



Full wwPDB X-ray Structure Validation Report i

Nov 14, 2023 – 01:31 AM JST

PDB ID : 5YP1
Title : Crystal structure of dipeptidyl peptidase IV (DPP IV) 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 : 2.47 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 i 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

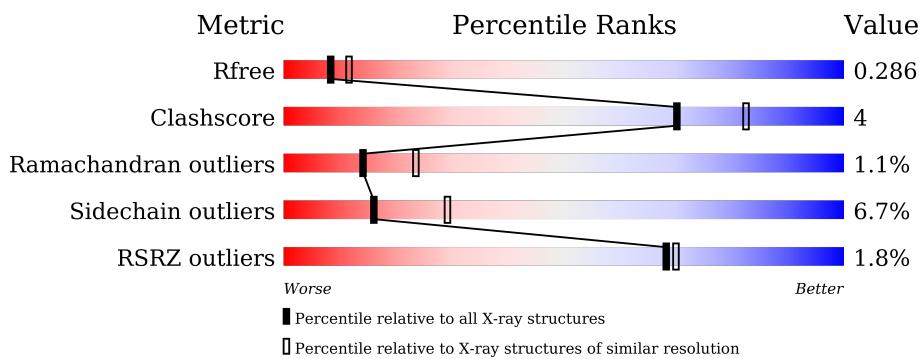
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

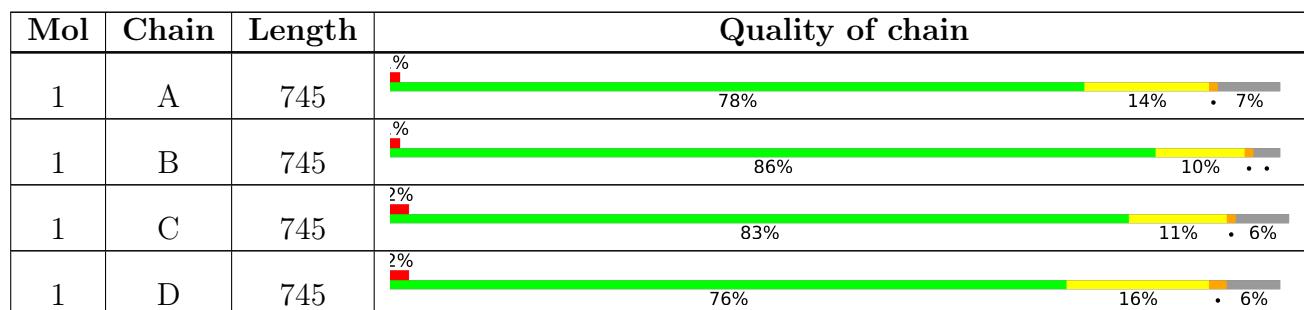
The reported resolution of this entry is 2.47 Å.

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}	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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 <=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.



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 22690 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.

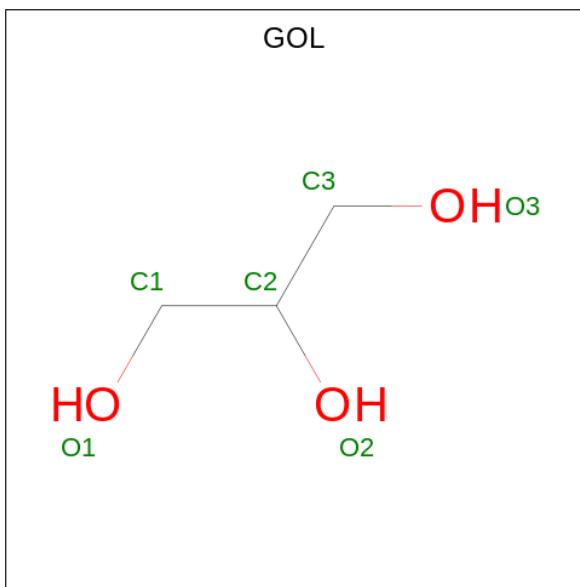
- Molecule 1 is a protein called Dipeptidyl aminopeptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	695	5426	3445	943	1028	10	0	0	0
1	B	724	5660	3580	994	1076	10	0	0	0
1	C	704	5497	3485	960	1042	10	0	0	0
1	D	703	5492	3482	959	1041	10	0	0	0

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 (three-letter code: GOL) (formula: C₃H₈O₃).



