



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:18 AM UTC

PDB ID : 5FCH / pdb_00005fch
Title : Crystal Structure of Xaa-Pro dipeptidase from Xanthomonas campestris, phosphate and Zn bound
Authors : Kumar, A.; Are, V.; Ghosh, B.; Jamdar, S.; Makde, R.D.
Deposited on : 2015-12-15
Resolution : 1.95 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

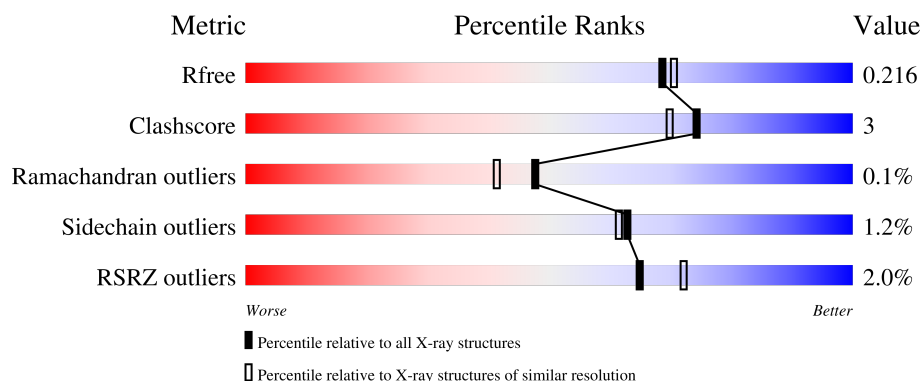
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	399	33% 67%
1	B	399	3% 85% 13%
2	C	3	33% 67%

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
6	PEG	B	404	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6271 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 Proline dipeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	0	0
			2979	1882	530	550	17			
1	B	395	Total	C	N	O	S	0	1	0
			2978	1877	532	552	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q8P839
B	1	SER	-	expression tag	UNP Q8P839

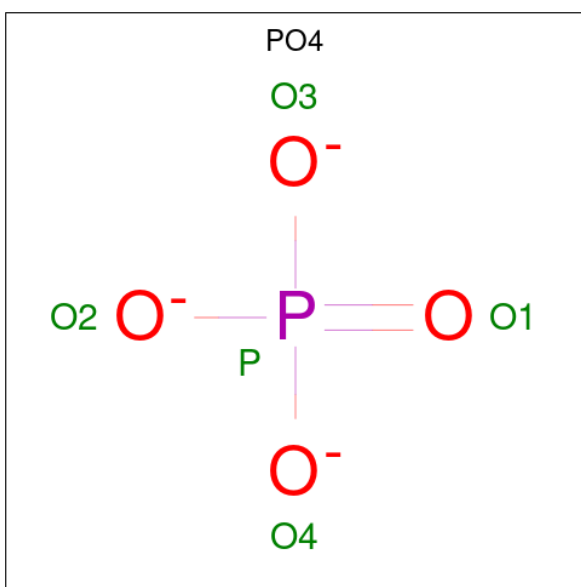
- Molecule 2 is a protein called GLY-GLY-GLY.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			13	6	3	4			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

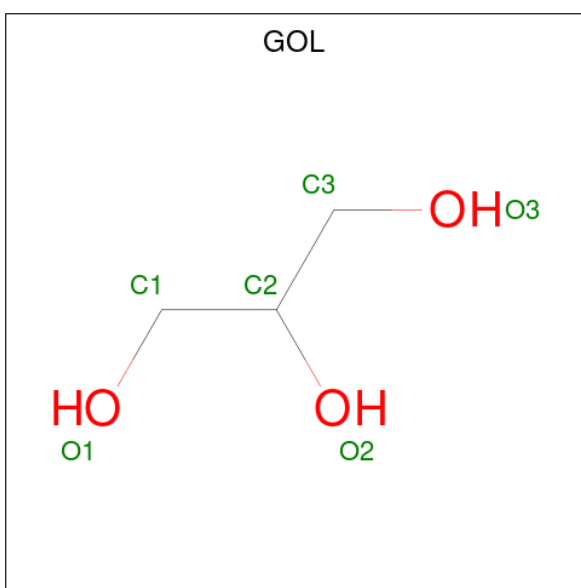
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		
3	B	2	Total	Zn	0	0
			2	2		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



