J	838	0	874	8	0
4	K	838	0	874	5	0
5	F	764	0	747	8	0
5	L	764	0	747	8	0
6	A	6	8	8	0	0
6	B	18	24	24	0	0
6	D	6	8	8	0	0
6	F	6	8	8	0	0
6	H	12	16	16	0	0
6	J	6	8	8	1	0
7	A	74	0	0	0	0
7	B	101	0	0	0	0
7	C	32	0	0	0	0
7	D	30	0	0	0	0
7	E	25	0	0	0	0
7	F	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	22	0	0	0	0
7	H	86	0	0	0	0
7	I	52	0	0	0	0
7	J	25	0	0	0	0
7	K	18	0	0	0	0
7	L	19	0	0	0	0
All	All	15084	72	14306	57	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 2.

All (57) 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)
4:K:73:MET:HE1	5:L:66:LEU:HD11	1.53	0.90
2:H:45:LEU:O	2:H:49:THR:HG22	1.90	0.71
4:K:14:THR:HG23	5:L:93:PRO:HG3	1.79	0.64
1:G:36:LEU:HD22	1:G:104:TYR:HB2	1.80	0.63
2:H:49:THR:HG23	2:H:65:GLY:H	1.65	0.62
3:C:119:LEU:HB2	4:E:63:PRO:HB3	1.83	0.60
1:A:36:LEU:HD22	1:A:104:TYR:HB2	1.84	0.58
4:K:2:VAL:HG22	4:K:3:PRO:HD2	1.85	0.58
4:J:2:VAL:HG22	4:J:3:PRO:HD2	1.85	0.58
4:D:2:VAL:HG22	4:D:3:PRO:HD2	1.85	0.58
3:I:198:ILE:HD12	4:J:90:GLU:HG3	1.86	0.57
4:E:2:VAL:HG22	4:E:3:PRO:HD2	1.86	0.57
2:H:119:LEU:HB2	4:J:63:PRO:HB3	1.87	0.56
3:I:112:LEU:HB3	3:I:120:CYS:HB2	1.91	0.53
3:I:148:ALA:HB2	4:J:54:LYS:HE2	1.91	0.52
3:C:49:THR:HG23	3:C:55:TYR:HE2	1.74	0.52
5:F:71:ALA:HB3	5:F:90:GLN:HB3	1.92	0.51
2:H:112:LEU:HB3	2:H:120:CYS:HB2	1.93	0.51
5:L:71:ALA:HB3	5:L:90:GLN:HB3	1.92	0.51
2:B:52:TRP:CG	4:J:93:PRO:HB3	2.47	0.50
1:A:69:GLN:HG3	4:E:37:LEU:HD23	1.94	0.50
2:B:112:LEU:HB3	2:B:120:CYS:HB2	1.94	0.49
2:H:155:LEU:HD22	5:L:61:ILE:HG23	1.94	0.49
5:L:30:ALA:HB3	5:L:38:VAL:HB	1.95	0.49
5:L:2:LEU:N	5:L:3:PRO:HD3	2.28	0.49
5:F:30:ALA:HB3	5:F:38:VAL:HB	1.95	0.49
3:C:112:LEU:HB3	3:C:120:CYS:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:12:LEU:HD21	3:C:92:TYR:HB2	1.95	0.48
5:F:2:LEU:N	5:F:3:PRO:HD3	2.28	0.48
1:G:9:LYS:HB2	1:G:53:THR:HG22	1.95	0.48
3:I:12:LEU:HD21	3:I:92:TYR:HB2	1.96	0.47
2:B:119:LEU:HB2	4:D:63:PRO:HB3	1.98	0.46
3:C:148:ALA:HB2	4:D:54:LYS:HE2	1.98	0.46
2:H:110:ARG:HH21	4:J:79:ARG:HH12	1.65	0.45
2:B:155:LEU:HD22	5:F:61:ILE:HG23	1.98	0.45
1:A:42:GLN:HB2	1:A:45:SER:HB3	1.99	0.44
4:K:2:VAL:HG12	4:K:84:PRO:HA	2.00	0.44
4:E:2:VAL:HG12	4:E:84:PRO:HA	2.00	0.44
1:A:193:ARG:HH11	1:A:223:MET:HG3	1.83	0.44
1:G:23:PHE:HB2	1:G:136:ILE:HB	1.99	0.44
4:D:2:VAL:HG12	4:D:84:PRO:HA	2.00	0.44
1:G:138:PRO:HA	1:G:141:ILE:HD12	2.00	0.44
1:G:193:ARG:HH11	1:G:223:MET:HG3	1.82	0.44
1:G:195:ALA:HB1	4:K:75:GLN:CG	2.49	0.43
4:J:2:VAL:HG12	4:J:84:PRO:HA	2.00	0.43
5:F:44:ASP:C	5:F:47:HIS:HB2	2.42	0.43
2:H:49:THR:CG2	2:H:65:GLY:H	2.31	0.43
4:E:73:MET:SD	5:F:66:LEU:HD21	2.58	0.43
4:E:69:ARG:O	4:E:73:MET:HG2	2.20	0.42
4:J:58:ARG:HB3	6:J:201:GOL:H31	2.02	0.42
5:F:75:GLU:HB2	5:F:87:LEU:HD11	2.02	0.41
5:L:14:GLU:HB2	5:L:29:THR:HB	2.02	0.41
5:L:75:GLU:HB2	5:L:87:LEU:HD11	2.03	0.41
5:F:14:GLU:HB2	5:F:29:THR:HB	2.01	0.41
1:A:50:PHE:HB3	1:A:131:LEU:HB3	2.03	0.41
2:H:10:GLN:HG3	2:H:41:LEU:HD13	2.03	0.41
1:G:50:PHE:HB3	1:G:131:LEU:HB3	2.03	0.41

