



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:33 PM UTC

PDB ID : 5YP4 / pdb_00005yp4
Title : Crystal structure of dipeptidyl peptidase IV (DPP IV) with Lys-Pro from Pseudoxanthomonas mexicana WO24
Authors : Roppongi, S.; Suzuki, Y.; Tateoka, C.; Fuimoto, M.; Morisawa, S.; Iizuka, I.; Nakamura, A.; Honma, N.; Shida, Y.; Ogasawara, W.; Tanaka, N.; Sakamoto, Y.; Nonaka, T.
Deposited on : 2017-11-01
Resolution : 1.90 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

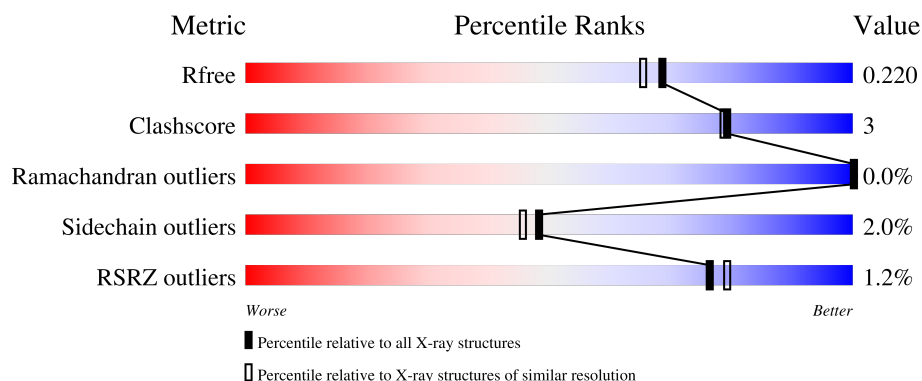
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	745	88% 9% • •
1	B	745	90% 6% • •
1	C	745	2% 85% 6% • 8%
1	D	745	89% 6% • •

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	B	807	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25338 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 Dipeptidyl aminopeptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	724	Total	C	N	O	S	0	0	0
			5660	3580	994	1076	10			
1	B	724	Total	C	N	O	S	0	0	0
			5660	3580	994	1076	10			
1	C	687	Total	C	N	O	S	0	1	0
			5379	3419	937	1013	10			
1	D	714	Total	C	N	O	S	0	0	0
			5571	3523	981	1057	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	ILE	MET	see sequence details	UNP Q6F3I7
B	12	ILE	MET	see sequence details	UNP Q6F3I7
C	12	ILE	MET	see sequence details	UNP Q6F3I7
D	12	ILE	MET	see sequence details	UNP Q6F3I7

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



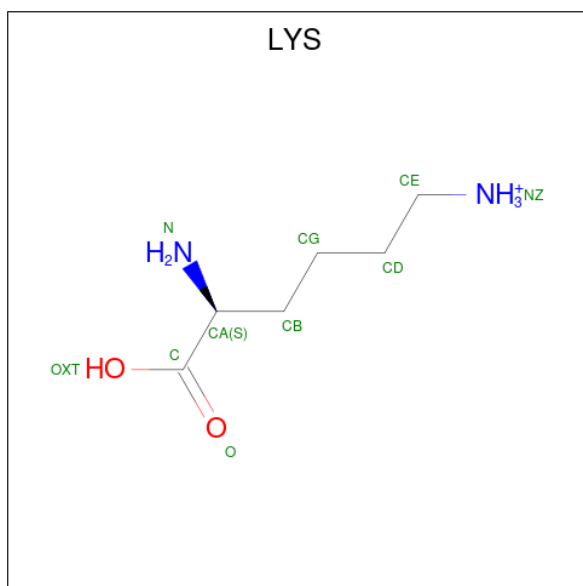
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total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

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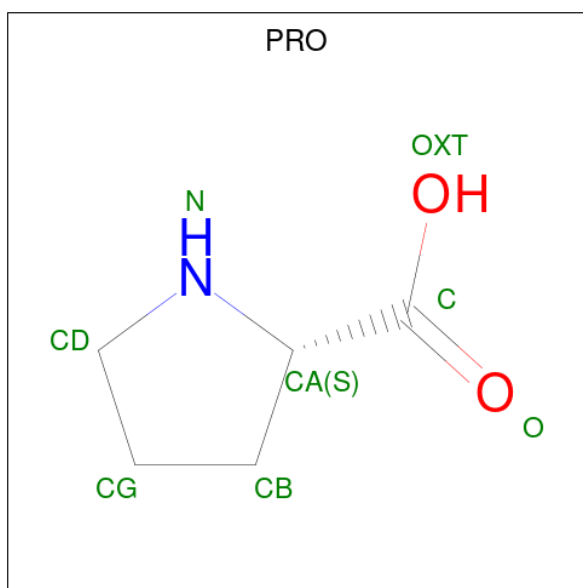
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is LYSINE (CCD ID: LYS) (formula: $C_6H_{15}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	6	2	1		
3	B	1	Total	C	N	O	0	0
			9	6	2	1		
3	C	1	Total	C	N	O	0	0
			9	6	2	1		
3	D	1	Total	C	N	O	0	0
			9	6	2	1		

- Molecule 4 is PROLINE (CCD ID: PRO) (formula: $C_5H_9NO_2$).