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

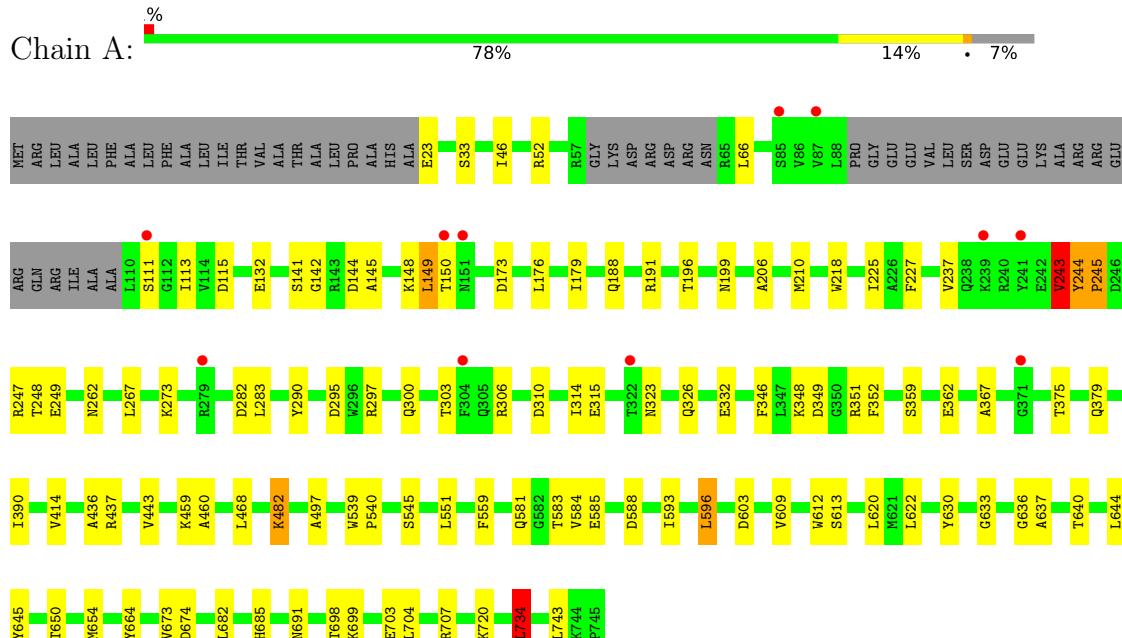
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	100	Total O 100 100	0	0
3	B	221	Total O 221 221	0	0
3	C	190	Total O 190 190	0	0
3	D	98	Total O 98 98	0	0

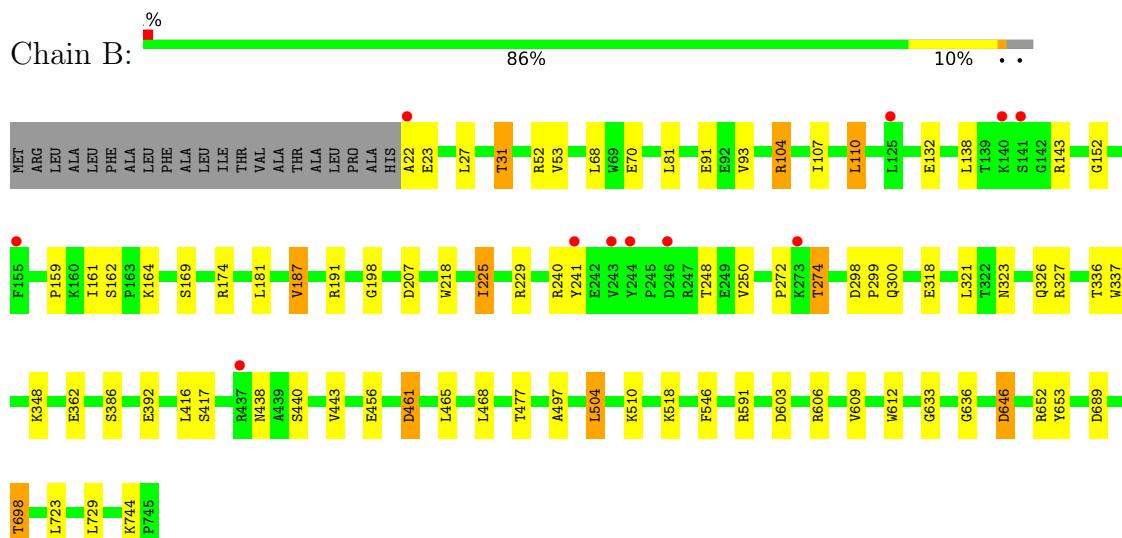
3 Residue-property plots [\(i\)](#)

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.