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	220/269 (82%)	215 (98%)	5 (2%)	0	100	100
1	G	218/269 (81%)	213 (98%)	5 (2%)	0	100	100
2	B	195/226 (86%)	188 (96%)	7 (4%)	0	100	100
2	H	197/226 (87%)	190 (96%)	7 (4%)	0	100	100
3	C	195/227 (86%)	190 (97%)	4 (2%)	1 (0%)	24	19
3	I	194/227 (86%)	189 (97%)	3 (2%)	2 (1%)	12	7
4	D	108/152 (71%)	107 (99%)	1 (1%)	0	100	100
4	E	108/152 (71%)	108 (100%)	0	0	100	100
4	J	108/152 (71%)	106 (98%)	2 (2%)	0	100	100
4	K	108/152 (71%)	106 (98%)	2 (2%)	0	100	100
5	F	96/133 (72%)	94 (98%)	1 (1%)	1 (1%)	12	7
5	L	96/133 (72%)	92 (96%)	3 (3%)	1 (1%)	12	7
All	All	1843/2318 (80%)	1798 (98%)	40 (2%)	5 (0%)	36	33

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	49	HIS
3	I	51	GLY
3	C	110	ARG
3	I	110	ARG
5	L	45	ALA

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	184/216 (85%)	182 (99%)	2 (1%)	65	71
1	G	182/216 (84%)	179 (98%)	3 (2%)	55	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	164/189 (87%)	155 (94%)	9 (6%)	19	15
2	H	166/189 (88%)	157 (95%)	9 (5%)	20	15
3	C	156/181 (86%)	150 (96%)	6 (4%)	29	28
3	I	155/181 (86%)	150 (97%)	5 (3%)	34	35
4	D	94/124 (76%)	93 (99%)	1 (1%)	65	71
4	E	94/124 (76%)	92 (98%)	2 (2%)	47	51
4	J	94/124 (76%)	93 (99%)	1 (1%)	65	71
4	K	94/124 (76%)	91 (97%)	3 (3%)	34	35
5	F	83/110 (76%)	82 (99%)	1 (1%)	63	69
5	L	83/110 (76%)	81 (98%)	2 (2%)	43	45
All	All	1549/1888 (82%)	1505 (97%)	44 (3%)	38	39

