



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:16 PM UTC

PDB ID : 5FCF / pdb\_00005fcf  
Title : Crystal Structure of Xaa-Pro dipeptidase from Xanthomonas campestris, phosphate and Mn bound  
Authors : Kumar, A.; Are, V.; Ghosh, B.; Jamdar, S.; Makde, R.D.  
Deposited on : 2015-12-15  
Resolution : 1.85 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](mailto: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>.

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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

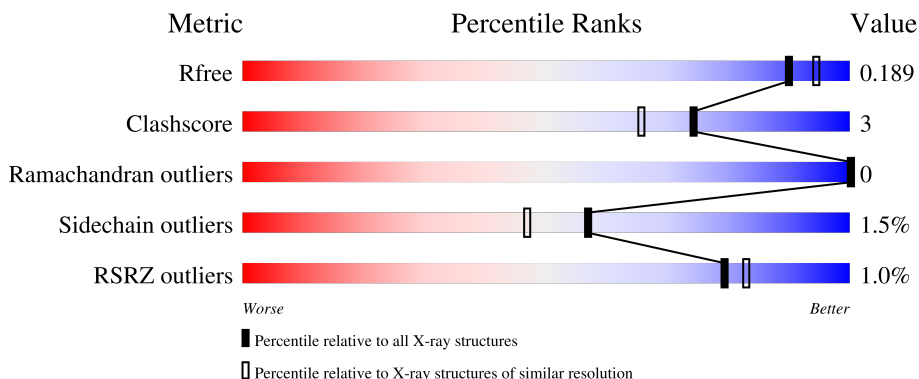
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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  $\geq 3$ , 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	 88% 11% ..
1	B	399	 2% 83% 15% ..
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 i

There are 7 unique types of molecules in this entry. The entry contains 6415 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
			Total	C	N	O	S			
1	A	397	Total	C	N	O	S	0	0	0
			2989	1884	537	551	17			
1	B	396	Total	C	N	O	S	0	0	0
			2986	1882	537	550	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
			Total	C	N	O			
2	C	3	Total	C	N	O	0	0	0
			13	6	3	4			

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



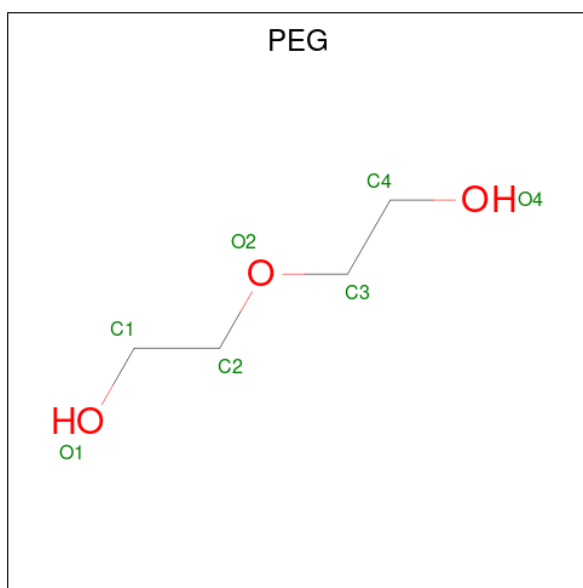
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- 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 7 4 3	0	0


- Molecule 7 is water.

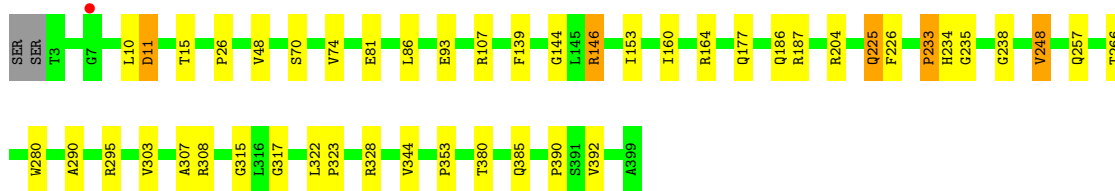
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	174	Total O 174 174	0	0
7	B	218	Total O 218 218	0	0
7	C	2	Total O 2 2	0	0

