Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:18 PM UTC

PDB ID	:	6QSC / pdb_00006qsc
Title	:	Crystal Structure of Arg470His mutant of Human Prolidase with Mn ions and GlyPro ligand
Authors	:	Wilk, P.; Wator, E.; Weiss, M.S.
Deposited on	:	2019-02-20
Resolution	:	1.57 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:

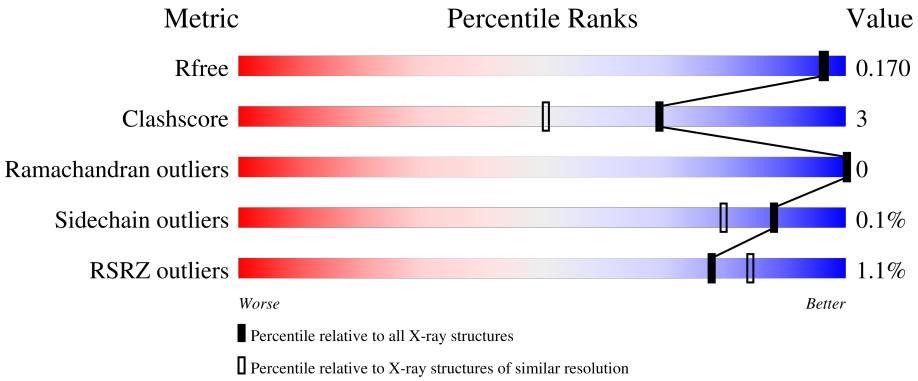
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

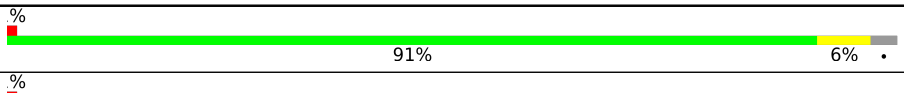
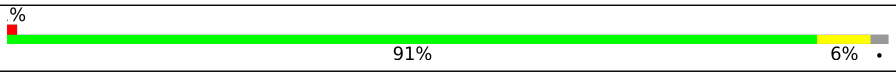
The reported resolution of this entry is 1.57 Å.

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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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.

Mol	Chain	Length	Quality of chain
1	A	493	
1	B	493	

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
3	MH2	A	500	-	-	X	-
4	GOL	A	504	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16478 atoms, of which 7613 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 Xaa-Pro dipeptidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	477	Total	C	H	N	O	S	0	22	0
			7585	2419	3766	660	708	32			
1	B	483	Total	C	H	N	O	S	0	16	0
			7607	2427	3775	660	713	32			

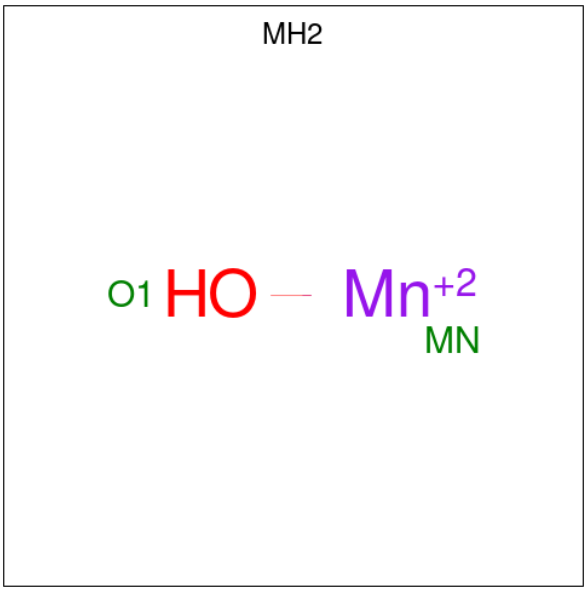
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	470	HIS	ARG	engineered mutation	UNP P12955
B	470	HIS	ARG	engineered mutation	UNP P12955