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	GLU
1	A	118	ILE
2	B	7	ILE
2	B	13	ILE
2	B	88	ILE
2	B	91	THR
2	B	94	THR
2	B	118	ARG
2	B	162	SER
2	B	182	GLU
2	B	198	LEU
3	C	36	ARG
3	C	45	LEU
3	C	65	GLN
3	C	81	ILE
3	C	88	ILE
3	C	105	LYS
4	D	23	VAL
4	E	1	ASP
4	E	23	VAL
5	F	42	LEU
1	G	37	THR
1	G	52	SER

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Mol	Chain	Res	Type
1	G	75	GLU
2	H	7	ILE
2	H	13	ILE
2	H	41	LEU
2	H	88	ILE
2	H	91	THR
2	H	94	THR
2	H	162	SER
2	H	182	GLU
2	H	198	LEU
3	I	36	ARG
3	I	45	LEU
3	I	81	ILE
3	I	88	ILE
3	I	163	VAL
4	J	23	VAL
4	K	14	THR
4	K	23	VAL
4	K	106	LYS
5	L	6	LEU
5	L	79	TYR

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

Mol	Chain	Res	Type
1	A	29	ASN
1	A	47	ASN
1	A	69	GLN
1	A	83	HIS
1	A	96	ASN
1	A	133	HIS
1	A	170	GLN
2	B	12	GLN
2	B	15	GLN
2	B	42	GLN
2	B	193	ASN
3	C	16	GLN
3	C	101	HIS
4	D	10	ASN
4	D	75	GLN
4	E	10	ASN
5	F	90	GLN

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Mol	Chain	Res	Type
1	G	69	GLN
1	G	83	HIS
1	G	170	GLN
2	H	12	GLN
2	H	15	GLN
2	H	42	GLN
3	I	101	HIS
3	I	128	GLN
3	I	193	ASN
4	J	10	ASN
4	K	10	ASN
5	L	23	ASN
5	L	90	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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](#)

9 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	$\# Z > 2$
6	GOL	J	201	-	5,5,5	0.06	0	5,5,5	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	GOL	B	202	-	5,5,5	0.05	0	5,5,5	0.21	0
6	GOL	D	201	-	5,5,5	0.06	0	5,5,5	0.10	0
6	GOL	H	202	-	5,5,5	0.07	0	5,5,5	0.22	0
6	GOL	B	203	-	5,5,5	0.04	0	5,5,5	0.21	0
6	GOL	F	101	-	5,5,5	0.08	0	5,5,5	0.17	0
6	GOL	A	301	-	5,5,5	0.05	0	5,5,5	0.17	0
6	GOL	B	201	-	5,5,5	0.12	0	5,5,5	0.13	0
6	GOL	H	201	-	5,5,5	0.06	0	5,5,5	0.15	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
6	GOL	J	201	-	-	0/4/4/4	-
6	GOL	B	202	-	-	0/4/4/4	-
6	GOL	D	201	-	-	0/4/4/4	-
6	GOL	H	202	-	-	0/4/4/4	-
6	GOL	B	203	-	-	0/4/4/4	-
6	GOL	F	101	-	-	0/4/4/4	-
6	GOL	A	301	-	-	0/4/4/4	-
6	GOL	B	201	-	-	0/4/4/4	-
6	GOL	H	201	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	201	GOL	1	0