### 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.

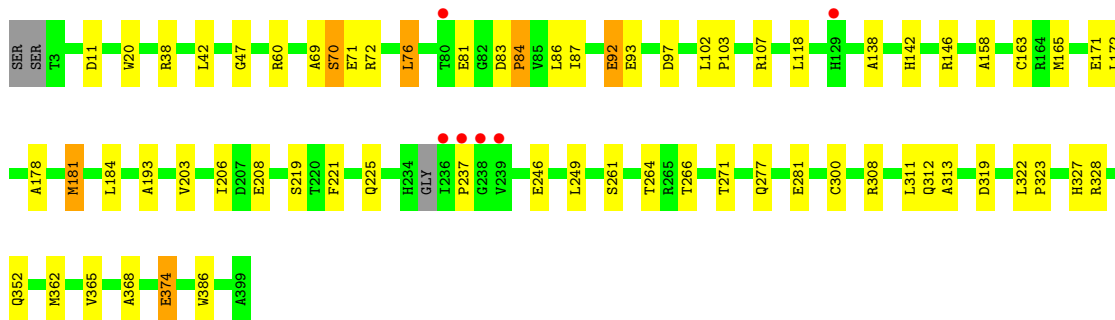
- Molecule 1: Proline dipeptidase

Chain A:  88% 11% ..



- Molecule 1: Proline dipeptidase

Chain B:  2% 83% 15% ..



- Molecule 2: GLY-GLY-GLY

Chain C:  33% 33% 67%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.96Å 104.28Å 112.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 1.85 45.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.00-1.85) 99.7 (45.00-1.85)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 1.86Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.159 , 0.196 (Not available) , 0.189	Depositor DCC
$R_{free}$ test set	4080 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.1	Xtrriage
Anisotropy	0.052	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 34.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6415	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MN, PO4, PEG, 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	1.67	29/3059 (0.9%)	1.38	11/4170 (0.3%)
1	B	1.79	46/3055 (1.5%)	1.41	10/4163 (0.2%)
2	C	4.02	3/12 (25.0%)	2.30	0/12
All	All	1.74	78/6126 (1.3%)	1.40	21/8345 (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	2
All	All	0	3