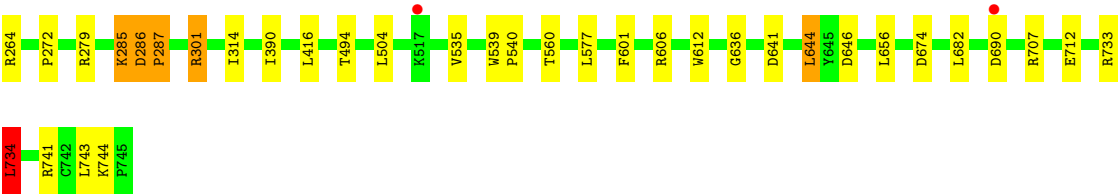
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			7	5	1	1		
4	B	1	Total	C	N	O	0	0
			7	5	1	1		
4	C	1	Total	C	N	O	0	0
			8	5	1	2		
4	D	1	Total	C	N	O	0	0
			7	5	1	1		

- Molecule 5 is water.

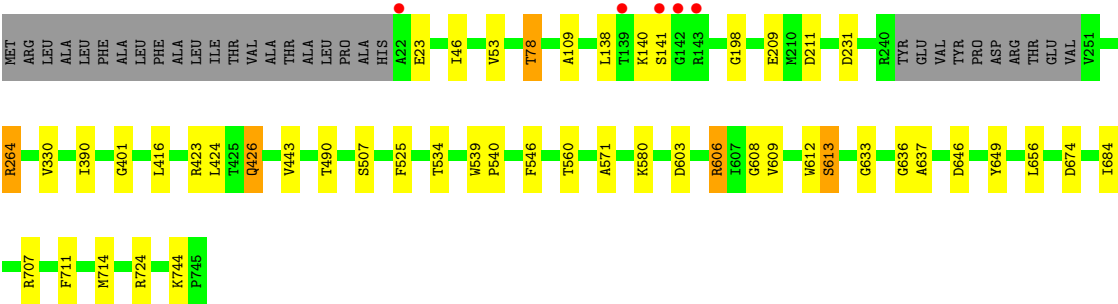
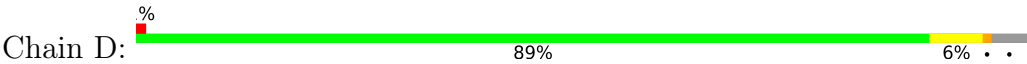
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	817	Total	O	0	0
			817	817		
5	B	685	Total	O	0	0
			685	685		
5	C	611	Total	O	0	0
			611	611		
5	D	764	Total	O	0	0
			764	764		

- Molecule 1: Dipeptidyl aminopeptidase 4





● Molecule 1: Dipeptidyl aminopeptidase 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	88.66Å 104.49Å 112.84Å 67.42° 68.83° 65.46°	Depositor
Resolution (Å)	40.00 – 1.90 40.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.2 (40.00-1.90) 94.2 (40.00-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.164 , 0.213 0.174 , 0.220	Depositor DCC
R_{free} test set	12223 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	16.8	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for h,h-k,h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25338	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.77% 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 [i](#)