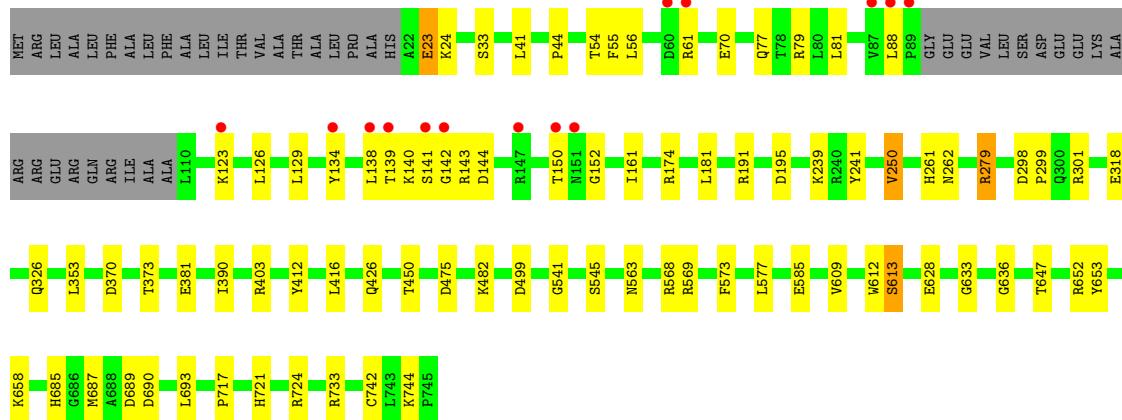
- Molecule 1: Dipeptidyl aminopeptidase 4



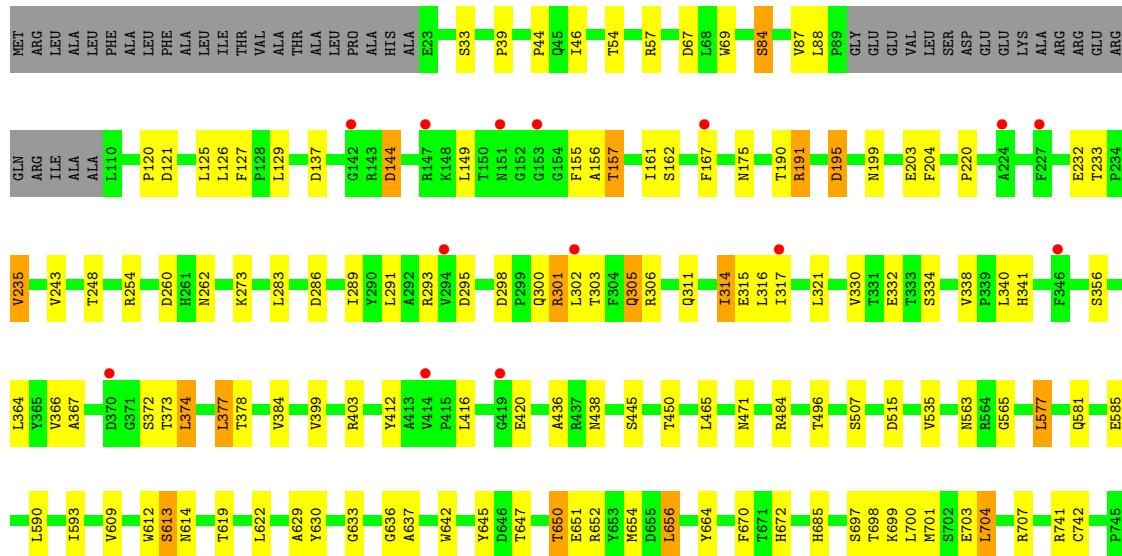
- Molecule 1: Dipeptidyl aminopeptidase 4



- Molecule 1: Dipeptidyl aminopeptidase 4



- Molecule 1: Dipeptidyl aminopeptidase 4



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	149.73Å 326.19Å 71.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.47 55.15 – 2.47	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-2.47) 99.8 (55.15-2.47)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	2.07 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R , R_{free}	0.217 , 0.284 0.223 , 0.286	Depositor DCC
R_{free} test set	6289 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.4	EDS
L-test for twinning ²	$< L > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22690	wwPDB-VP
Average B, all atoms (Å ²)	45.0	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 20.36 % 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 8.8489e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $< |L| >$, $< L^2 >$ 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	0.66	0/5562	0.85	3/7569 (0.0%)
1	B	0.74	1/5799 (0.0%)	0.89	6/7887 (0.1%)
1	C	0.75	0/5635	0.88	6/7668 (0.1%)
1	D	0.66	0/5630	0.85	2/7661 (0.0%)
All	All	0.70	1/22626 (0.0%)	0.87	17/30785 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	417	SER	CB-OG	-5.67	1.34	1.42