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	83	ASP	CA-C	8.42	1.62	1.53
1	B	93	GLU	C-O	8.35	1.33	1.24
1	A	390	PRO	CA-C	-8.09	1.43	1.52
2	C	3	GLY	N-CA	-8.01	1.32	1.45
1	B	281	GLU	CG-CD	7.38	1.70	1.52
1	A	392	VAL	N-CA	7.03	1.54	1.45
1	B	181	MET	SD-CE	-6.95	1.62	1.79
1	A	70	SER	N-CA	6.93	1.55	1.46
1	B	246	GLU	C-O	6.78	1.31	1.23
1	B	311	LEU	N-CA	-6.76	1.38	1.46
1	A	238	GLY	N-CA	6.76	1.52	1.45
1	B	386	TRP	C-O	6.65	1.31	1.23
1	B	118	LEU	N-CA	-6.62	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	81	GLU	C-O	-6.60	1.15	1.23
1	B	138	ALA	CA-C	6.45	1.61	1.52
1	B	92	GLU	N-CA	6.43	1.54	1.46
1	B	281	GLU	CD-OE2	6.42	1.37	1.25
1	B	158	ALA	C-O	6.40	1.31	1.24
1	A	144	GLY	C-O	-6.36	1.16	1.23
1	B	102	LEU	CA-C	6.36	1.58	1.52
1	B	311	LEU	C-O	6.33	1.31	1.24
1	B	374	GLU	CA-C	-6.30	1.45	1.52
1	A	225	GLN	N-CA	-6.28	1.38	1.45
1	A	390	PRO	N-CA	6.25	1.54	1.47
1	B	300	CYS	C-O	6.12	1.31	1.24
1	B	103	PRO	N-CA	-6.09	1.40	1.47
1	B	368	ALA	CA-C	6.02	1.57	1.52
1	B	60	ARG	CZ-NH1	-6.00	1.24	1.32
1	B	163	CYS	C-O	-6.00	1.17	1.24
1	A	280	TRP	C-O	5.96	1.30	1.24
1	B	261	SER	N-CA	5.94	1.52	1.45
1	A	353	PRO	CA-C	-5.90	1.45	1.52
1	A	234	HIS	C-O	-5.87	1.16	1.24
1	B	219	SER	C-O	-5.85	1.16	1.23
1	B	178	ALA	CA-C	5.79	1.60	1.52
1	A	204	ARG	N-CA	5.61	1.53	1.46
1	B	352	GLN	CD-OE1	5.60	1.34	1.23
1	A	93	GLU	N-CA	5.59	1.53	1.46
1	B	221	PHE	C-O	5.56	1.30	1.23
1	A	380	THR	N-CA	5.53	1.52	1.45
1	B	11	ASP	CA-CB	5.49	1.61	1.53
1	B	97	ASP	C-O	-5.49	1.17	1.24
1	B	184	LEU	C-O	5.44	1.30	1.24
1	B	281	GLU	CD-OE1	5.41	1.35	1.25
1	B	172	LEU	C-O	-5.41	1.17	1.24
1	A	233	PRO	C-O	5.40	1.31	1.24
2	C	3	GLY	CA-C	-5.38	1.42	1.52
1	B	47	GLY	C-O	-5.37	1.16	1.24
1	A	144	GLY	CA-C	5.36	1.57	1.52
1	A	160	ILE	N-CA	5.35	1.52	1.46
1	A	107	ARG	CZ-NH1	5.32	1.40	1.32
1	B	225	GLN	CD-NE2	-5.30	1.22	1.33
1	B	84	PRO	C-O	-5.29	1.17	1.23
1	B	266	THR	CA-C	5.29	1.58	1.52
1	A	226	PHE	CA-C	5.27	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	328	ARG	C-O	5.26	1.31	1.23
1	A	146	ARG	CA-C	-5.24	1.45	1.52
1	B	165	MET	C-O	-5.21	1.18	1.24
1	A	344	VAL	CA-C	-5.18	1.46	1.52
1	B	76	LEU	CA-C	-5.16	1.46	1.52
1	A	307	ALA	CA-C	5.15	1.59	1.52
1	A	248	VAL	C-O	-5.14	1.18	1.24
1	B	70	SER	CA-C	-5.13	1.46	1.53
1	B	365	VAL	CA-C	-5.13	1.48	1.53
1	A	315	GLY	C-O	-5.12	1.17	1.24
1	B	171	GLU	CA-C	5.12	1.59	1.52
1	A	290	ALA	C-O	-5.11	1.18	1.24
1	B	193	ALA	CA-C	5.11	1.59	1.52
1	B	203	VAL	N-CA	5.10	1.52	1.46
1	A	177	GLN	CA-C	5.09	1.59	1.52
1	A	187	ARG	CZ-NH1	5.08	1.39	1.32
1	B	300	CYS	N-CA	-5.07	1.40	1.46
1	B	277	GLN	C-O	5.06	1.29	1.24
1	B	47	GLY	N-CA	5.05	1.52	1.45
1	B	271	THR	C-O	-5.03	1.18	1.24
2	C	3	GLY	C-O	5.02	1.33	1.23
1	A	186	GLN	C-O	5.02	1.29	1.24
1	A	238	GLY	C-O	-5.00	1.19	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	GLU	N-CA-C	9.66	123.53	109.14
1	B	181	MET	CG-SD-CE	-8.78	81.58	100.90
1	B	208	GLU	CB-CG-CD	8.03	126.26	112.60
1	B	206	ILE	N-CA-C	6.75	117.50	110.62
1	A	295	ARG	CG-CD-NE	-6.74	97.17	112.00
1	B	308	ARG	CG-CD-NE	-6.30	98.14	112.00
1	A	164	ARG	N-CA-C	6.26	119.09	111.82
1	A	234	HIS	N-CA-C	6.26	120.22	112.59
1	A	11	ASP	CB-CA-C	6.08	123.02	110.31
1	B	76	LEU	CD1-CG-CD2	-6.07	97.44	110.80
1	A	187	ARG	NE-CZ-NH2	-5.92	113.88	119.20
1	A	107	ARG	NE-CZ-NH1	5.70	127.20	121.50
1	B	107	ARG	NE-CZ-NH2	-5.50	114.25	119.20
1	A	303	VAL	N-CA-C	-5.43	105.24	110.72
1	B	313	ALA	N-CA-C	-5.39	105.51	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	PHE	N-CA-C	5.20	118.41	111.75
1	B	71	GLU	N-CA-C	5.06	119.30	113.18
1	A	317	GLY	N-CA-C	-5.05	102.03	112.34
1	B	69	ALA	CA-C-O	-5.04	116.20	121.55
1	A	295	ARG	CA-C-N	-5.02	114.58	119.76
1	A	295	ARG	C-N-CA	-5.02	114.58	119.76