5.1 Standard geometry [i](#)

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	1.30	15/5799 (0.3%)	1.10	5/7887 (0.1%)
1	B	1.22	3/5799 (0.1%)	1.09	7/7887 (0.1%)
1	C	1.23	6/5515 (0.1%)	1.09	6/7501 (0.1%)
1	D	1.24	5/5706 (0.1%)	1.10	8/7757 (0.1%)
All	All	1.25	29/22819 (0.1%)	1.10	26/31032 (0.1%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	255	TYR	C-O	-6.78	1.18	1.24
1	C	744	LYS	C-O	6.28	1.26	1.23
1	A	606	ARG	CD-NE	-6.15	1.37	1.46
1	B	256	PRO	CA-C	6.03	1.58	1.52
1	A	494	THR	CA-C	-6.02	1.45	1.52
1	C	287	PRO	C-O	6.01	1.32	1.24
1	D	53	VAL	CA-CB	-5.83	1.47	1.54
1	A	272	PRO	CA-C	5.82	1.58	1.52
1	A	507	SER	C-O	5.78	1.31	1.23
1	A	523	VAL	N-CA	5.64	1.53	1.46
1	B	362	GLU	CA-C	5.58	1.60	1.52
1	A	350	GLY	C-O	-5.46	1.16	1.24
1	A	386	SER	C-O	-5.41	1.17	1.23
1	D	608	GLY	N-CA	5.33	1.50	1.44
1	D	606	ARG	CD-NE	-5.28	1.38	1.46
1	A	730	HIS	C-O	5.26	1.30	1.24
1	A	633	GLY	C-O	5.26	1.29	1.24
1	A	296	TRP	N-CA	5.22	1.52	1.46
1	A	541	GLY	C-O	5.22	1.31	1.23
1	C	158	ASP	CA-C	-5.18	1.50	1.53
1	A	636	GLY	CA-C	-5.14	1.48	1.52
1	A	158	ASP	CA-CB	5.14	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	711	PHE	CA-C	-5.13	1.46	1.52
1	B	561	LEU	C-O	-5.09	1.18	1.23
1	C	301	ARG	CD-NE	-5.07	1.39	1.46
1	C	272	PRO	CA-C	5.07	1.57	1.52
1	D	198	GLY	CA-C	-5.04	1.48	1.52
1	C	734	LEU	CA-C	5.03	1.59	1.52
1	A	473	VAL	CA-C	5.03	1.60	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	606	ARG	NE-CZ-NH2	-8.06	111.94	119.20
1	C	286	ASP	CA-C-N	6.99	126.69	119.56
1	C	286	ASP	C-N-CA	6.99	126.69	119.56
1	B	584	VAL	N-CA-CB	-6.79	102.97	110.51
1	A	606	ARG	NE-CZ-NH1	6.55	128.06	121.50
1	D	78	THR	CB-CA-C	6.29	120.69	109.38
1	B	724	ARG	NE-CZ-NH1	-6.20	115.30	121.50
1	D	656	LEU	N-CA-C	6.15	117.64	109.83
1	D	606	ARG	NE-CZ-NH2	-6.14	113.67	119.20
1	A	590	LEU	CD1-CG-CD2	5.79	123.53	110.80
1	A	543	SER	N-CA-C	-5.72	98.62	110.80
1	C	601	PHE	N-CA-C	5.62	119.77	113.02
1	B	256	PRO	CB-CA-C	-5.47	107.28	111.87
1	D	330	VAL	CB-CA-C	-5.43	101.25	111.30
1	B	78	THR	CB-CA-C	5.34	119.49	109.71
1	C	242	GLU	N-CA-C	5.33	117.76	108.76
1	C	301	ARG	NE-CZ-NH2	-5.24	114.48	119.20
1	B	75	SER	N-CA-C	5.23	119.37	112.89
1	A	590	LEU	CA-CB-CG	-5.16	98.25	116.30
1	B	584	VAL	N-CA-C	5.15	115.77	110.36
1	D	401	GLY	N-CA-C	5.15	118.99	110.55
1	D	606	ARG	NE-CZ-NH1	5.13	126.63	121.50
1	D	571	ALA	N-CA-C	5.07	116.88	111.36
1	B	557	VAL	N-CA-C	-5.06	102.33	109.21
1	C	167	PHE	N-CA-C	5.05	116.86	109.24
1	D	264	ARG	NE-CZ-NH2	5.01	123.71	119.20

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	5660	0	5521	40	0
1	B	5660	0	5521	27	0
1	C	5379	0	5251	31	0
1	D	5571	0	5441	22	0
2	A	24	0	32	3	0
2	B	60	0	80	5	0
2	C	12	0	16	1	0
2	D	30	0	40	0	0
3	A	9	0	12	0	0
3	B	9	0	12	0	0
3	C	9	0	12	0	0
3	D	9	0	12	0	0
4	A	7	0	7	0	0
4	B	7	0	7	0	0
4	C	8	0	7	0	0
4	D	7	0	7	0	0
5	A	817	0	0	10	0
5	B	685	0	0	5	0
5	C	611	0	0	8	0
5	D	764	0	0	5	0
All	All	25338	0	21978	121	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 3.