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

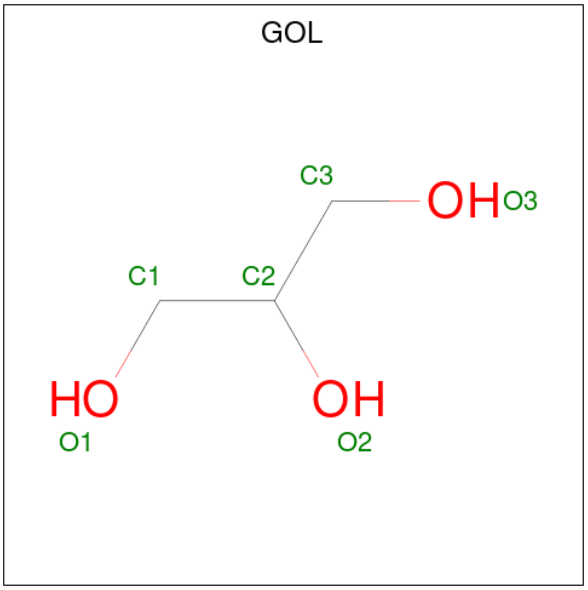
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		

- Molecule 3 is MANGANESE ION, 1 HYDROXYL COORDINATED (CCD ID: MH2) (formula: HMnO).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 11 3 5 3	0	0
4	A	1	Total C H O 11 3 5 3	0	0

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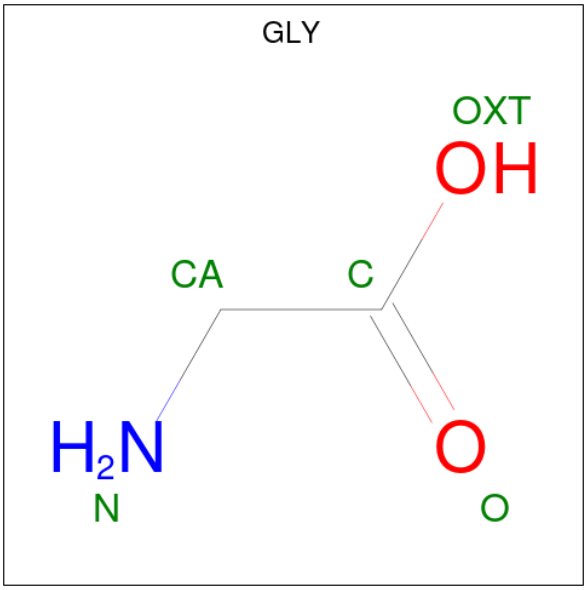
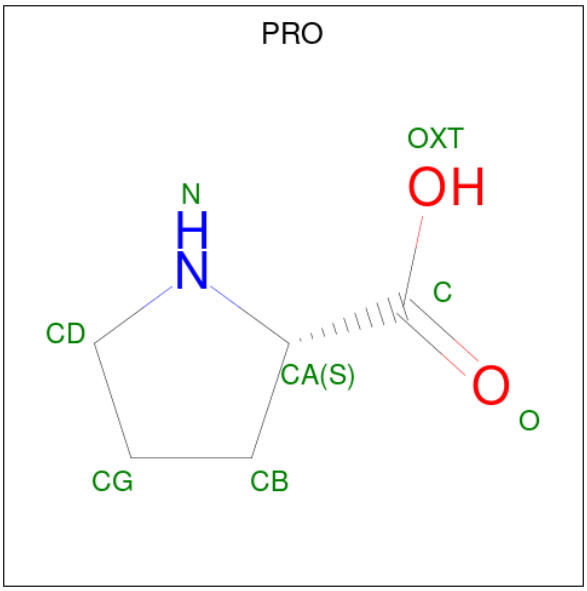
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			11	3	5	3		
4	B	1	Total	C	H	O	0	0
			11	3	5	3		
4	B	1	Total	C	H	O	0	0
			11	3	5	3		
4	B	1	Total	C	H	O	0	0
			11	3	5	3		
4	B	1	Total	C	H	O	0	0
			11	3	5	3		
4	B	1	Total	C	H	O	0	0
			11	3	5	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			9	2	5	1	1		
5	B	1	Total	C	H	N	O	0	0
			9	2	5	1	1		

- Molecule 6 is PROLINE (CCD ID: PRO) (formula: $C_5H_9NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H N O 15 5 7 1 2	0	0
6	B	1	Total C H N O 15 5 7 1 2	0	0

