



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:29 PM UTC

PDB ID : 5YP1 / pdb_00005yp1
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 ⓘ 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

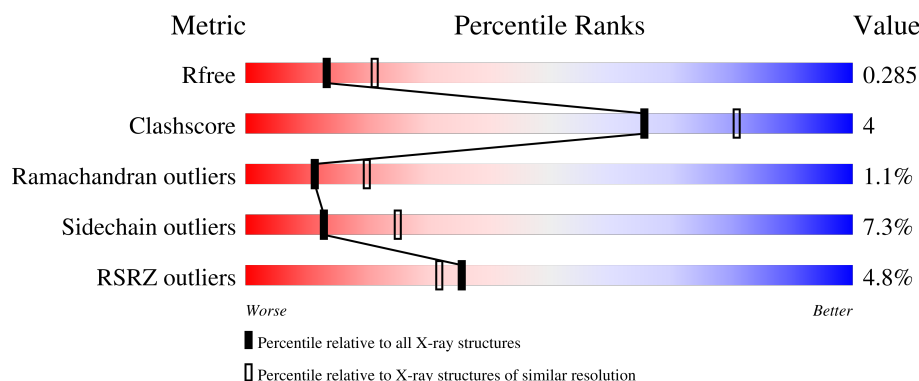
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (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 $\leq 5\%$. 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	5% 76% 16% • 7%
1	B	745	2% 85% 11% • •
1	C	745	3% 83% 11% • 6%
1	D	745	8% 75% 16% • 6%

2 Entry composition

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
1	A	695	Total	C	N	O	S	0	0	0
			5426	3445	943	1028	10			
1	B	724	Total	C	N	O	S	0	0	0
			5660	3580	994	1076	10			
1	C	704	Total	C	N	O	S	0	0	0
			5497	3485	960	1042	10			
1	D	703	Total	C	N	O	S	0	0	0
			5492	3482	959	1041	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	B	1	Total	C	O	0	0
			6	3	3		

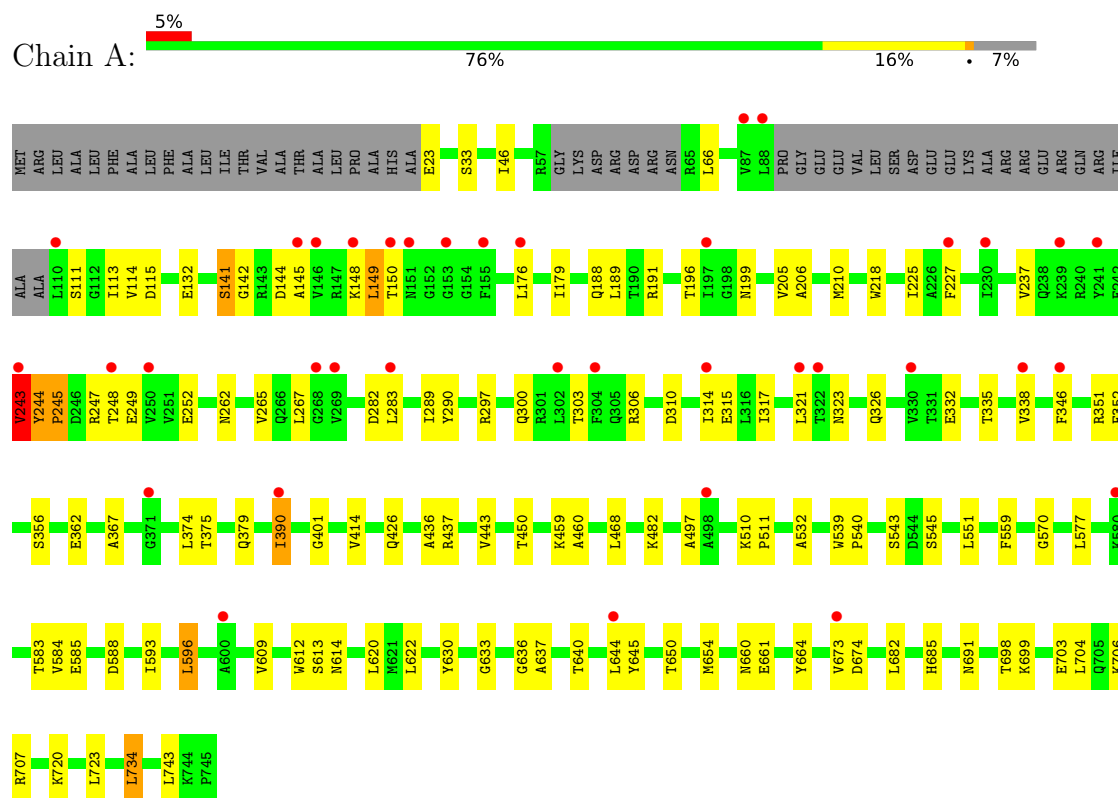
- Molecule 3 is water.