5.7 Other polymers [i](#)

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	224/269 (83%)	1.23	38 (16%) 4 5	37, 57, 80, 122	0
1	G	222/269 (82%)	1.75	77 (34%) 1 1	63, 89, 114, 133	0
2	B	197/226 (87%)	0.92	17 (8%) 16 18	34, 52, 68, 77	0
2	H	199/226 (88%)	1.01	13 (6%) 25 29	41, 54, 69, 78	0
3	C	197/227 (86%)	2.30	104 (52%) 0 0	41, 69, 103, 117	0
3	I	196/227 (86%)	1.31	34 (17%) 4 5	45, 63, 87, 100	0
4	D	110/152 (72%)	1.25	20 (18%) 3 4	37, 53, 76, 91	0
4	E	110/152 (72%)	1.86	43 (39%) 1 1	37, 60, 83, 89	0
4	J	110/152 (72%)	1.15	11 (10%) 12 14	42, 55, 83, 90	0
4	K	110/152 (72%)	1.28	20 (18%) 3 4	47, 63, 87, 91	0
5	F	98/133 (73%)	1.41	25 (25%) 1 2	40, 56, 90, 106	0
5	L	98/133 (73%)	1.30	16 (16%) 4 5	47, 65, 84, 90	0
All	All	1871/2318 (80%)	1.41	418 (22%) 2 3	34, 61, 98, 133	0

All (418) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	63	LEU	7.8
4	E	2	VAL	7.6
3	C	67	TYR	6.5
4	E	41	ALA	6.0
5	F	49	HIS	5.6
3	C	55	TYR	5.3
3	C	62	TYR	5.1
3	C	45	LEU	5.1
3	C	52	TRP	5.0
3	C	64	GLY	5.0
3	C	70	ILE	5.0