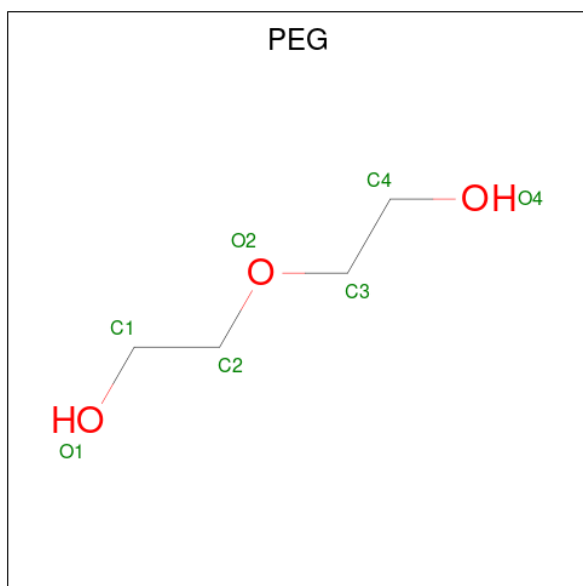
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			7	4	3		

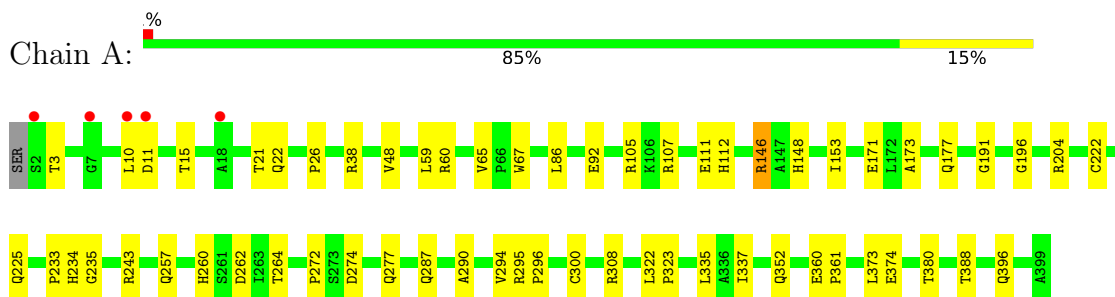
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	115	Total	O	0	0
			115	115		
7	B	146	Total	O	0	0
			146	146		
7	C	1	Total	O	0	0
			1	1		

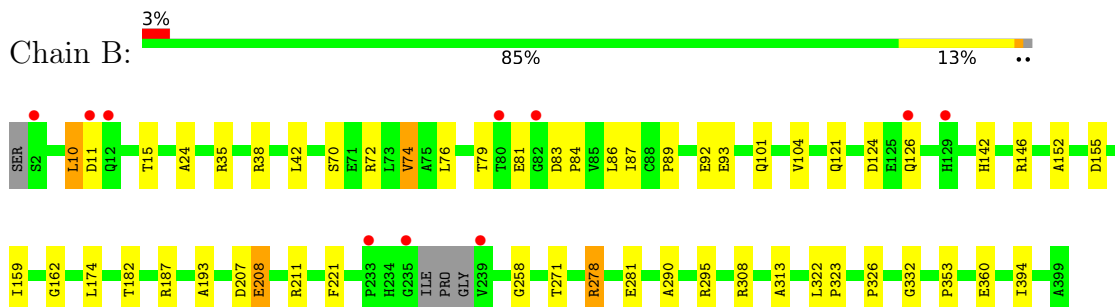
3 Residue-property plots

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.