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

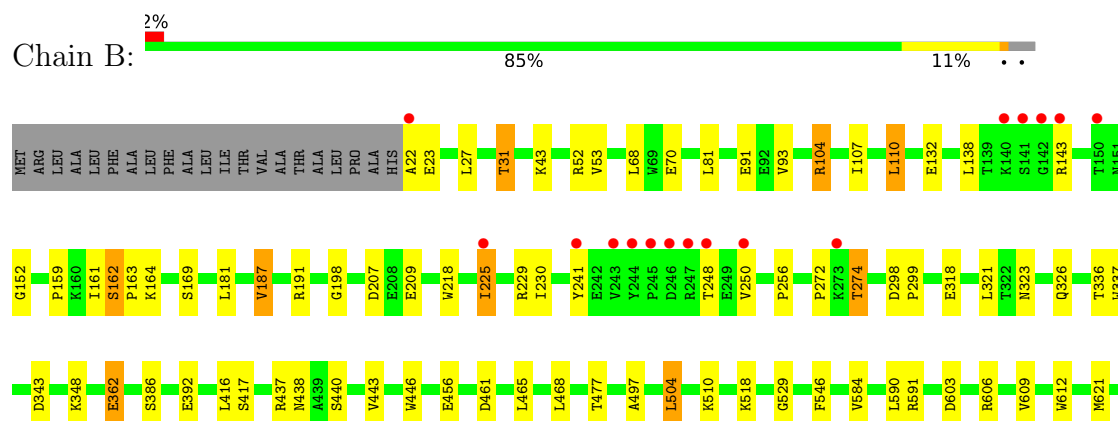
3 Residue-property plots

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: Dipeptidyl aminopeptidase 4

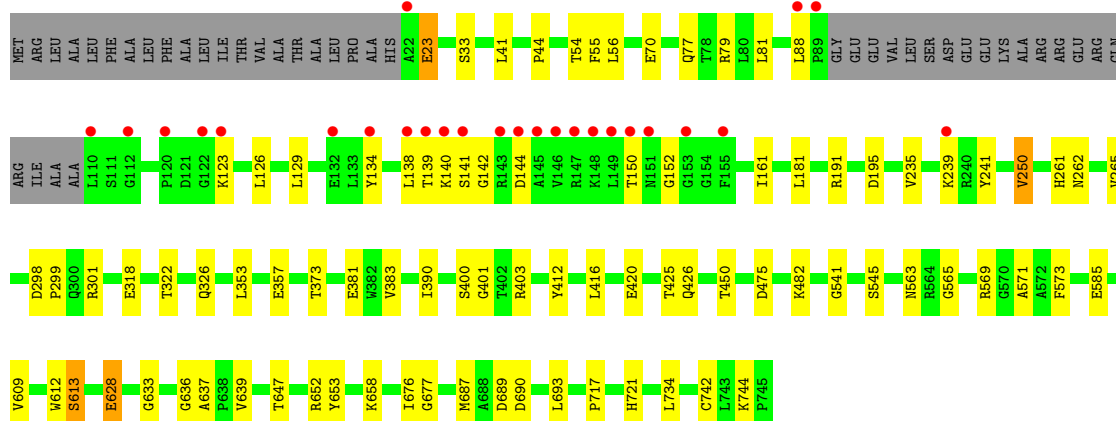
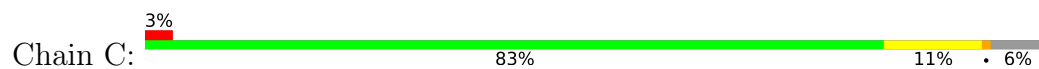