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Mol	Chain	Res	Type	RSRZ
3	C	86	PHE	5.0
3	I	66	ALA	5.0
4	E	44	PRO	5.0
5	L	2	LEU	5.0
3	C	82	TYR	4.9
3	I	67	TYR	4.9
4	E	1	ASP	4.8
3	C	32	VAL	4.8
3	C	53	SER	4.8
3	C	13	PHE	4.7
3	C	56	GLY	4.7
3	I	199	CYS	4.7
4	E	110	PRO	4.6
3	C	54	ILE	4.6
3	C	87	CYS	4.6
3	C	199	CYS	4.6
4	K	110	PRO	4.6
4	J	59	PRO	4.5
3	C	50	PRO	4.4
1	G	222	ALA	4.4
3	C	19	ALA	4.4
3	C	41	LEU	4.3
4	J	104	SER	4.3
3	C	71	ILE	4.3
3	C	49	THR	4.3
3	C	25	ASN	4.2
4	E	37	LEU	4.2
1	G	152	ILE	4.2
2	H	49	THR	4.1
1	G	209	SER	4.1
1	G	10	TYR	4.1
1	A	118	ILE	4.1
5	F	27	CYS	4.1
3	C	81	ILE	4.1
2	H	86	PHE	4.0
3	I	50	PRO	4.0
3	C	5	ILE	4.0
3	C	88	ILE	4.0
5	F	78	PRO	3.9
1	G	136	ILE	3.9
3	C	80	PHE	3.9
3	C	20	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
3	C	17	GLY	3.9
1	G	19	PHE	3.8
3	C	79	GLY	3.8
5	L	78	PRO	3.8
5	L	51	THR	3.8
4	E	43	SER	3.8
1	G	158	THR	3.8
5	L	19	LEU	3.8
3	I	17	GLY	3.8
4	E	4	TYR	3.7
3	C	89	THR	3.7
3	C	6	VAL	3.7
3	C	48	ILE	3.7
1	G	179	THR	3.7
3	C	14	THR	3.7
5	F	50	ASP	3.6
3	C	57	LEU	3.6
1	G	161	TYR	3.6
4	J	51	CYS	3.6
1	G	157	THR	3.6
5	F	2	LEU	3.6
3	I	48	ILE	3.5
4	K	69	ARG	3.5
3	C	9	PRO	3.5
2	B	49	THR	3.5
1	G	141	ILE	3.5
4	D	38	GLY	3.5
4	E	38	GLY	3.5
5	F	81	GLY	3.5
3	C	7	ILE	3.4
1	G	23	PHE	3.4
5	L	46	GLY	3.4
3	C	61	THR	3.4
3	C	91	ILE	3.4
5	F	80	PRO	3.4
4	E	57	LYS	3.4
2	H	199	CYS	3.4
5	F	41	CYS	3.4
1	G	126	TYR	3.4
3	C	92	TYR	3.4
4	E	3	PRO	3.4
3	C	51	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
3	I	82	TYR	3.4
3	C	3	PRO	3.4
4	K	2	VAL	3.3
1	G	133	HIS	3.3
1	G	154	GLY	3.3
5	F	51	THR	3.3
3	C	8	PRO	3.3
4	E	83	GLY	3.3
3	C	167	VAL	3.3
3	C	66	ALA	3.3
3	C	35	LEU	3.3
4	D	37	LEU	3.3
3	C	72	LYS	3.3
1	G	159	THR	3.2
3	I	89	THR	3.2
3	I	192	CYS	3.2
3	C	34	GLU	3.2
3	C	44	TYR	3.2
4	J	37	LEU	3.2
1	A	186	SER	3.2
1	A	44	GLY	3.2
4	J	2	VAL	3.2
3	I	54	ILE	3.2
2	B	65	GLY	3.2
1	A	222	ALA	3.2
1	A	152	ILE	3.2
1	G	118	ILE	3.2
4	E	87	LEU	3.2
3	C	69	GLY	3.1
3	C	22	ARG	3.1
4	E	27	ARG	3.1
4	E	45	ASP	3.1
3	C	30	LEU	3.1
3	I	55	TYR	3.1
4	E	64	MET	3.1
1	A	110	THR	3.1
1	G	81	THR	3.1
5	F	26	PHE	3.1
1	G	93	ALA	3.1
1	G	156	THR	3.1
1	G	97	PHE	3.1
1	G	13	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
3	C	185	ALA	3.1
1	A	202	MET	3.1
1	A	161	TYR	3.0
3	C	173	TYR	3.0
4	E	88	THR	3.0
1	G	160	GLU	3.0
4	D	51	CYS	3.0
4	K	23	VAL	3.0
4	D	110	PRO	3.0
4	J	25	PRO	3.0
3	C	65	GLN	3.0
2	B	3	PRO	3.0
5	F	47	HIS	3.0
4	E	84	PRO	3.0
4	K	89	PHE	3.0
1	A	232	ALA	2.9
3	I	195	ALA	2.9
5	L	41	CYS	2.9