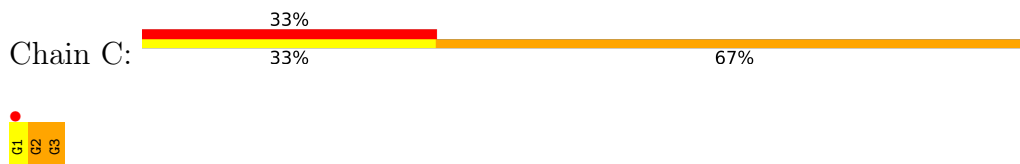
• Molecule 1: Proline dipeptidase



• Molecule 1: Proline dipeptidase



• Molecule 2: GLY-GLY-GLY



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.03Å 104.08Å 112.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 1.95 45.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.00-1.95) 99.9 (45.00-1.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.172 , 0.211 0.183 , 0.216	Depositor DCC
R_{free} test set	3488 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 32.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6271	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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: PO4, GOL, ZN, PEG

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	1.66	31/3049 (1.0%)	1.32	12/4158 (0.3%)
1	B	1.73	26/3046 (0.9%)	1.35	16/4150 (0.4%)
2	C	3.07	2/12 (16.7%)	1.94	0/12
All	All	1.70	59/6107 (1.0%)	1.33	28/8320 (0.3%)

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
2	C	0	1
All	All	0	2

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	83	ASP	CA-C	12.88	1.66	1.53
1	B	211	ARG	N-CA	8.27	1.56	1.46
1	A	171	GLU	N-CA	8.08	1.55	1.46
1	B	353	PRO	CA-CB	7.82	1.64	1.53
1	A	146	ARG	CA-C	-7.18	1.42	1.52
1	A	59	LEU	N-CA	7.14	1.55	1.46
2	C	3	GLY	N-CA	-7.07	1.34	1.45
1	B	35	ARG	N-CA	6.81	1.54	1.46
1	A	272	PRO	C-O	-6.68	1.16	1.23
1	A	380	THR	N-CA	6.60	1.53	1.45
1	B	290	ALA	C-O	-6.55	1.16	1.24
1	A	335	LEU	C-O	-6.52	1.15	1.24
1	B	281	GLU	CG-CD	6.52	1.68	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	ARG	N-CA	6.50	1.54	1.46
1	A	277	GLN	CA-C	-6.47	1.44	1.52
1	B	394	ILE	N-CA	6.43	1.54	1.46
1	B	281	GLU	CD-OE2	6.40	1.37	1.25
1	A	173	ALA	C-O	-6.34	1.16	1.24
1	A	396	GLN	C-O	6.32	1.31	1.24
1	B	193	ALA	CA-C	6.27	1.60	1.52
1	B	187	ARG	CZ-NH1	6.26	1.41	1.32
1	B	221	PHE	C-O	6.07	1.31	1.23
1	A	300	CYS	N-CA	6.05	1.53	1.46
1	B	155	ASP	CA-C	6.05	1.60	1.52
1	B	182	THR	CA-C	6.03	1.60	1.52
1	B	332	GLY	N-CA	5.99	1.52	1.45
1	A	112	HIS	C-O	-5.92	1.16	1.24
1	A	177	GLN	CA-C	5.82	1.60	1.52
1	A	274	ASP	C-O	-5.80	1.17	1.24
1	B	281	GLU	CA-CB	5.76	1.62	1.53
1	A	287	GLN	CA-C	5.75	1.60	1.52
1	A	148	HIS	C-O	-5.71	1.17	1.24
1	A	287	GLN	N-CA	5.68	1.53	1.46
1	A	361	PRO	CA-C	5.68	1.58	1.53
1	A	105	ARG	C-O	5.68	1.30	1.24
1	A	38	ARG	CD-NE	5.66	1.54	1.46
1	A	294	VAL	CA-C	5.60	1.59	1.52
1	A	21	THR	C-O	-5.55	1.17	1.23
1	B	295	ARG	N-CA	5.51	1.51	1.46
1	B	258	GLY	CA-C	5.50	1.59	1.51
1	A	290	ALA	C-O	-5.50	1.17	1.24
1	B	152	ALA	N-CA	-5.48	1.39	1.46
1	B	74	VAL	C-O	5.40	1.30	1.24
1	B	93	GLU	C-O	5.40	1.30	1.24
1	A	222	CYS	CA-C	-5.39	1.46	1.52
1	A	337	ILE	N-CA	-5.38	1.40	1.46
1	B	104	VAL	C-O	-5.37	1.18	1.23
2	C	3	GLY	CA-C	-5.36	1.42	1.52
1	B	81	GLU	CA-C	5.36	1.59	1.52
1	A	388	THR	C-N	5.30	1.39	1.33
1	B	87	ILE	CA-C	5.30	1.58	1.52
1	B	101	GLN	N-CA	5.25	1.52	1.46
1	A	352	GLN	N-CA	5.20	1.50	1.45
1	A	264	THR	C-O	5.11	1.30	1.24
1	B	124	ASP	CA-C	5.11	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	TRP	CA-C	5.09	1.59	1.52
1	B	159	ILE	C-O	5.08	1.29	1.24
1	A	296	PRO	C-O	-5.06	1.17	1.23
1	A	243	ARG	CZ-NH1	5.02	1.39	1.32