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	734	LEU	CA-CB-CG	6.78	130.90	115.30
1	B	689	ASP	CB-CG-OD1	6.64	124.27	118.30
1	B	174	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	C	733	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	243	VAL	C-N-CA	5.69	135.92	121.70
1	C	499	ASP	CB-CG-OD1	5.66	123.39	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	568	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	C	370	ASP	CB-CG-OD1	5.49	123.24	118.30
1	D	191	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	B	327	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	D	484	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	C	279	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	646	ASP	CB-CA-C	-5.20	100.01	110.40
1	A	603	ASP	CB-CG-OD1	5.19	122.97	118.30
1	C	174	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	B	174	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	240	ARG	NE-CZ-NH2	-5.05	117.77	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	243	VAL	Peptide
1	B	22	ALA	Peptide

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 MolProbit. 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	5426	0	5289	44	0
1	B	5660	0	5520	34	0
1	C	5497	0	5358	28	0
1	D	5492	0	5353	54	0
2	B	6	0	8	1	0
3	A	100	0	0	0	0
3	B	221	0	0	2	0
3	C	190	0	0	2	0
3	D	98	0	0	0	0
All	All	22690	0	21528	156	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 4.

All (156) 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:C:262:ASN:OD1	1:C:647:THR:HG21	1.84	0.78
1:A:46:ILE:HD11	1:A:443:VAL:HG23	1.72	0.70
1:D:367:ALA:HB2	1:D:374:LEU:HD12	1.75	0.69
1:B:31:THR:HG21	1:B:729:LEU:HB2	1.76	0.66
1:D:593:ILE:HD11	1:D:630:TYR:CZ	2.31	0.65
1:A:243:VAL:HG11	1:A:249:GLU:N	2.12	0.65
1:A:612:TRP:CE3	1:A:636:GLY:HA3	2.33	0.64
1:D:609:VAL:HG13	1:D:619:THR:HG23	1.80	0.63
1:C:612:TRP:CE3	1:C:636:GLY:HA3	2.34	0.62
1:B:510:LYS:NZ	1:C:381:GLU:OE1	2.32	0.62
1:A:243:VAL:HG21	1:A:248:THR:HG23	1.81	0.62
1:D:306:ARG:NH2	1:D:315:GLU:OE1	2.33	0.62
1:A:314:ILE:HG13	1:A:332:GLU:HB2	1.82	0.61
1:A:245:PRO:O	1:B:698:THR:CG2	2.49	0.60
1:C:123:LYS:HA	1:C:138:LEU:HD12	1.84	0.60
1:B:187:VAL:HG23	1:B:274:THR:HG23	1.84	0.59
1:A:243:VAL:HG11	1:A:249:GLU:H	1.68	0.58
1:D:314:ILE:HG22	1:D:332:GLU:HB2	1.84	0.58
1:D:88:LEU:HD11	1:D:129:LEU:HD23	1.87	0.57
1:D:612:TRP:CE3	1:D:636:GLY:HA3	2.41	0.56
1:C:70:GLU:OE1	1:C:81:LEU:HD13	2.06	0.56
1:A:46:ILE:HG21	1:A:436:ALA:HB2	1.89	0.55
1:B:438:ASN:ND2	1:B:440:SER:OG	2.40	0.55
1:B:104:ARG:HG2	1:B:207:ASP:HB3	1.86	0.55
1:D:232:GLU:O	1:D:235:VAL:HG13	2.07	0.55
1:A:539:TRP:CD2	1:A:540:PRO:HD2	2.41	0.55
1:A:645:TYR:O	1:A:650:THR:OG1	2.23	0.54
1:D:127:PHE:HB3	1:D:129:LEU:HD13	1.89	0.54
1:D:637:ALA:HA	1:D:685:HIS:CD2	2.42	0.54
1:D:565:GLY:HA3	1:D:577:LEU:HD13	1.89	0.54
1:C:652:ARG:HD2	1:C:653:TYR:CZ	2.43	0.54