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	308	ARG	Sidechain
2	C	2	GLY	Peptide,Mainchain

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2989	0	2929	11	0
1	B	2986	0	2927	25	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	12	0	16	1	0
6	B	7	0	10	8	0
7	A	174	0	0	0	0
7	B	218	0	0	1	0
7	C	2	0	0	0	0
All	All	6415	0	5893	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	1.29	0.94
1:B:146:ARG:HH11	2:C:3:GLY:CA	1.89	0.85
1:B:72:ARG:HH11	6:B:404:PEG:H32	1.48	0.78
1:B:70:SER:CB	6:B:404:PEG:H41	2.22	0.70
1:B:72:ARG:HH11	6:B:404:PEG:C3	2.04	0.69
1:B:76:LEU:HD11	1:B:84:PRO:HB2	1.75	0.69
1:B:72:ARG:NH1	6:B:404:PEG:H32	2.09	0.67
1:B:146:ARG:NH1	2:C:3:GLY:HA2	2.08	0.64
1:A:74:VAL:HG21	5:A:405:GOL:H32	1.80	0.62
1:B:20:TRP:HB2	1:B:181:MET:HE3	1.83	0.60
1:B:70:SER:HB2	6:B:404:PEG:H41	1.81	0.60
1:B:38:ARG:HH11	1:B:42:LEU:HD11	1.66	0.60
1:B:70:SER:HB2	6:B:404:PEG:C4	2.33	0.59
1:B:142:HIS:NE2	2:C:3:GLY:HA3	2.22	0.55
1:B:322:LEU:HA	1:B:323:PRO:C	2.32	0.54
1:A:146:ARG:HH11	2:C:2:GLY:CA	2.20	0.54
1:A:225:GLN:NE2	1:A:235:GLY:CA	2.70	0.54
1:B:70:SER:CB	6:B:404:PEG:C4	2.86	0.53
1:B:38:ARG:NH1	1:B:42:LEU:HD11	2.25	0.52
1:B:327:HIS:HD2	1:B:328:ARG:O	1.96	0.48
1:A:26:PRO:HB3	1:A:257:GLN:NE2	2.29	0.48
1:B:76:LEU:HD11	1:B:84:PRO:CB	2.42	0.48
1:A:146:ARG:HH11	2:C:2:GLY:N	2.13	0.46
1:A:11:ASP:O	1:A:15:THR:HG23	2.15	0.46
1:A:322:LEU:HA	1:A:323:PRO:C	2.41	0.45
1:B:146:ARG:HH11	2:C:3:GLY:HA3	1.76	0.45
1:B:312:GLN:NE2	1:B:319:ASP:H	2.15	0.45
1:B:362:MET:HE1	7:B:544:HOH:O	2.17	0.45
1:A:225:GLN:HE21	1:A:235:GLY:CA	2.30	0.44
2:C:1:GLY:HA2	2:C:2:GLY:O	2.17	0.44
1:A:225:GLN:NE2	1:A:235:GLY:HA2	2.32	0.43
1:B:264:THR:H	1:B:374:GLU:HB3	1.83	0.43
1:A:153:ILE:H	2:C:1:GLY:N	2.17	0.42
1:A:248:VAL:O	1:A:266:THR:HA	2.21	0.41
1:B:249:LEU:C	1:B:249:LEU:HD23	2.47	0.41
1:B:146:ARG:NH1	2:C:3:GLY:CA	2.70	0.40
1:B:92:GLU:OE2	6:B:404:PEG:H22	2.21	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	395/399 (99%)	386 (98%)	9 (2%)	0	100	100
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	788/801 (98%)	769 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	298/302 (99%)	292 (98%)	6 (2%)	48	36
1	B	298/302 (99%)	295 (99%)	3 (1%)	68	60
All	All	596/604 (99%)	587 (98%)	9 (2%)	57	47