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	GLU	N-CA-C	9.56	123.39	109.14
1	B	187	ARG	NE-CZ-NH2	-8.28	111.75	119.20
1	B	187	ARG	NE-CZ-NH1	7.20	128.70	121.50
1	A	295	ARG	CG-CD-NE	-6.31	98.11	112.00
1	A	60	ARG	NE-CZ-NH2	-6.23	113.59	119.20
1	B	83	ASP	CA-C-O	6.10	126.51	120.17
1	A	234	HIS	N-CA-C	6.09	120.74	112.88
1	B	308	ARG	CG-CD-NE	-6.02	98.76	112.00
1	A	111	GLU	N-CA-C	5.98	118.56	111.33
1	A	107	ARG	CG-CD-NE	-5.82	99.19	112.00
1	A	3	THR	N-CA-C	5.67	120.05	113.18
1	B	271	THR	CA-C-N	-5.64	114.78	120.31
1	B	271	THR	C-N-CA	-5.64	114.78	120.31
1	B	278	ARG	NE-CZ-NH1	5.62	127.12	121.50
1	B	208	GLU	CB-CG-CD	5.57	122.07	112.60
1	B	360	GLU	N-CA-C	5.56	116.76	108.76
1	B	207	ASP	N-CA-C	5.46	116.92	110.97
1	A	22	GLN	CB-CA-C	-5.42	103.99	112.12
1	B	121	GLN	CB-CG-CD	-5.41	103.40	112.60
1	B	162	GLY	N-CA-C	-5.34	106.25	113.24
1	B	278	ARG	NE-CZ-NH2	-5.33	114.40	119.20
1	B	313	ALA	N-CA-C	-5.28	105.64	111.71
1	A	65	VAL	CA-C-N	-5.25	114.95	120.94
1	A	65	VAL	C-N-CA	-5.25	114.95	120.94
1	A	308	ARG	NE-CZ-NH1	-5.24	116.26	121.50
1	A	191	GLY	N-CA-C	5.18	119.15	112.83
1	A	196	GLY	N-CA-C	5.16	122.40	115.59
1	B	308	ARG	NE-CZ-NH2	5.11	123.80	119.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	260	HIS	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	C	2	GLY	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	2979	0	2908	15	0
1	B	2978	0	2904	22	0
2	C	13	0	11	10	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	18	0	24	1	0
6	B	7	0	10	5	0
7	A	115	0	0	1	0
7	B	146	0	0	0	0
7	C	1	0	0	0	0
All	All	6271	0	5857	37	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 (37) 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:B:146:ARG:HH11	2:C:3:GLY:HA2	1.42	0.83
1:B:146:ARG:HH11	2:C:3:GLY:CA	1.94	0.80