All (121) 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:744:LYS:HB2	5:A:1318:HOH:O	1.18	1.29
1:D:744:LYS:HB2	5:D:1357:HOH:O	1.20	1.27
1:D:211:ASP:HB2	5:D:1501:HOH:O	1.53	1.07
1:A:744:LYS:CB	5:A:1318:HOH:O	1.84	0.91
1:A:648:HIS:HD2	1:A:652:ARG:HH21	1.20	0.88
1:A:22:ALA:N	5:A:901:HOH:O	2.06	0.88
1:C:712:GLU:OE2	1:C:741[B]:ARG:NH2	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:ASP:OD2	1:A:606:ARG:HD3	1.80	0.82
1:A:648:HIS:CD2	1:A:652:ARG:HH21	1.98	0.81
1:D:525:PHE:O	1:D:560:THR:HG23	1.83	0.77
1:B:648:HIS:HD2	1:B:652:ARG:HH21	1.34	0.75
1:D:674:ASP:OD1	1:D:707:ARG:NH1	2.20	0.74
1:B:109:ALA:HB2	1:B:724:ARG:HD3	1.70	0.74
1:B:277:ARG:NH1	5:B:902:HOH:O	2.23	0.70
1:B:648:HIS:CD2	1:B:652:ARG:HH21	2.11	0.69
1:B:293:ARG:HD2	2:B:808:GOL:H11	1.73	0.69
1:A:62:ASP:OD1	5:A:902:HOH:O	2.12	0.68
1:A:175:ASN:HD21	1:A:193:GLY:H	1.39	0.68
1:A:307:GLN:NE2	1:A:648:HIS:HE1	1.95	0.64
1:D:109:ALA:HB2	1:D:724:ARG:HD2	1.81	0.63
1:B:293:ARG:HD2	2:B:808:GOL:C1	2.30	0.61
1:A:109:ALA:HB3	2:A:803:GOL:H31	1.83	0.60
1:D:744:LYS:CB	5:D:1357:HOH:O	2.03	0.59
1:A:603:ASP:OD2	1:A:606:ARG:CD	2.50	0.59
1:C:641:ASP:O	1:C:644:LEU:HD12	2.04	0.58
1:A:744:LYS:CG	5:A:1318:HOH:O	2.34	0.57
1:B:603:ASP:OD2	1:B:606:ARG:HD3	2.05	0.57
1:D:603:ASP:OD2	1:D:606:ARG:HD3	2.04	0.57
1:B:70:GLU:OE2	1:B:79:ARG:NH1	2.39	0.56
1:B:201:VAL:HB	2:B:811:GOL:H32	1.86	0.56
1:A:307:GLN:HE22	1:A:648:HIS:HE1	1.52	0.56
1:C:690:ASP:HB3	5:C:1343:HOH:O	2.06	0.55
1:A:34:ALA:HB1	1:A:35:PRO:HD2	1.87	0.55
1:A:606:ARG:HD2	5:A:974:HOH:O	2.07	0.55
1:B:211:ASP:HB2	5:B:1341:HOH:O	2.06	0.55
1:C:208:GLU:OE1	5:C:901:HOH:O	2.18	0.55
1:A:670:PHE:CZ	1:A:699:LYS:HG2	2.42	0.54
1:C:149:LEU:HB3	1:C:179:ILE:HD13	1.90	0.54
1:B:42:THR:HG23	1:B:43:LYS:HG3	1.89	0.53
1:B:46:ILE:HD11	1:B:443:VAL:HG23	1.90	0.53
1:C:204:PHE:CE1	1:C:208:GLU:HG3	2.44	0.53
1:A:279:ARG:NH2	1:A:321:LEU:O	2.42	0.53
1:B:744:LYS:HB2	1:C:285:LYS:HD3	1.91	0.52
1:B:298:ASP:HB2	1:B:299:PRO:CD	2.40	0.52
1:B:307:GLN:OE1	1:B:648:HIS:HE1	1.92	0.51
2:B:811:GOL:H11	5:B:1114:HOH:O	2.11	0.51
1:C:612:TRP:CE3	1:C:636:GLY:HA3	2.46	0.51
1:D:231:ASP:HB3	1:D:264:ARG:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:GLN:HE21	1:C:253:GLN:HE21	1.60	0.49
1:C:88:LEU:HD11	1:C:129:LEU:HD13	1.95	0.49
1:B:42:THR:HG22	1:B:56:LEU:HB2	1.95	0.49
1:C:238:GLN:HE21	1:C:253:GLN:NE2	2.10	0.49
1:D:46:ILE:HD11	1:D:443:VAL:HG23	1.94	0.49
1:A:648:HIS:HD2	1:A:652:ARG:NH2	2.01	0.48
1:C:264:ARG:NH2	1:C:287:PRO:HB3	2.28	0.48
1:C:494:THR:HA	1:C:504:LEU:O	2.14	0.47
1:A:603:ASP:CG	1:A:606:ARG:HD3	2.38	0.47
1:D:423:ARG:NH2	1:D:426:GLN:NE2	2.62	0.47
1:A:613:SER:HA	1:A:637:ALA:O	2.15	0.47
1:B:390:ILE:HD11	1:B:416:LEU:HD21	1.96	0.47
1:B:209:GLU:CD	1:B:649:TYR:HB2	2.40	0.47
1:C:535:VAL:HG22	1:C:560:THR:HG23	1.96	0.47
1:C:734:LEU:HD13	5:C:913:HOH:O	2.14	0.46
1:A:107:ILE:HA	2:A:803:GOL:H32	1.97	0.46
1:A:539:TRP:CD2	1:A:540:PRO:HD2	2.50	0.46
1:C:28:GLU:OE2	1:C:733:ARG:NH2	2.49	0.46