1	G	18	VAL	2.9
1	G	144	VAL	2.9
3	C	94	THR	2.9
4	D	25	PRO	2.9
3	C	16	GLN	2.9
1	A	168	SER	2.9
1	A	28	ASN	2.9
1	G	49	ALA	2.9
4	D	91	GLY	2.9
1	A	126	TYR	2.9
4	K	4	TYR	2.9
3	C	39	ALA	2.9
3	C	68	GLY	2.9
5	L	6	LEU	2.9
4	E	16	VAL	2.9
2	B	94	THR	2.9
3	C	90	THR	2.9
4	E	58	ARG	2.9
4	K	24	THR	2.9
3	C	84	GLU	2.9
3	C	78	ALA	2.9
5	F	74	VAL	2.8
1	A	235	PHE	2.8
2	H	4	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
4	E	91	GLY	2.8
4	D	103	CYS	2.8
1	G	208	SER	2.8
4	E	42	SER	2.8
1	A	169	GLN	2.8
4	K	38	GLY	2.8
1	G	25	ALA	2.8
4	D	56	LEU	2.8
5	F	42	LEU	2.8
3	I	52	TRP	2.8
3	I	87	CYS	2.8
1	A	45	SER	2.8
1	A	207	GLU	2.8
1	G	84	PHE	2.8
3	C	60	GLY	2.8
2	B	67	TYR	2.8
3	I	63	LEU	2.8
4	E	95	LEU	2.8
1	G	9	LYS	2.8
5	F	34	GLY	2.7
3	I	70	ILE	2.7
3	I	129	SER	2.7
2	B	77	GLY	2.7
3	C	10	LYS	2.7
3	I	14	THR	2.7
4	J	24	THR	2.7
3	C	24	PRO	2.7
4	D	59	PRO	2.7
1	A	147	VAL	2.7
4	K	57	LYS	2.7
5	F	46	GLY	2.7
1	A	5	ALA	2.7
4	E	46	ALA	2.7
1	G	137	PRO	2.7
3	C	38	ASN	2.7
1	G	88	ILE	2.7
1	G	226	VAL	2.7
4	E	48	VAL	2.7
4	E	51	CYS	2.7
1	A	26	TRP	2.7
1	G	145	THR	2.6
3	C	43	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	209	SER	2.6
1	A	167	VAL	2.6
1	G	91	VAL	2.6
3	C	130	VAL	2.6
1	A	134	ARG	2.6
2	B	43	GLU	2.6
1	G	83	HIS	2.6
2	B	41	LEU	2.6
1	G	7	VAL	2.6
3	I	94	THR	2.6
4	K	58	ARG	2.6
3	C	198	ILE	2.6
1	A	210	GLU	2.6
1	G	112	GLY	2.6
5	L	27	CYS	2.6
3	C	93	LYS	2.6
2	H	94	THR	2.6
4	K	40	ALA	2.6
4	K	44	PRO	2.6
1	G	162	SER	2.6
1	G	184	VAL	2.5
2	B	5	ILE	2.5
1	A	166	TYR	2.5
1	G	202	MET	2.5
2	B	95	GLY	2.5
5	L	45	ALA	2.5
2	B	86	PHE	2.5
3	I	13	PHE	2.5
5	L	74	VAL	2.5
3	C	101	HIS	2.5
4	D	57	LYS	2.5
4	E	85	LYS	2.5
1	G	29	ASN	2.5
5	L	98	CYS	2.5
1	G	6	THR	2.5
3	C	31	THR	2.5
3	I	49	THR	2.5
4	D	24	THR	2.5
1	G	26	TRP	2.5
3	C	18	GLY	2.5
1	G	32	VAL	2.5
3	C	46	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
5	F	98	CYS	2.5
5	F	85	ASP	2.5
5	F	44	ASP	2.4
1	A	171	THR	2.4
4	K	20	PRO	2.4
1	G	164	ALA	2.4
1	A	143	ARG	2.4
4	J	58	ARG	2.4
1	G	233	TYR	2.4
3	C	23	CYS	2.4
3	C	142	TYR	2.4
5	F	77	SER	2.4
4	E	56	LEU	2.4
3	C	178	ASP	2.4
1	G	110	THR	2.4
1	G	153	THR	2.4
4	E	21	TYR	2.4
4	D	39	ALA	2.4
3	C	15	GLN	2.4
3	C	95	GLY	2.4
5	L	34	GLY	2.4
5	L	50	ASP	2.4
1	G	188	VAL	2.4
4	E	92	LYS	2.4
2	B	52	TRP	2.4
2	H	2	THR	2.4
4	K	25	PRO	2.4
1	G	148	TYR	2.3
1	A	25	ALA	2.3
1	G	203	ALA	2.3
3	C	12	LEU	2.3
2	H	127	GLY	2.3
3	C	129	SER	2.3
3	C	131	ILE	2.3
3	I	53	SER	2.3
4	E	98	ILE	2.3
1	A	43	VAL	2.3
1	G	43	VAL	2.3
1	A	137	PRO	2.3
1	G	125	THR	2.3
4	D	26	THR	2.3