1:D:156:ALA:O	1:D:157:THR:HG23	2.08	0.54
1:A:243:VAL:HG12	1:A:244:TYR:HD2	1.73	0.53
1:B:107:ILE:HB	1:B:110:LEU:HD22	1.90	0.53
1:A:314:ILE:HD11	1:A:332:GLU:CG	2.39	0.52
1:D:203:GLU:O	1:D:204:PHE:C	2.47	0.52
1:A:581:GLN:N	1:A:654:MET:HE1	2.24	0.52
1:B:362:GLU:CG	3:B:995:HOH:O	2.56	0.52
1:B:132:GLU:OE2	1:B:152:GLY:HA2	2.09	0.52
1:B:386:SER:HA	2:B:801:GOL:H11	1.92	0.52
1:A:262:ASN:ND2	1:A:290:TYR:OH	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ASP:HB3	1:A:326:GLN:HE22	1.75	0.51
1:A:227:PHE:O	1:A:267:LEU:HD12	2.11	0.51
1:B:603:ASP:OD2	1:B:606:ARG:HD3	2.11	0.51
1:C:77:GLN:NE2	1:C:79:ARG:HD3	2.25	0.51
1:C:318:GLU:O	1:C:326:GLN:HA	2.10	0.51
1:D:593:ILE:HD13	1:D:629:ALA:HB1	1.92	0.51
1:C:44:PRO:HA	1:C:54:THR:O	2.10	0.51
1:D:289:ILE:HD12	1:D:289:ILE:O	2.10	0.51
1:D:46:ILE:HG21	1:D:436:ALA:HB2	1.93	0.50
1:A:188:GLN:HE21	1:A:191:ARG:HA	1.76	0.50
1:A:148:LYS:HB3	1:A:179:ILE:HD13	1.92	0.50
1:B:27:LEU:O	1:B:31:THR:HB	2.12	0.50
1:B:612:TRP:CE3	1:B:636:GLY:HA3	2.46	0.49
1:A:176:LEU:HD21	1:A:225:ILE:HG21	1.93	0.49
1:A:23:GLU:HA	1:A:482:LYS:O	2.12	0.49
1:D:195:ASP:N	1:D:195:ASP:OD1	2.46	0.49
1:C:77:GLN:HE21	1:C:79:ARG:HD3	1.78	0.48
1:A:559:PHE:CD2	1:A:596:LEU:HD21	2.48	0.48
1:C:41:LEU:HD22	1:C:55:PHE:CG	2.48	0.48
1:C:353:LEU:HD11	1:C:390:ILE:HD13	1.96	0.48
1:B:318:GLU:O	1:B:326:GLN:HA	2.13	0.48
1:B:652:ARG:HD2	1:B:653:TYR:CZ	2.49	0.48
1:C:241:TYR:CD2	1:C:250:VAL:HG12	2.49	0.48
1:D:316:LEU:HB3	1:D:330:VAL:HG12	1.96	0.48
1:A:609:VAL:O	1:A:633:GLY:HA2	2.13	0.48
1:D:609:VAL:O	1:D:633:GLY:HA2	2.14	0.47
1:D:175:ASN:HA	1:D:199:ASN:HD22	1.79	0.47
1:D:295:ASP:O	1:D:303:THR:HB	2.13	0.47
1:A:132:GLU:OE1	1:A:149:LEU:HD23	2.15	0.47
1:D:235:VAL:O	1:D:254:ARG:NH1	2.48	0.47
1:D:384:VAL:HG13	1:D:399:VAL:HB	1.97	0.47
1:D:332:GLU:OE2	1:D:356:SER:HB2	2.15	0.47
1:B:159:PRO:HA	1:B:169:SER:O	2.14	0.47
1:B:362:GLU:HG3	3:B:995:HOH:O	2.15	0.47
1:D:403:ARG:HB3	1:D:412:TYR:CZ	2.50	0.47
1:B:70:GLU:HB3	1:B:81:LEU:HD11	1.97	0.47
1:B:606:ARG:NH2	1:B:744:LYS:O	2.48	0.47
1:C:129:LEU:HD12	1:C:134:TYR:CD1	2.50	0.47
1:A:497:ALA:HB1	1:A:588:ASP:OD1	2.15	0.46
1:D:126:LEU:HB2	1:D:161:ILE:HD11	1.96	0.46
1:A:637:ALA:HA	1:A:685:HIS:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ILE:HD11	1:A:332:GLU:HG3	1.97	0.46
1:C:687:MET:HE3	1:C:717:PRO:N	2.30	0.46
1:B:104:ARG:HG2	1:B:207:ASP:CB	2.46	0.46
1:B:609:VAL:O	1:B:633:GLY:HA2	2.15	0.46
1:C:563:ASN:ND2	1:C:585:GLU:HB2	2.31	0.46
1:D:698:THR:O	1:D:701:MET:HB2	2.16	0.46
1:B:298:ASP:HB2	1:B:299:PRO:HD2	1.98	0.45
1:D:654:MET:HB3	1:D:664:TYR:CE1	2.50	0.45
1:A:297:ARG:HA	1:A:346:PHE:CD2	2.51	0.45
1:A:243:VAL:HG11	1:A:248:THR:HA	1.98	0.45
1:A:682:LEU:HD21	1:A:734:LEU:HD12	1.99	0.45
1:D:298:ASP:OD2	1:D:301:ARG:NE	2.34	0.45
1:A:654:MET:HB3	1:A:664:TYR:CE1	2.52	0.45
1:A:218:TRP:CZ2	1:A:225:ILE:HD11	2.52	0.45
1:C:239:LYS:HA	3:C:812:HOH:O	2.16	0.45