1:C:734:LEU:HD22	5:D:1286:HOH:O	2.15	0.46
1:D:209:GLU:CD	1:D:649:TYR:HB2	2.41	0.46
1:B:733:ARG:HD2	5:B:1187:HOH:O	2.15	0.46
1:C:656:LEU:HB3	5:C:1340:HOH:O	2.16	0.46
1:B:312:LYS:O	1:B:333:THR:HA	2.15	0.46
1:C:674:ASP:OD1	1:C:707:ARG:NE	2.45	0.46
1:A:109:ALA:CB	2:A:803:GOL:H31	2.44	0.45
1:D:534:THR:HB	1:D:560:THR:HG21	1.98	0.45
1:B:374:LEU:HD11	5:B:931:HOH:O	2.16	0.45
1:B:449:ASP:OD2	2:B:810:GOL:O1	2.30	0.45
2:C:803:GOL:H32	5:C:1389:HOH:O	2.16	0.45
1:C:237:VAL:CG1	1:C:252:GLU:HG3	2.47	0.45
1:D:613:SER:HA	1:D:637:ALA:O	2.17	0.45
1:C:52:ARG:HD3	1:C:70:GLU:OE1	2.17	0.45
1:D:612:TRP:CE3	1:D:636:GLY:HA3	2.52	0.45
1:C:390:ILE:CD1	1:C:416:LEU:HD21	2.46	0.44
1:C:577:LEU:C	1:C:577:LEU:HD12	2.41	0.44
1:B:609:VAL:O	1:B:633:GLY:HA2	2.17	0.44
1:C:644:LEU:HD23	5:C:1344:HOH:O	2.17	0.44
1:A:353:LEU:HD11	1:A:390:ILE:HG12	2.00	0.44
1:A:537:ARG:NE	5:A:910:HOH:O	2.42	0.43
1:A:494:THR:HA	1:A:504:LEU:O	2.18	0.43
1:A:61:ARG:HG2	5:A:1245:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:534:THR:OG1	1:D:560:THR:CG2	2.67	0.43
1:C:286:ASP:HA	1:C:287:PRO:HD2	1.88	0.43
1:A:42:THR:HG22	1:A:56:LEU:HB2	2.01	0.43
1:C:539:TRP:CD2	1:C:540:PRO:HD2	2.54	0.42
1:A:78:THR:HG21	5:A:1311:HOH:O	2.19	0.42
1:C:682:LEU:HD21	1:C:734:LEU:HD12	2.02	0.42
1:A:209:GLU:OE2	1:A:646:ASP:OD2	2.38	0.42
1:B:495:LEU:C	1:B:495:LEU:HD12	2.45	0.42
1:C:191:ARG:NH2	5:C:929:HOH:O	2.52	0.42
1:A:46:ILE:HD11	1:A:443:VAL:HG23	2.02	0.42
1:D:609:VAL:O	1:D:633:GLY:HA2	2.20	0.42
1:C:741[A]:ARG:NH2	5:C:913:HOH:O	2.42	0.41
1:A:307:GLN:HE22	1:A:648:HIS:CE1	2.35	0.41
1:A:535:VAL:HG22	1:A:560:THR:HG23	2.01	0.41
1:A:684:ILE:HA	1:A:714:MET:O	2.19	0.41
1:D:534:THR:OG1	1:D:560:THR:HG22	2.20	0.41
1:A:614:ASN:ND2	5:A:943:HOH:O	2.53	0.41
1:A:34:ALA:HB1	1:A:35:PRO:CD	2.50	0.41
1:A:612:TRP:CE3	1:A:636:GLY:HA3	2.56	0.41
1:D:490:THR:CG2	1:D:507:SER:HB2	2.50	0.41
1:B:703:GLU:OE2	1:B:707:ARG:NE	2.47	0.41
1:D:580:LYS:HE2	5:D:1304:HOH:O	2.19	0.41
1:D:539:TRP:CD2	1:D:540:PRO:HD2	2.55	0.41
1:B:290:TYR:HB2	1:B:307:GLN:HB3	2.02	0.41
1:C:159:PRO:HA	1:C:169:SER:O	2.20	0.41
1:D:140:LYS:O	1:D:141:SER:C	2.63	0.41
1:D:684:ILE:HA	1:D:714:MET:O	2.20	0.41
1:A:566:THR:HB	1:A:567:PRO:HD2	2.03	0.40
1:B:533:GLN:OE1	1:B:568:ARG:HD3	2.21	0.40
1:A:533:GLN:OE1	1:A:568:ARG:HD3	2.22	0.40
1:C:606:ARG:HD2	1:C:743:LEU:O	2.22	0.40
1:A:506:TYR:CD1	1:A:506:TYR:C	3.00	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	722/745 (97%)	697 (96%)	25 (4%)	0	100	100
1	B	722/745 (97%)	694 (96%)	28 (4%)	0	100	100
1	C	676/745 (91%)	655 (97%)	21 (3%)	0	100	100
1	D	710/745 (95%)	685 (96%)	24 (3%)	1 (0%)	48	40
All	All	2830/2980 (95%)	2731 (96%)	98 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	613	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	587/602 (98%)	574 (98%)	13 (2%)	45	42
1	B	587/602 (98%)	573 (98%)	14 (2%)	43	38
1	C	558/602 (93%)	547 (98%)	11 (2%)	48	46
1	D	577/602 (96%)	568 (98%)	9 (2%)	55	54
All	All	2309/2408 (96%)	2262 (98%)	47 (2%)	48	46