• Molecule 1: Dipeptidyl aminopeptidase 4

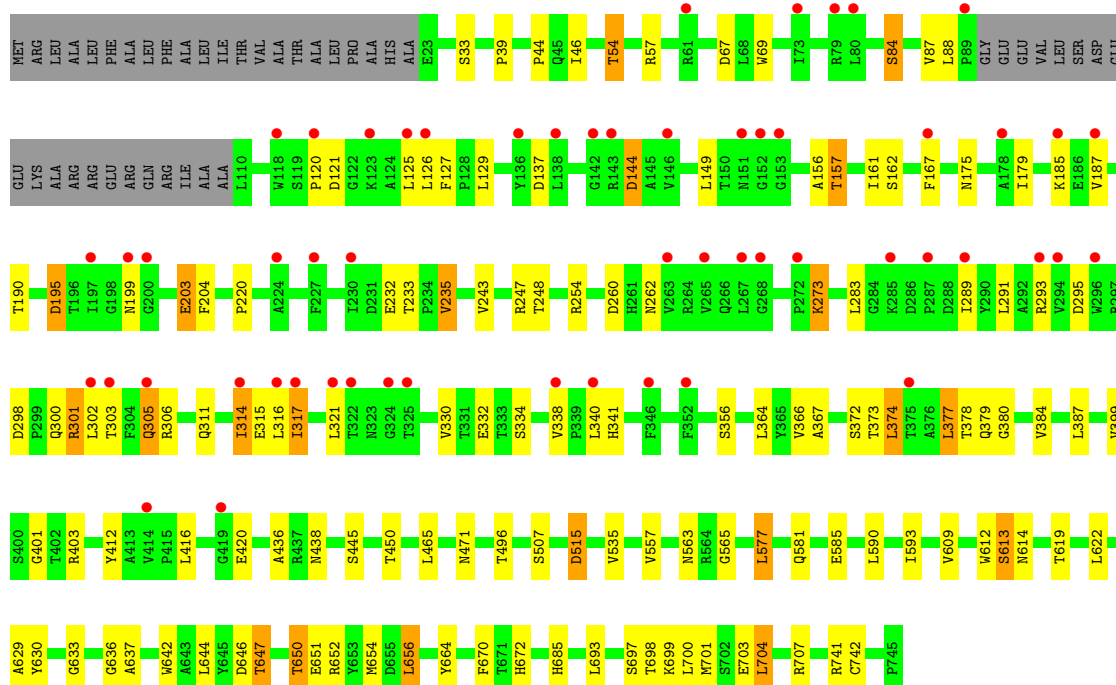
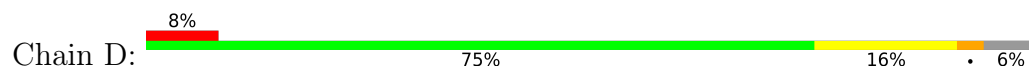




• Molecule 1: Dipeptidyl aminopeptidase 4



• Molecule 1: Dipeptidyl aminopeptidase 4



4 Data and refinement statistics

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 40.00 – 2.47	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-2.47) 99.8 (40.00-2.47)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.217 , 0.284 0.222 , 0.285	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)	0.29 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	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 $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.91	0/5562	1.05	16/7569 (0.2%)
1	B	1.01	2/5799 (0.0%)	1.06	8/7887 (0.1%)
1	C	1.01	2/5635 (0.0%)	1.03	7/7668 (0.1%)
1	D	0.92	0/5630	1.03	7/7661 (0.1%)
All	All	0.96	4/22626 (0.0%)	1.04	38/30785 (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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	43	LYS	CA-C	7.56	1.59	1.53
1	B	256	PRO	C-O	-6.66	1.18	1.24
1	C	400	SER	N-CA	-5.35	1.39	1.46
1	C	637	ALA	N-CA	-5.20	1.42	1.46