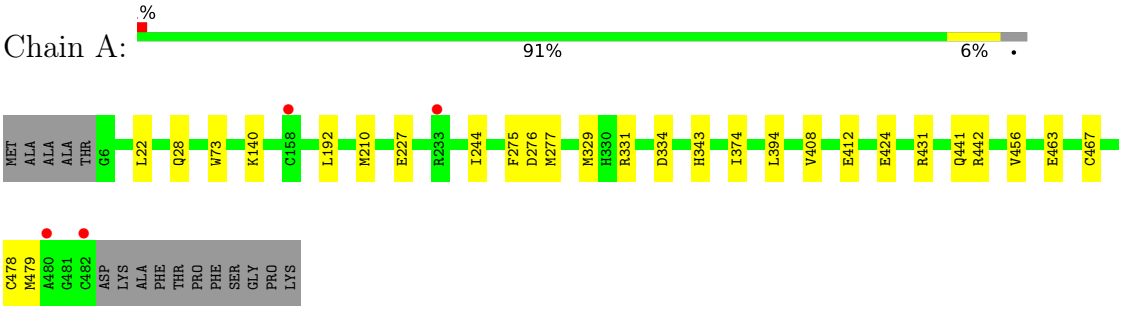
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	572	Total O 572 572	0	0
7	B	558	Total O 558 558	0	0

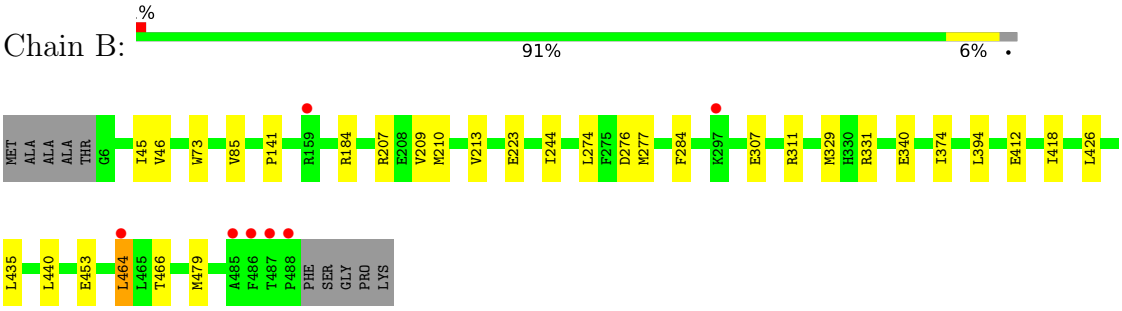
3 Residue-property plots (i)

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: Xaa-Pro dipeptidase



• Molecule 1: Xaa-Pro dipeptidase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	103.54Å 108.71Å 211.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.35 – 1.57 48.35 – 1.57	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.35-1.57) 99.8 (48.35-1.57)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 1.57Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.147 , 0.167 0.148 , 0.170	Depositor DCC
R_{free} test set	2100 reflections (1.27%)	wwPDB-VP
Wilson B-factor (Å^2)	22.8	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 49.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	16478	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MH2, GOL, MN