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	ILE
1	A	78	THR
1	A	79	ARG
1	A	141	SER
1	A	143	ARG

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Mol	Chain	Res	Type
1	A	144	ASP
1	A	251	VAL
1	A	273	LYS
1	A	390	ILE
1	A	416	LEU
1	A	425	THR
1	A	546	PHE
1	A	744	LYS
1	B	28	GLU
1	B	42	THR
1	B	46	ILE
1	B	78	THR
1	B	191	ARG
1	B	277	ARG
1	B	374	LEU
1	B	416	LEU
1	B	424	LEU
1	B	426	GLN
1	B	470	VAL
1	B	546	PHE
1	B	580	LYS
1	B	584	VAL
1	C	114	VAL
1	C	191	ARG
1	C	238	GLN
1	C	252	GLU
1	C	279	ARG
1	C	285	LYS
1	C	301	ARG
1	C	314	ILE
1	C	644	LEU
1	C	646	ASP
1	C	734	LEU
1	D	23	GLU
1	D	78	THR
1	D	138	LEU
1	D	390	ILE
1	D	416	LEU
1	D	424	LEU
1	D	426	GLN
1	D	546	PHE
1	D	646	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	175	ASN
1	A	262	ASN
1	A	300	GLN
1	A	307	GLN
1	A	342	ASN
1	A	426	GLN
1	A	554	GLN
1	A	614	ASN
1	A	648	HIS
1	A	691	ASN
1	A	705	GLN
1	B	45	GLN
1	B	64	ASN
1	B	300	GLN
1	B	326	GLN
1	B	342	ASN
1	B	426	GLN
1	B	519	GLN
1	B	614	ASN
1	B	648	HIS
1	C	45	GLN
1	C	64	ASN
1	C	238	GLN
1	C	253	GLN
1	C	261	HIS
1	C	262	ASN
1	C	548	ASN
1	C	599	GLN
1	D	151	ASN
1	D	199	ASN
1	D	266	GLN
1	D	300	GLN
1	D	426	GLN
1	D	548	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