1:B:76:LEU:HD11	1:B:84:PRO:HB2	1.65	0.77
1:B:70:SER:OG	6:B:404:PEG:H31	1.88	0.73
1:B:89:PRO:HB2	1:B:92[B]:GLU:HG3	1.83	0.59
1:A:146:ARG:HH11	2:C:2:GLY:CA	2.18	0.56
1:B:72:ARG:HH11	6:B:404:PEG:H32	1.70	0.56
1:B:79:THR:OG1	1:B:126:GLN:OE1	2.15	0.55
1:B:38:ARG:HH11	1:B:42:LEU:HD11	1.71	0.54
1:B:70:SER:CB	6:B:404:PEG:H31	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:ARG:HH11	2:C:3:GLY:HA3	1.72	0.52
1:B:146:ARG:NH1	2:C:3:GLY:HA2	2.20	0.52
1:B:92[B]:GLU:CD	6:B:404:PEG:H22	2.35	0.51
1:B:322:LEU:HD21	1:B:326:PRO:HB3	1.91	0.51
1:A:26:PRO:HB3	1:A:257:GLN:NE2	2.27	0.50
1:A:11:ASP:O	1:A:15:THR:HG23	2.15	0.47
1:A:257:GLN:NE2	7:A:502:HOH:O	2.48	0.46
1:B:10:LEU:HD23	1:B:10:LEU:HA	1.82	0.46
1:B:142:HIS:NE2	2:C:3:GLY:HA3	2.30	0.46
1:B:76:LEU:HD11	1:B:84:PRO:CB	2.40	0.46
1:A:322:LEU:HA	1:A:323:PRO:C	2.41	0.45
1:A:146:ARG:HH11	2:C:2:GLY:N	2.14	0.45
1:B:74:VAL:HG21	6:B:404:PEG:H12	1.99	0.44
1:B:11:ASP:O	1:B:15:THR:HG23	2.18	0.44
1:A:360:GLU:HB3	1:A:374:GLU:HB2	2.00	0.44
1:A:10:LEU:HD23	1:A:10:LEU:HA	1.91	0.43
1:A:225:GLN:HE21	1:A:235:GLY:CA	2.31	0.43
1:A:225:GLN:NE2	1:A:235:GLY:CA	2.82	0.43
1:A:92:GLU:OE2	5:A:405:GOL:H2	2.19	0.43
1:A:360:GLU:HA	1:A:373:LEU:O	2.18	0.43
1:B:322:LEU:HA	1:B:323:PRO:C	2.44	0.42
1:B:146:ARG:NH1	2:C:3:GLY:CA	2.74	0.42
1:B:24:ALA:HB3	1:B:174:LEU:HD23	2.01	0.42
1:A:153:ILE:H	2:C:1:GLY:H2	1.69	0.41
1:B:38:ARG:NH1	1:B:42:LEU:HD11	2.36	0.41
1:A:153:ILE:H	2:C:1:GLY:N	2.18	0.40
1:A:26:PRO:HB3	1:A:257:GLN:HE22	1.85	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	396/399 (99%)	386 (98%)	9 (2%)	1 (0%)	36	28
1	B	392/399 (98%)	383 (98%)	9 (2%)	0	100	100
2	C	1/3 (33%)	0	1 (100%)	0	100	100
All	All	789/801 (98%)	769 (98%)	19 (2%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	ASP