1:A:188:GLN:NE2	1:A:191:ARG:HA	2.33	0.44
1:A:622:LEU:HB3	1:A:630:TYR:CE2	2.53	0.44
1:D:262:ASN:HD21	1:D:647:THR:HG21	1.82	0.44
1:A:352:PHE:CE1	1:A:367:ALA:HB3	2.52	0.44
1:B:241:TYR:HA	1:B:250:VAL:HA	1.98	0.44
1:D:613:SER:OG	1:D:614:ASN:N	2.49	0.44
1:D:651:GLU:OE1	1:D:656:LEU:HD22	2.17	0.44
1:C:298:ASP:OD1	1:C:301:ARG:N	2.51	0.44
1:C:475:ASP:OD1	1:C:475:ASP:C	2.56	0.44
1:D:670:PHE:CZ	1:D:699:LYS:HG2	2.52	0.44
1:B:612:TRP:CH2	1:B:723:LEU:HD13	2.52	0.44
1:B:218:TRP:CE3	1:B:225:ILE:HG22	2.53	0.43
1:C:261:HIS:HB3	3:C:974:HOH:O	2.17	0.43
1:C:609:VAL:O	1:C:633:GLY:HA2	2.19	0.43
1:D:507:SER:HB3	1:D:535:VAL:HG13	2.01	0.43
1:B:53:VAL:HG11	1:B:443:VAL:HG21	2.01	0.43
1:C:628:GLU:H	1:C:628:GLU:CD	2.20	0.43
1:D:162:SER:HB2	1:D:167:PHE:HB2	2.00	0.43
1:C:403:ARG:HB3	1:C:412:TYR:CZ	2.54	0.43
1:D:565:GLY:CA	1:D:577:LEU:HD13	2.48	0.43
1:B:336:THR:OG1	1:B:337:TRP:N	2.52	0.43
1:D:44:PRO:HA	1:D:54:THR:O	2.19	0.42
1:D:67:ASP:OD1	1:D:84:SER:HB3	2.19	0.42
1:D:642:TRP:O	1:D:650:THR:HG21	2.20	0.42
1:D:703:GLU:OE1	1:D:707:ARG:NH1	2.46	0.42
1:A:703:GLU:OE1	1:A:707:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:ASP:HB2	1:B:299:PRO:CD	2.50	0.42
1:D:311:GLN:NE2	1:D:652:ARG:HG3	2.34	0.42
1:C:23:GLU:HA	1:C:482:LYS:O	2.19	0.42
1:D:88:LEU:CD1	1:D:129:LEU:HD23	2.49	0.42
1:D:137:ASP:N	1:D:144:ASP:OD2	2.52	0.42
1:D:314:ILE:HB	1:D:338:VAL:HG21	2.02	0.42
1:B:198:GLY:O	1:B:229:ARG:HA	2.19	0.42
1:A:245:PRO:HA	1:B:698:THR:HG23	2.01	0.42
1:A:593:ILE:HD11	1:A:630:TYR:CE1	2.55	0.42
1:C:298:ASP:HB2	1:C:299:PRO:HD2	2.01	0.42
1:D:235:VAL:HG22	1:D:254:ARG:HD2	2.01	0.42
1:D:293:ARG:HB2	1:D:305:GLN:NE2	2.35	0.42
1:D:57:ARG:HB3	1:D:69:TRP:CD1	2.55	0.41
1:A:149:LEU:HD22	1:A:149:LEU:N	2.34	0.41
1:A:237:VAL:O	1:A:237:VAL:HG23	2.20	0.41
1:C:569:ARG:HB2	1:C:573:PHE:CD1	2.56	0.41
1:A:66:LEU:HD12	1:A:113:ILE:O	2.20	0.41
1:B:348:LYS:N	1:B:392:GLU:OE2	2.52	0.41
1:C:689:ASP:OD2	1:C:721:HIS:HA	2.20	0.41
1:D:367:ALA:CB	1:D:374:LEU:HD12	2.48	0.41
1:A:306:ARG:NH2	1:A:315:GLU:OE1	2.49	0.41
1:D:39:PRO:HD2	1:D:471:ASN:OD1	2.21	0.41
1:D:175:ASN:OD1	1:D:199:ASN:ND2	2.54	0.41
1:D:364:LEU:N	1:D:378:THR:OG1	2.44	0.41
1:A:583:THR:OG1	1:A:584:VAL:N	2.54	0.41
1:C:126:LEU:HB2	1:C:161:ILE:HD11	2.02	0.41
1:D:190:THR:OG1	1:D:199:ASN:ND2	2.53	0.41
1:B:161:ILE:HG22	1:B:162:SER:N	2.37	0.40
1:D:366:VAL:HG12	1:D:377:LEU:HD11	2.03	0.40
1:B:497:ALA:HB2	1:B:504:LEU:CD1	2.51	0.40
1:D:700:LEU:HG	1:D:704:LEU:HD22	2.02	0.40
1:A:245:PRO:O	1:B:698:THR:HG22	2.22	0.40
1:A:206:ALA:HB2	1:A:210:MET:CE	2.52	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	689/745 (92%)	623 (90%)	56 (8%)	10 (2%)	10 16
1	B	722/745 (97%)	672 (93%)	46 (6%)	4 (1%)	25 40
1	C	700/745 (94%)	657 (94%)	36 (5%)	7 (1%)	15 26
1	D	699/745 (94%)	631 (90%)	59 (8%)	9 (1%)	12 19
All	All	2810/2980 (94%)	2583 (92%)	197 (7%)	30 (1%)	14 23