29 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	B	812	-	5,5,5	0.27	0	5,5,5	0.98	0
2	GOL	B	803	-	5,5,5	0.29	0	5,5,5	1.37	1 (20%)
2	GOL	A	805	-	5,5,5	1.17	0	5,5,5	0.82	0
2	GOL	B	808	-	5,5,5	0.31	0	5,5,5	1.23	1 (20%)
2	GOL	B	811	-	5,5,5	0.49	0	5,5,5	1.92	2 (40%)
3	LYS	A	801	4	7,8,9	0.67	0	3,8,10	0.76	0
2	GOL	D	803	-	5,5,5	0.24	0	5,5,5	0.26	0
2	GOL	A	804	-	5,5,5	0.48	0	5,5,5	1.20	0
3	LYS	D	801	4	7,8,9	0.53	0	3,8,10	0.84	0
4	PRO	C	802	3	8,8,8	0.91	1 (12%)	10,10,10	1.46	1 (10%)
3	LYS	C	801	4	7,8,9	0.72	0	3,8,10	0.59	0
2	GOL	B	807	-	5,5,5	1.00	0	5,5,5	2.34	3 (60%)
2	GOL	B	805	-	5,5,5	0.32	0	5,5,5	1.00	0
2	GOL	A	803	-	5,5,5	0.55	0	5,5,5	0.68	0
2	GOL	C	803	-	5,5,5	0.73	0	5,5,5	0.58	0
2	GOL	B	806	-	5,5,5	0.70	0	5,5,5	1.49	1 (20%)
2	GOL	C	804	-	5,5,5	0.42	0	5,5,5	0.83	0
4	PRO	A	802	1,3	6,7,8	0.65	0	7,8,10	1.78	1 (14%)
2	GOL	B	809	-	5,5,5	0.15	0	5,5,5	0.56	0
2	GOL	D	807	-	5,5,5	0.33	0	5,5,5	0.56	0
2	GOL	D	804	-	5,5,5	0.87	0	5,5,5	1.36	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PRO	D	802	1,3	6,7,8	0.67	0	7,8,10	2.41	1 (14%)
4	PRO	B	802	1,3	6,7,8	0.91	1 (16%)	7,8,10	2.02	1 (14%)
2	GOL	B	804	-	5,5,5	0.44	0	5,5,5	0.61	0
2	GOL	D	805	-	5,5,5	0.46	0	5,5,5	0.81	0
2	GOL	B	810	-	5,5,5	0.35	0	5,5,5	0.44	0
3	LYS	B	801	4	7,8,9	0.50	0	3,8,10	0.73	0
2	GOL	D	806	-	5,5,5	0.42	0	5,5,5	0.41	0
2	GOL	A	806	-	5,5,5	0.37	0	5,5,5	0.51	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	GOL	B	812	-	-	2/4/4/4	-
2	GOL	B	803	-	-	2/4/4/4	-
2	GOL	A	805	-	-	1/4/4/4	-
2	GOL	B	808	-	-	0/4/4/4	-
2	GOL	B	811	-	-	0/4/4/4	-
3	LYS	A	801	4	-	0/6/7/9	-
2	GOL	D	803	-	-	4/4/4/4	-
2	GOL	A	804	-	-	1/4/4/4	-
3	LYS	D	801	4	-	0/6/7/9	-
4	PRO	C	802	3	-	0/4/11/11	0/1/1/1
3	LYS	C	801	4	-	0/6/7/9	-
2	GOL	B	807	-	-	4/4/4/4	-
2	GOL	B	805	-	-	2/4/4/4	-
2	GOL	A	803	-	-	3/4/4/4	-
2	GOL	C	803	-	-	0/4/4/4	-
2	GOL	B	806	-	-	2/4/4/4	-
2	GOL	C	804	-	-	2/4/4/4	-
4	PRO	A	802	1,3	-	0/0/9/11	0/1/1/1
2	GOL	B	809	-	-	3/4/4/4	-
2	GOL	D	807	-	-	3/4/4/4	-
2	GOL	D	804	-	-	2/4/4/4	-
4	PRO	D	802	1,3	-	0/0/9/11	0/1/1/1
4	PRO	B	802	1,3	-	0/0/9/11	0/1/1/1
2	GOL	B	804	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	D	805	-	-	2/4/4/4	-
2	GOL	B	810	-	-	2/4/4/4	-
3	LYS	B	801	4	-	0/6/7/9	-
2	GOL	D	806	-	-	1/4/4/4	-
2	GOL	A	806	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	802	PRO	CA-N	-2.11	1.45	1.48
4	C	802	PRO	OXT-C	-2.10	1.24	1.30

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	802	PRO	CB-CA-C	-6.21	104.13	112.66
4	B	802	PRO	CB-CA-C	-5.09	105.67	112.66
4	A	802	PRO	CB-CA-C	-4.29	106.77	112.66
2	B	807	GOL	O3-C3-C2	-3.73	93.59	110.38
4	C	802	PRO	OXT-C-O	-3.15	116.93	124.08
2	B	811	GOL	C3-C2-C1	-2.90	101.16	111.80
2	D	804	GOL	O2-C2-C3	-2.69	98.03	109.18
2	B	808	GOL	O1-C1-C2	2.63	122.23	110.38
2	B	806	GOL	O3-C3-C2	2.52	121.74	110.38
2	B	807	GOL	C3-C2-C1	-2.34	103.22	111.80
2	B	807	GOL	O2-C2-C1	2.32	118.78	109.18
2	B	811	GOL	O2-C2-C1	2.29	118.68	109.18
2	B	803	GOL	O1-C1-C2	-2.03	101.22	110.38