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	VAL	CA-C-N	7.90	135.92	121.70
1	A	243	VAL	C-N-CA	7.90	135.92	121.70
1	D	273	LYS	N-CA-C	7.29	120.24	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	401	GLY	N-CA-C	6.50	121.20	110.55
1	A	511	PRO	N-CA-C	6.40	120.49	111.33
1	B	417	SER	N-CA-C	6.39	120.65	112.34
1	A	317	ILE	N-CA-C	6.32	116.76	106.72
1	A	141	SER	N-CA-C	6.21	121.70	114.62
1	A	532	ALA	N-CA-C	6.18	117.68	107.73
1	A	321	LEU	N-CA-C	6.16	120.92	112.04
1	A	401	GLY	N-CA-C	6.16	120.72	111.42
1	C	401	GLY	N-CA-C	6.07	119.99	111.19
1	B	446	TRP	N-CA-C	6.04	117.96	108.96
1	B	741	ARG	N-CA-C	5.96	117.44	111.07
1	B	162	SER	CA-C-N	5.88	125.08	118.97
1	B	162	SER	C-N-CA	5.88	125.08	118.97
1	A	614	ASN	N-CA-C	-5.83	104.35	112.45
1	D	557	VAL	N-CA-C	-5.60	100.51	108.58
1	A	390	ILE	CB-CA-C	-5.52	102.47	110.63
1	C	677	GLY	N-CA-C	5.51	117.81	111.36
1	A	510	LYS	CA-C-N	5.48	126.25	120.11
1	A	510	LYS	C-N-CA	5.48	126.25	120.11
1	A	265	VAL	N-CA-C	5.47	116.44	107.24
1	A	570	GLY	CA-C-O	-5.47	118.67	122.22
1	A	356	SER	N-CA-C	5.46	116.44	108.14
1	D	380	GLY	N-CA-C	5.44	117.12	111.95
1	C	235	VAL	N-CA-C	-5.38	104.00	108.63
1	B	529	GLY	CA-C-N	5.32	125.03	119.82
1	B	529	GLY	C-N-CA	5.32	125.03	119.82
1	C	565	GLY	N-CA-C	-5.31	108.16	114.48
1	C	676	ILE	CA-C-N	5.25	124.96	119.92
1	C	676	ILE	C-N-CA	5.25	124.96	119.92
1	D	317	ILE	N-CA-C	5.24	115.59	107.78
1	B	646	ASP	CB-CA-C	-5.23	100.01	110.42
1	D	515	ASP	CB-CA-C	5.20	116.68	108.88
1	A	374	LEU	N-CA-C	-5.15	101.36	109.50
1	D	647	THR	N-CA-C	5.06	117.19	111.02
1	C	639	VAL	N-CA-C	-5.04	103.07	109.58

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 ⓘ

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	5426	0	5289	46	0
1	B	5660	0	5520	37	0
1	C	5497	0	5358	31	0
1	D	5492	0	5353	57	0
2	B	6	0	8	2	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	165	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 (165) 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:206:ALA:HB2	1:A:210:MET:HE3	1.66	0.77
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:ILE:HG22	1:D:332:GLU:HB2	1.84	0.58
1:D:203:GLU:O	1:D:204:PHE:C	2.47	0.57
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:206:ALA:CB	1:A:210:MET:HE3	2.35	0.55
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: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: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
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:475:ASP:OD1	1:C:475:ASP:C	2.56	0.48
1:C:77:GLN:HE21	1:C:79:ARG:HD3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:628:GLU:H	1:C:628:GLU:CD	2.20	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:C:687:MET:HE1	1:D:701:MET:CE	2.44	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:D:646:ASP:O	1:D:650:THR:OG1	2.25	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
1:A:314:ILE:HD11	1:A:332:GLU:HG3	1.97	0.46
1:A:654:MET:HA	1:A:654:MET:HE2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:209:GLU:CD	1:B:649:TYR:HB2	2.43	0.43
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: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:A:645:TYR:O	1:A:650:THR:OG1	2.23	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:687:MET:HE1	1:D:701:MET:HE1	2.03	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:B:343:ASP:OD2	2:B:801:GOL:O1	2.34	0.41
1:D:39:PRO:HD2	1:D:471:ASN:OD1	2.21	0.41
1:C:357:GLU:CD	1:C:571:ALA:HB2	2.45	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:B:621:MET:HE1	1:B:672:HIS:CD2	2.56	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:C:687:MET:HE3	1:C:717:PRO:CA	2.51	0.40
1:A:660:ASN:O	1:A:661:GLU:C	2.64	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

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%)	8 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	722/745 (97%)	672 (93%)	46 (6%)	4 (1%)	21	35
1	C	700/745 (94%)	657 (94%)	36 (5%)	7 (1%)	12	22
1	D	699/745 (94%)	631 (90%)	59 (8%)	9 (1%)	9	16
All	All	2810/2980 (94%)	2583 (92%)	197 (7%)	30 (1%)	11	20

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
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 ⓘ

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%)	514 (91%)	50 (9%)	9	18
1	B	587/602 (98%)	553 (94%)	34 (6%)	18	35
1	C	571/602 (95%)	543 (95%)	28 (5%)	22	42
1	D	571/602 (95%)	515 (90%)	56 (10%)	7	14
All	All	2293/2408 (95%)	2125 (93%)	168 (7%)	13	25