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	SER
1	A	244	TYR
1	A	323	ASN
1	B	646	ASP
1	C	150	THR
1	A	142	GLY
1	A	145	ALA
1	A	613	SER
1	B	461	ASP
1	C	141	SER
1	C	613	SER
1	D	87	VAL
1	D	149	LEU
1	A	245	PRO
1	A	351	ARG
1	C	140	LYS
1	D	120	PRO
1	D	233	THR
1	D	372	SER
1	D	445	SER
1	A	674	ASP
1	D	144	ASP

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Mol	Chain	Res	Type
1	D	291	LEU
1	A	460	ALA
1	B	23	GLU
1	B	272	PRO
1	C	142	GLY
1	C	541	GLY
1	D	220	PRO
1	C	152	GLY

5.3.2 Protein sidechains [\(i\)](#)

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	564/602 (94%)	519 (92%)	45 (8%)	12 21
1	B	587/602 (98%)	557 (95%)	30 (5%)	24 42
1	C	571/602 (95%)	543 (95%)	28 (5%)	25 44
1	D	571/602 (95%)	521 (91%)	50 (9%)	10 18
All	All	2293/2408 (95%)	2140 (93%)	153 (7%)	16 29

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	SER
1	A	52	ARG
1	A	115	ASP
1	A	141	SER
1	A	144	ASP
1	A	149	LEU
1	A	150	THR
1	A	173	ASP
1	A	196	THR
1	A	199	ASN
1	A	243	VAL
1	A	247	ARG
1	A	273	LYS

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Mol	Chain	Res	Type
1	A	283	LEU
1	A	295	ASP
1	A	300	GLN
1	A	303	THR
1	A	310	ASP
1	A	348	LYS
1	A	349	ASP
1	A	359	SER
1	A	362	GLU
1	A	375	THR
1	A	379	GLN
1	A	390	ILE
1	A	414	VAL
1	A	437	ARG
1	A	459	LYS
1	A	468	LEU
1	A	482	LYS
1	A	545	SER
1	A	551	LEU
1	A	585	GLU
1	A	596	LEU
1	A	620	LEU
1	A	640	THR
1	A	644	LEU
1	A	673	VAL
1	A	691	ASN
1	A	698	THR
1	A	699	LYS
1	A	704	LEU
1	A	720	LYS
1	A	734	LEU
1	A	743	LEU
1	B	31	THR
1	B	52	ARG
1	B	68	LEU
1	B	91	GLU
1	B	93	VAL
1	B	104	ARG
1	B	110	LEU
1	B	138	LEU
1	B	143	ARG
1	B	164	LYS

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Mol	Chain	Res	Type
1	B	181	LEU
1	B	187	VAL
1	B	191	ARG
1	B	225	ILE
1	B	248	THR
1	B	274	THR
1	B	300	GLN
1	B	321	LEU
1	B	323	ASN
1	B	416	LEU
1	B	456	GLU
1	B	461	ASP
1	B	465	LEU
1	B	468	LEU
1	B	477	THR
1	B	504	LEU
1	B	518	LYS
1	B	546	PHE
1	B	591	ARG
1	B	698	THR
1	C	23	GLU
1	C	24	LYS
1	C	33	SER
1	C	56	LEU
1	C	61	ARG
1	C	88	LEU
1	C	139	THR
1	C	143	ARG
1	C	144	ASP
1	C	181	LEU
1	C	191	ARG
1	C	195	ASP
1	C	250	VAL
1	C	279	ARG
1	C	373	THR
1	C	416	LEU
1	C	426	GLN
1	C	450	THR
1	C	545	SER
1	C	577	LEU
1	C	613	SER
1	C	658	LYS