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	806	GOL	O1-C1-C2-C3
2	B	803	GOL	C1-C2-C3-O3
2	B	803	GOL	O2-C2-C3-O3
2	B	804	GOL	O1-C1-C2-C3
2	B	807	GOL	O1-C1-C2-C3
2	B	809	GOL	O1-C1-C2-O2
2	B	809	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	B	812	GOL	C1-C2-C3-O3
2	C	804	GOL	O1-C1-C2-C3
2	D	804	GOL	C1-C2-C3-O3
2	D	807	GOL	C1-C2-C3-O3
2	B	805	GOL	O2-C2-C3-O3
2	B	806	GOL	O2-C2-C3-O3
2	A	803	GOL	O1-C1-C2-C3
2	B	805	GOL	C1-C2-C3-O3
2	B	806	GOL	C1-C2-C3-O3
2	B	807	GOL	C1-C2-C3-O3
2	B	810	GOL	O1-C1-C2-C3
2	D	803	GOL	O1-C1-C2-C3
2	D	803	GOL	C1-C2-C3-O3
2	D	805	GOL	O1-C1-C2-C3
2	A	806	GOL	O1-C1-C2-O2
2	B	804	GOL	O1-C1-C2-O2
2	B	807	GOL	O1-C1-C2-O2
2	B	807	GOL	O2-C2-C3-O3
2	B	810	GOL	O1-C1-C2-O2
2	D	803	GOL	O2-C2-C3-O3
2	D	804	GOL	O2-C2-C3-O3
2	D	807	GOL	O2-C2-C3-O3
2	B	812	GOL	O2-C2-C3-O3
2	C	804	GOL	O1-C1-C2-O2
2	D	805	GOL	O1-C1-C2-O2
2	A	804	GOL	O2-C2-C3-O3
2	A	803	GOL	O1-C1-C2-O2
2	A	803	GOL	C1-C2-C3-O3
2	A	805	GOL	O1-C1-C2-C3
2	B	809	GOL	C1-C2-C3-O3
2	D	803	GOL	O1-C1-C2-O2
2	D	807	GOL	O1-C1-C2-O2
2	D	806	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	808	GOL	2	0
2	B	811	GOL	2	0
2	A	803	GOL	3	0
2	C	803	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	810	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	724/745 (97%)	-0.33	8 (1%) 78 80	9, 18, 35, 79	0
1	B	724/745 (97%)	-0.18	6 (0%) 82 85	11, 21, 39, 70	0
1	C	687/745 (92%)	-0.10	16 (2%) 61 65	11, 20, 46, 75	1 (0%)
1	D	714/745 (95%)	-0.33	5 (0%) 84 86	9, 19, 37, 79	0
All	All	2849/2980 (95%)	-0.24	35 (1%) 76 79	9, 20, 40, 79	1 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	745	PRO	5.0
1	A	745	PRO	4.8
1	A	241	TYR	4.7
1	C	250	VAL	4.1
1	C	241	TYR	3.9
1	B	152	GLY	3.6
1	C	251	VAL	3.5
1	D	142	GLY	3.2
1	C	145	ALA	3.2
1	C	136	TYR	3.1
1	B	22	ALA	2.9
1	A	141	SER	2.8
1	C	155	PHE	2.7
1	A	22	ALA	2.6
1	C	22	ALA	2.6
1	C	238	GLN	2.6
1	B	151	ASN	2.6
1	C	40	THR	2.6
1	A	142	GLY	2.5
1	C	248	THR	2.5
1	D	139	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	517	LYS	2.5
1	C	62	ASP	2.4
1	B	241	TYR	2.3
1	A	243	VAL	2.3
1	C	88	LEU	2.3
1	B	142	GLY	2.3
1	D	22	ALA	2.2
1	D	141	SER	2.2
1	C	237	VAL	2.2
1	C	125	LEU	2.2
1	A	144	ASP	2.2
1	A	245	PRO	2.2
1	C	690	ASP	2.1
1	D	143	ARG	2.1

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 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
2	GOL	B	806	6/6	0.78	0.19	47,48,56,59	0
2	GOL	B	805	6/6	0.81	0.16	39,47,51,58	0
2	GOL	A	803	6/6	0.81	0.14	27,35,54,54	0
2	GOL	B	807	6/6	0.82	0.13	25,28,32,36	0
2	GOL	B	809	6/6	0.84	0.15	40,50,54,57	0
2	GOL	B	803	6/6	0.85	0.14	39,41,46,47	0
2	GOL	B	810	6/6	0.85	0.15	32,44,50,53	0
2	GOL	C	804	6/6	0.86	0.12	38,41,45,49	0
2	GOL	D	806	6/6	0.87	0.14	32,34,36,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	B	804	6/6	0.89	0.13	30,33,36,37	0
2	GOL	D	804	6/6	0.89	0.12	26,28,37,44	0
2	GOL	D	805	6/6	0.89	0.12	43,50,51,54	0
2	GOL	B	808	6/6	0.89	0.15	37,48,51,52	0
3	LYS	C	801	9/10	0.89	0.12	18,25,36,38	0
2	GOL	B	812	6/6	0.90	0.10	32,36,37,38	0
2	GOL	A	804	6/6	0.91	0.10	32,34,37,41	0
2	GOL	A	806	6/6	0.91	0.12	38,42,46,52	0
2	GOL	B	811	6/6	0.92	0.14	23,29,33,38	0
4	PRO	C	802	8/8	0.92	0.08	19,21,22,23	0
4	PRO	A	802	7/8	0.93	0.08	14,14,15,16	0
2	GOL	D	803	6/6	0.93	0.11	23,35,40,47	0
2	GOL	D	807	6/6	0.94	0.09	29,36,39,45	0
2	GOL	C	803	6/6	0.94	0.08	21,24,28,30	0
3	LYS	D	801	9/10	0.95	0.09	14,15,24,27	0
3	LYS	A	801	9/10	0.95	0.09	16,16,27,28	0
2	GOL	A	805	6/6	0.95	0.07	19,21,22,22	0
4	PRO	D	802	7/8	0.96	0.06	13,14,15,16	0
3	LYS	B	801	9/10	0.97	0.07	15,18,34,39	0
4	PRO	B	802	7/8	0.97	0.05	14,15,16,16	0

6.5 Other polymers

There are no such residues in this entry.