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	SER
1	A	114	VAL
1	A	115	ASP
1	A	141	SER
1	A	144	ASP
1	A	149	LEU
1	A	150	THR
1	A	189	LEU
1	A	196	THR
1	A	199	ASN
1	A	205	VAL
1	A	243	VAL
1	A	247	ARG
1	A	252	GLU
1	A	283	LEU
1	A	289	ILE
1	A	300	GLN
1	A	303	THR
1	A	310	ASP
1	A	335	THR
1	A	338	VAL
1	A	362	GLU
1	A	375	THR
1	A	379	GLN

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Mol	Chain	Res	Type
1	A	390	ILE
1	A	414	VAL
1	A	426	GLN
1	A	437	ARG
1	A	450	THR
1	A	459	LYS
1	A	468	LEU
1	A	543	SER
1	A	545	SER
1	A	551	LEU
1	A	577	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	706	LYS
1	A	720	LYS
1	A	723	LEU
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	163	PRO
1	B	164	LYS
1	B	181	LEU
1	B	187	VAL
1	B	191	ARG
1	B	225	ILE
1	B	230	ILE

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Mol	Chain	Res	Type
1	B	248	THR
1	B	274	THR
1	B	321	LEU
1	B	323	ASN
1	B	362	GLU
1	B	416	LEU
1	B	437	ARG
1	B	456	GLU
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	584	VAL
1	B	590	LEU
1	B	591	ARG
1	B	698	THR
1	C	23	GLU
1	C	33	SER
1	C	56	LEU
1	C	88	LEU
1	C	139	THR
1	C	144	ASP
1	C	181	LEU
1	C	191	ARG
1	C	195	ASP
1	C	250	VAL
1	C	265	VAL
1	C	322	THR
1	C	373	THR
1	C	383	VAL
1	C	416	LEU
1	C	420	GLU
1	C	425	THR
1	C	426	GLN
1	C	450	THR
1	C	545	SER
1	C	613	SER
1	C	628	GLU
1	C	658	LYS
1	C	690	ASP

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Mol	Chain	Res	Type
1	C	693	LEU
1	C	734	LEU
1	C	742	CYS
1	C	744	LYS
1	D	33	SER
1	D	54	THR
1	D	84	SER
1	D	121	ASP
1	D	125	LEU
1	D	157	THR
1	D	179	ILE
1	D	185	LYS
1	D	187	VAL
1	D	195	ASP
1	D	203	GLU
1	D	235	VAL
1	D	243	VAL
1	D	247	ARG
1	D	248	THR
1	D	260	ASP
1	D	273	LYS
1	D	283	LEU
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	379	GLN
1	D	387	LEU
1	D	416	LEU
1	D	420	GLU
1	D	438	ASN
1	D	450	THR
1	D	465	LEU

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Mol	Chain	Res	Type
1	D	496	THR
1	D	515	ASP
1	D	563	ASN
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	644	LEU
1	D	650	THR
1	D	656	LEU
1	D	672	HIS
1	D	693	LEU
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 (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	GLN
1	A	262	ASN
1	A	305	GLN
1	A	326	GLN
1	A	548	ASN
1	A	685	HIS
1	B	199	ASN
1	B	266	GLN
1	B	305	GLN
1	B	379	GLN
1	B	426	GLN
1	B	438	ASN
1	B	614	ASN
1	C	77	GLN
1	C	266	GLN
1	D	45	GLN
1	D	199	ASN
1	D	305	GLN
1	D	326	GLN
1	D	454	GLN

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Mol	Chain	Res	Type
1	D	548	ASN
1	D	648	HIS
1	D	685	HIS
1	D	691	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 oligosaccharides 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	0.90	0	5,5,5	1.74	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($^{\circ}$)	Ideal($^{\circ}$)
2	B	801	GOL	C3-C2-C1	2.24	120.00	111.80