4	J	39	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
5	F	79	TYR	2.3
2	B	68	GLY	2.3
3	I	69	GLY	2.3
4	K	43	SER	2.3
3	I	5	ILE	2.3
4	E	101	VAL	2.3
3	I	65	GLN	2.3
4	E	25	PRO	2.3
3	C	192	CYS	2.3
3	C	98	ALA	2.3
4	E	40	ALA	2.3
3	C	143	ARG	2.3
3	I	37	GLY	2.3
1	A	184	VAL	2.3
3	C	194	PRO	2.3
3	C	116	ASN	2.3
2	H	46	ARG	2.3
1	G	131	LEU	2.3
1	G	89	TYR	2.3
3	C	42	GLN	2.2
3	C	47	GLN	2.2
1	A	97	PHE	2.2
3	C	83	ARG	2.2
3	C	118	ARG	2.2
4	D	58	ARG	2.2
2	B	199	CYS	2.2
3	I	51	GLY	2.2
4	J	38	GLY	2.2
2	H	142	TYR	2.2
1	G	171	THR	2.2
4	K	106	LYS	2.2
5	F	20	LYS	2.2
3	C	26	GLY	2.2
3	C	33	ALA	2.2
3	I	98	ALA	2.2
4	K	37	LEU	2.2
5	F	87	LEU	2.2
1	G	8	TYR	2.2
1	A	159	THR	2.2
4	J	110	PRO	2.2
4	D	2	VAL	2.2
4	D	23	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	77	ALA	2.2
3	C	11	ALA	2.2
2	B	47	HIS	2.2
3	C	96	GLN	2.2
4	D	29	LEU	2.2
1	G	168	SER	2.2
1	G	234	SER	2.2
2	H	1	SER	2.2
5	F	43	SER	2.2
1	G	194	MET	2.2
3	C	76	PRO	2.1
2	H	7	ILE	2.1
4	E	50	PHE	2.1
3	C	36	ARG	2.1
3	C	186	LEU	2.1
4	E	31	CYS	2.1
1	A	208	SER	2.1
1	G	59	TYR	2.1
3	C	85	THR	2.1
3	I	8	PRO	2.1
5	L	82	THR	2.1
4	E	86	GLN	2.1
1	G	235	PHE	2.1
1	G	51	VAL	2.1
1	G	147	VAL	2.1
2	H	47	HIS	2.1
4	D	53	GLY	2.1
3	C	99	ALA	2.1
1	G	52	SER	2.1
2	B	198	LEU	2.1
4	E	103	CYS	2.1
4	E	9	THR	2.1
1	A	146	ARG	2.1
3	C	37	GLY	2.1
3	I	46	ARG	2.1
1	G	50	PHE	2.1
3	I	86	PHE	2.1
4	K	39	ALA	2.1
1	G	180	SER	2.1
4	E	18	MET	2.1
5	F	48	GLU	2.1
1	A	95	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	20	GLN	2.1
1	G	60	THR	2.1
4	K	14	THR	2.1
5	F	82	THR	2.1
3	I	10	LYS	2.1
3	I	91	ILE	2.1
2	B	80	PHE	2.1
1	G	100	ALA	2.1
1	G	195	ALA	2.1
1	A	68	MET	2.0
4	K	6	LEU	2.0
4	E	10	ASN	2.0
1	A	109	ASP	2.0
1	G	142	ARG	2.0
1	A	145	THR	2.0
1	G	4	PRO	2.0
5	L	3	PRO	2.0
3	C	58	TYR	2.0
3	C	174	TYR	2.0
4	E	36	LYS	2.0
3	C	77	GLY	2.0
5	L	79	TYR	2.0
1	G	187	ILE	2.0
4	E	7	VAL	2.0
4	D	87	LEU	2.0
1	G	201	CYS	2.0
4	D	31	CYS	2.0
3	I	72	LYS	2.0
2	H	37	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 ⓘ

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(Å ²)	Q<0.9
6	GOL	A	301	6/6	0.49	0.27	91,91,91,91	0
6	GOL	H	202	6/6	0.64	0.16	96,97,97,97	0
6	GOL	J	201	6/6	0.75	0.22	93,93,94,94	0
6	GOL	D	201	6/6	0.76	0.21	86,86,87,87	0
6	GOL	B	201	6/6	0.79	0.25	111,111,111,111	0
6	GOL	B	203	6/6	0.81	0.16	81,82,83,83	0
6	GOL	B	202	6/6	0.83	0.26	95,96,97,97	0
6	GOL	H	201	6/6	0.87	0.19	81,81,82,82	0
6	GOL	F	101	6/6	0.88	0.18	99,99,100,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.