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	48	VAL
1	A	81	GLU
1	A	86	LEU
1	A	233	PRO
1	A	385	GLN
1	B	86	LEU

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Mol	Chain	Res	Type
1	B	87	ILE
1	B	237	PRO

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	225	GLN
1	A	257	GLN
1	A	305	GLN
1	B	46	GLN
1	B	225	GLN
1	B	312	GLN
1	B	327	HIS

### 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](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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
4	PO4	B	403	3	4,4,4	1.16	0	6,6,6	1.60	2 (33%)
5	GOL	A	405	-	5,5,5	0.18	0	5,5,5	1.16	0
6	PEG	B	404	-	6,6,6	0.73	0	5,5,5	1.88	2 (40%)
5	GOL	A	404	-	5,5,5	1.05	0	5,5,5	0.79	0
4	PO4	A	403	3	4,4,4	3.30	1 (25%)	6,6,6	2.18	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
6	PEG	B	404	-	-	2/4/4/4	-
5	GOL	A	404	-	-	0/4/4/4	-
5	GOL	A	405	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	403	PO4	P-O1	6.44	1.65	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403	PO4	O3-P-O1	4.64	127.36	110.95
6	B	404	PEG	O4-C4-C3	3.41	131.91	111.82
4	B	403	PO4	O4-P-O3	2.47	115.59	107.91
4	B	403	PO4	O2-P-O1	-2.43	102.37	110.95
6	B	404	PEG	O2-C2-C1	-2.18	100.53	110.11

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	405	GOL	1	0
6	B	404	PEG	8	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	397/399 (99%)	-0.15	1 (0%) 90 92	15, 24, 41, 58	0
1	B	396/399 (99%)	-0.26	6 (1%) 72 76	13, 20, 38, 59	0
2	C	3/3 (100%)	2.17	1 (33%) 1 1	25, 25, 30, 38	0
All	All	796/801 (99%)	-0.19	8 (1%) 79 83	13, 22, 40, 59	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	1	GLY	4.1
1	B	236	ILE	3.7
1	B	237	PRO	2.9
1	B	80	THR	2.6
1	B	238	GLY	2.1
1	A	7	GLY	2.1
1	B	129	HIS	2.1
1	B	239	VAL	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	PEG	B	404	7/7	0.89	0.13	26,32,39,40	0
5	GOL	A	404	6/6	0.93	0.11	22,28,32,37	0
5	GOL	A	405	6/6	0.94	0.10	25,35,38,40	0
4	PO4	B	403	5/5	0.98	0.07	14,15,18,19	0
4	PO4	A	403	5/5	0.98	0.06	17,18,22,23	0
3	MN	A	401	1/1	0.99	0.02	18,18,18,18	0
3	MN	B	402	1/1	1.00	0.02	15,15,15,15	0
3	MN	A	402	1/1	1.00	0.02	18,18,18,18	0
3	MN	B	401	1/1	1.00	0.02	14,14,14,14	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.