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Mol	Chain	Res	Type
1	C	685	HIS
1	C	690	ASP
1	C	693	LEU
1	C	724	ARG
1	C	742	CYS
1	C	744	LYS
1	D	33	SER
1	D	84	SER
1	D	121	ASP
1	D	125	LEU
1	D	155	PHE
1	D	157	THR
1	D	191	ARG
1	D	195	ASP
1	D	235	VAL
1	D	243	VAL
1	D	248	THR
1	D	260	ASP
1	D	273	LYS
1	D	283	LEU
1	D	286	ASP
1	D	300	GLN
1	D	301	ARG
1	D	302	LEU
1	D	305	GLN
1	D	314	ILE
1	D	317	ILE
1	D	321	LEU
1	D	334	SER
1	D	340	LEU
1	D	341	HIS
1	D	373	THR
1	D	374	LEU
1	D	377	LEU
1	D	416	LEU
1	D	420	GLU
1	D	438	ASN
1	D	450	THR
1	D	465	LEU
1	D	496	THR
1	D	515	ASP
1	D	563	ASN

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Mol	Chain	Res	Type
1	D	577	LEU
1	D	581	GLN
1	D	585	GLU
1	D	590	LEU
1	D	613	SER
1	D	622	LEU
1	D	645	TYR
1	D	650	THR
1	D	656	LEU
1	D	672	HIS
1	D	697	SER
1	D	704	LEU
1	D	741	ARG
1	D	742	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	262	ASN
1	A	305	GLN
1	A	326	GLN
1	A	548	ASN
1	A	554	GLN
1	A	685	HIS
1	B	305	GLN
1	B	438	ASN
1	C	77	GLN
1	C	253	GLN
1	C	266	GLN
1	D	77	GLN
1	D	199	ASN
1	D	305	GLN
1	D	311	GLN
1	D	326	GLN
1	D	438	ASN
1	D	548	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	B	801	-	5,5,5	0.86	0	5,5,5	1.66	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	B	801	-	-	4/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	GOL	C3-C2-C1	2.13	120.00	111.70

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	GOL	O1-C1-C2-C3
2	B	801	GOL	O1-C1-C2-O2
2	B	801	GOL	C1-C2-C3-O3
2	B	801	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	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 i

6.1 Protein, DNA and RNA chains i

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	695/745 (93%)	-0.08	11 (1%) 72 73	27, 51, 79, 117	0
1	B	724/745 (97%)	-0.22	11 (1%) 73 75	13, 32, 65, 110	0
1	C	704/745 (94%)	-0.24	14 (1%) 65 67	15, 31, 75, 140	0
1	D	703/745 (94%)	0.07	14 (1%) 65 67	28, 55, 84, 117	0
All	All	2826/2980 (94%)	-0.12	50 (1%) 68 70	13, 44, 79, 140	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	22	ALA	11.4
1	C	150	THR	8.0
1	D	153	GLY	7.2
1	A	371	GLY	5.5
1	B	141	SER	5.0
1	A	150	THR	4.6
1	B	246	ASP	4.2
1	C	138	LEU	4.2
1	A	151	ASN	3.7
1	D	414	VAL	3.5
1	C	60	ASP	3.5
1	A	241	TYR	3.5
1	D	151	ASN	3.5
1	C	141	SER	3.4
1	C	151	ASN	3.2
1	D	227	PHE	3.0
1	C	123	LYS	2.9
1	D	419	GLY	2.8
1	C	88	LEU	2.8
1	D	346	PHE	2.8
1	B	241	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	89	PRO	2.6
1	B	243	VAL	2.6
1	D	294	VAL	2.5
1	B	155	PHE	2.5
1	C	87	VAL	2.5
1	A	322	THR	2.5
1	A	279	ARG	2.4
1	C	139	THR	2.4
1	A	111	SER	2.4
1	A	304	PHE	2.4
1	B	140	LYS	2.4
1	C	147	ARG	2.4
1	D	142	GLY	2.3
1	D	224	ALA	2.3
1	D	147	ARG	2.3
1	B	125	LEU	2.3
1	B	244	TYR	2.3
1	A	239	LYS	2.2
1	D	317	ILE	2.2
1	B	437	ARG	2.2
1	C	142	GLY	2.2
1	A	87	VAL	2.2
1	A	85	SER	2.2
1	B	273	LYS	2.2
1	C	134	TYR	2.2
1	C	61	ARG	2.1
1	D	167	PHE	2.1
1	D	370	ASP	2.1
1	D	302	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides 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
2	GOL	B	801	6/6	0.90	0.14	39,47,49,52	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.