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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	GOL	2	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	695/745 (93%)	0.61	37 (5%)	32	28	27, 51, 79, 117	0
1	B	724/745 (97%)	-0.10	16 (2%)	62	59	13, 32, 65, 110	0
1	C	704/745 (94%)	-0.09	26 (3%)	45	41	15, 31, 75, 140	0
1	D	703/745 (94%)	0.75	56 (7%)	18	16	28, 55, 84, 117	0
All	All	2826/2980 (94%)	0.29	135 (4%)	35	32	13, 44, 79, 140	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	22	ALA	7.7
1	C	150	THR	6.5
1	B	243	VAL	5.4
1	D	138	LEU	4.5
1	A	88	LEU	4.4
1	B	241	TYR	4.2
1	C	148	LYS	3.8
1	B	245	PRO	3.8
1	C	138	LEU	3.6
1	A	248	THR	3.6
1	C	155	PHE	3.6
1	C	139	THR	3.5
1	C	151	ASN	3.4
1	C	149	LEU	3.4
1	C	123	LYS	3.4
1	D	178	ALA	3.4
1	A	304	PHE	3.4
1	A	371	GLY	3.4
1	B	248	THR	3.3
1	C	22	ALA	3.3
1	C	120	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	375	THR	3.2
1	A	338	VAL	3.2
1	A	283	LEU	3.2
1	A	241	TYR	3.2
1	D	352	PHE	3.1
1	D	89	PRO	3.1
1	C	145	ALA	3.1
1	A	148	LYS	3.1
1	C	239	LYS	3.1
1	B	250	VAL	3.1
1	D	146	VAL	3.1
1	D	294	VAL	3.0
1	C	88	LEU	3.0
1	C	140	LYS	3.0
1	D	153	GLY	3.0
1	A	146	VAL	3.0
1	C	110	LEU	3.0
1	D	414	VAL	2.9
1	D	324	GLY	2.9
1	A	145	ALA	2.8
1	D	346	PHE	2.8
1	A	150	THR	2.8
1	A	110	LEU	2.8
1	D	340	LEU	2.8
1	A	322	THR	2.7
1	B	142	GLY	2.7
1	D	322	THR	2.7
1	B	143	ARG	2.7
1	D	230	ILE	2.7
1	A	330	VAL	2.7
1	D	227	PHE	2.7
1	D	338	VAL	2.6
1	D	136	TYR	2.6
1	A	644	LEU	2.6
1	A	250	VAL	2.6
1	D	224	ALA	2.6
1	A	580	LYS	2.6
1	A	268	GLY	2.5
1	A	155	PHE	2.5
1	D	316	LEU	2.5
1	D	321	LEU	2.5
1	A	243	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	134	TYR	2.5
1	A	390	ILE	2.5
1	B	140	LYS	2.5
1	C	143	ARG	2.5
1	D	151	ASN	2.5
1	C	89	PRO	2.4
1	A	87	VAL	2.4
1	D	197	ILE	2.4
1	D	143	ARG	2.4
1	B	150	THR	2.4
1	B	141	SER	2.4
1	A	197	ILE	2.4
1	D	289	ILE	2.4
1	D	79	ARG	2.4
1	C	146	VAL	2.4
1	B	273	LYS	2.4
1	A	230	ILE	2.4
1	D	142	GLY	2.3
1	B	247	ARG	2.3
1	D	314	ILE	2.3
1	A	673	VAL	2.3
1	A	600	ALA	2.3
1	C	112	GLY	2.3
1	D	317	ILE	2.3
1	D	293	ARG	2.3
1	C	122	GLY	2.3
1	C	141	SER	2.3
1	D	305	GLN	2.3
1	D	267	LEU	2.3
1	D	302	LEU	2.3
1	D	268	GLY	2.3
1	C	144	ASP	2.3
1	C	132	GLU	2.3
1	B	244	TYR	2.3
1	D	303	THR	2.2
1	D	285	LYS	2.2
1	D	167	PHE	2.2
1	D	61	ARG	2.2
1	A	498	ALA	2.2
1	D	325	THR	2.2
1	A	302	LEU	2.2
1	D	296	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	120	PRO	2.2
1	D	187	VAL	2.2
1	A	176	LEU	2.2
1	B	225	ILE	2.2
1	B	246	ASP	2.2
1	C	153	GLY	2.1
1	D	73	ILE	2.1
1	D	287	PRO	2.1
1	D	80	LEU	2.1
1	D	126	LEU	2.1
1	D	419	GLY	2.1
1	D	272	PRO	2.1
1	A	227	PHE	2.1
1	D	263	VAL	2.1
1	A	151	ASN	2.1
1	A	239	LYS	2.1
1	D	123	LYS	2.1
1	D	265	VAL	2.1
1	D	152	GLY	2.1
1	A	314	ILE	2.1
1	A	346	PHE	2.0
1	D	125	LEU	2.0
1	A	153	GLY	2.0
1	D	118	TRP	2.0
1	D	200	GLY	2.0
1	D	185	LYS	2.0
1	A	269	VAL	2.0
1	C	147	ARG	2.0
1	A	321	LEU	2.0
1	D	199	ASN	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($\text{\AA}^2$)	Q<0.9
2	GOL	B	801	6/6	0.92	0.12	39,47,49,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.