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	294/302 (97%)	291 (99%)	3 (1%)	68	67
1	B	295/302 (98%)	291 (99%)	4 (1%)	59	56
All	All	589/604 (98%)	582 (99%)	7 (1%)	63	61

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	VAL
1	A	86	LEU
1	A	233	PRO
1	B	10	LEU
1	B	86	LEU
1	B	208	GLU
1	B	278	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	225	GLN
1	A	257	GLN
1	A	305	GLN
1	A	349	GLN
1	B	225	GLN
1	B	312	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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	$\# Z > 2$
5	GOL	A	405	-	5,5,5	0.25	0	5,5,5	0.67	0
6	PEG	B	404	-	6,6,6	0.69	0	5,5,5	0.42	0
4	PO4	B	403	3	4,4,4	1.29	1 (25%)	6,6,6	0.98	0
5	GOL	A	406	-	5,5,5	0.71	0	5,5,5	1.55	1 (20%)
5	GOL	A	404	-	5,5,5	0.73	0	5,5,5	1.06	0
4	PO4	A	403	3	4,4,4	1.01	0	6,6,6	1.80	1 (16%)

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
5	GOL	A	405	-	-	4/4/4/4	-
5	GOL	A	406	-	-	4/4/4/4	-
5	GOL	A	404	-	-	2/4/4/4	-
6	PEG	B	404	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	403	PO4	P-O4	-2.34	1.47	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403	PO4	O3-P-O1	3.71	124.08	110.95
5	A	406	GOL	O2-C2-C1	-2.53	98.70	109.18

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	404	GOL	O1-C1-C2-C3
5	A	406	GOL	O1-C1-C2-C3
5	A	406	GOL	C1-C2-C3-O3
5	A	405	GOL	O1-C1-C2-C3
5	A	405	GOL	C1-C2-C3-O3
5	A	405	GOL	O1-C1-C2-O2
5	A	406	GOL	O1-C1-C2-O2
5	A	406	GOL	O2-C2-C3-O3
6	B	404	PEG	O2-C3-C4-O4
5	A	404	GOL	O1-C1-C2-O2
5	A	405	GOL	O2-C2-C3-O3
6	B	404	PEG	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	405	GOL	1	0
6	B	404	PEG	5	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	398/399 (99%)	0.02	5 (1%) 75 81	15, 25, 41, 58	0
1	B	395/399 (98%)	-0.10	10 (2%) 58 65	10, 21, 41, 71	1 (0%)
2	C	3/3 (100%)	1.69	1 (33%) 1 0	26, 26, 33, 34	0
All	All	796/801 (99%)	-0.04	16 (2%) 65 72	10, 24, 41, 71	1 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	SER	6.2
1	B	235	GLY	5.0
1	A	10	LEU	3.9
1	B	126	GLN	3.7
1	B	80	THR	3.2
1	A	2	SER	3.0
1	B	82	GLY	2.7
2	C	1	GLY	2.7
1	A	7	GLY	2.6
1	B	11	ASP	2.6
1	B	239	VAL	2.5
1	B	129	HIS	2.4
1	B	12	GLN	2.3
1	A	11	ASP	2.2
1	A	18	ALA	2.2
1	B	233	PRO	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
6	PEG	B	404	7/7	0.85	0.18	38,39,44,45	0
5	GOL	A	406	6/6	0.87	0.16	33,37,38,38	0
5	GOL	A	405	6/6	0.92	0.11	30,40,42,46	0
5	GOL	A	404	6/6	0.94	0.11	27,31,36,42	0
4	PO4	A	403	5/5	0.99	0.06	18,22,24,27	0
4	PO4	B	403	5/5	0.99	0.07	16,19,20,22	0
3	ZN	B	401	1/1	1.00	0.02	17,17,17,17	0
3	ZN	B	402	1/1	1.00	0.05	21,21,21,21	0
3	ZN	A	401	1/1	1.00	0.02	21,21,21,21	0
3	ZN	A	402	1/1	1.00	0.04	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.