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	0.43	1/3981 (0.0%)	0.53	0/5386
1	B	0.44	0/3963	0.57	4/5362 (0.1%)
All	All	0.43	1/7944 (0.0%)	0.55	4/10748 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	140	LYS	C-O	-6.24	1.21	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	307[A]	GLU	CA-C-O	7.21	128.25	120.10
1	B	307[B]	GLU	CA-C-O	7.21	128.25	120.10
1	B	307[A]	GLU	N-CA-C	5.36	117.87	111.71
1	B	307[B]	GLU	N-CA-C	5.36	117.87	111.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3819	3766	3745	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3832	3775	3765	19	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	2	0
3	B	2	0	0	1	0
4	A	18	15	24	5	0
4	B	36	33	48	2	0
5	A	4	5	2	1	0
5	B	4	5	2	0	0
6	A	8	7	7	0	0
6	B	8	7	7	0	0
7	A	572	0	0	13	0
7	B	558	0	0	2	0
All	All	8865	7613	7600	53	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 (53) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331[B]:ARG:HD2	7:A:611:HOH:O	1.29	1.25
1:B:418:ILE:HG23	4:B:506:GOL:H31	1.53	0.89
4:A:503:GOL:H12	7:A:626:HOH:O	1.76	0.85
1:A:343[B]:HIS:CE1	7:A:608:HOH:O	2.33	0.81
1:A:478[B]:CYS:SG	7:A:793:HOH:O	2.38	0.80
1:A:467[A]:CYS:SG	7:A:1101:HOH:O	2.45	0.74
1:A:456[B]:VAL:CG2	1:A:463:GLU:HB3	2.19	0.72
1:B:464:LEU:HD22	1:B:466:THR:H	1.56	0.70
1:A:331[B]:ARG:CZ	1:A:394[B]:LEU:HD13	2.23	0.69
1:A:331[B]:ARG:CD	7:A:611:HOH:O	2.07	0.67
1:A:467[A]:CYS:SG	7:A:1045:HOH:O	2.54	0.65
1:A:408:VAL:HG22	1:A:456[B]:VAL:HG12	1.80	0.62
1:A:227:GLU:OE1	4:A:504:GOL:H2	2.00	0.61
1:A:331[B]:ARG:CZ	1:A:394[B]:LEU:CD1	2.80	0.59
1:A:73:TRP:HB2	1:A:374[B]:ILE:CD1	2.33	0.58
1:A:192:LEU:HD22	1:A:456[B]:VAL:HG11	1.86	0.58
1:A:331[B]:ARG:NH1	7:A:604:HOH:O	2.37	0.57
1:B:244:ILE:HB	1:B:276:ASP:HB3	1.87	0.57
4:A:504:GOL:H12	7:A:963:HOH:O	2.03	0.57
1:A:244:ILE:HB	1:A:276:ASP:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28[B]:GLN:NE2	7:A:602:HOH:O	1.63	0.56
1:B:207:ARG:HD3	7:B:664:HOH:O	2.06	0.55
1:A:456[B]:VAL:HG22	1:A:463:GLU:HB3	1.88	0.54
4:B:506:GOL:H12	7:B:959:HOH:O	2.07	0.54
1:B:45[B]:ILE:HD12	1:B:141:PRO:HB3	1.92	0.52
1:B:209:VAL:O	1:B:213[A]:VAL:HG23	2.10	0.51
1:A:331[B]:ARG:NH1	1:A:334:ASP:OD2	2.42	0.50
1:B:412:GLU:OE1	3:B:500:MH2:O1	2.29	0.49
1:A:331[B]:ARG:NH2	1:A:394[B]:LEU:HD13	2.28	0.49
1:A:210:MET:HG2	1:A:479:MET:HG2	1.95	0.48
1:A:412:GLU:OE1	3:A:500:MH2:O1	2.32	0.47
1:B:331:ARG:CZ	1:B:394:LEU:HD11	2.45	0.47
1:B:426:LEU:HG	1:B:435[B]:LEU:HD12	1.97	0.47
1:B:223:GLU:HA	1:B:277[A]:MET:HE1	1.97	0.46
4:A:504:GOL:H11	7:A:614:HOH:O	2.15	0.46
1:B:329:MET:HE2	1:B:329:MET:HA	1.97	0.46
1:B:453:GLU:OE1	1:B:464:LEU:HD11	2.14	0.46
1:A:22:LEU:C	1:A:22:LEU:HD23	2.41	0.46
1:A:424[B]:GLU:CD	1:A:431:ARG:HH22	2.23	0.46
1:A:275:PHE:HB3	1:A:277:MET:HE2	1.99	0.45
1:B:435[A]:LEU:HD12	1:B:440:LEU:HD22	1.99	0.45
1:A:331[A]:ARG:CZ	1:A:394[A]:LEU:HD11	2.46	0.44
1:B:311:ARG:NH1	1:B:340:GLU:OE2	2.48	0.44
4:A:504:GOL:H31	7:A:614:HOH:O	2.16	0.44
1:B:73:TRP:CD1	1:B:184:ARG:HG2	2.53	0.44
1:A:329:MET:HA	1:A:329:MET:HE2	2.01	0.43
1:B:284:PHE:CE2	1:B:374[A]:ILE:HD11	2.53	0.43
1:B:274:LEU:C	1:B:274:LEU:HD23	2.44	0.43
1:B:210:MET:HG2	1:B:479:MET:HG2	2.00	0.42
1:A:441[A]:GLN:HG3	1:A:442:ARG:N	2.34	0.42
1:B:46:VAL:O	1:B:85:VAL:HA	2.20	0.41
3:A:500:MH2:O1	5:A:506:GLY:C	2.64	0.41
1:A:331[A]:ARG:NH1	7:A:618:HOH:O	2.54	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	497/493 (101%)	488 (98%)	9 (2%)	0	100	100
1	B	497/493 (101%)	486 (98%)	11 (2%)	0	100	100
All	All	994/986 (101%)	974 (98%)	20 (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	421/410 (103%)	421 (100%)	0	100	100
1	B	418/410 (102%)	417 (100%)	1 (0%)	87	79
All	All	839/820 (102%)	838 (100%)	1 (0%)	88	80

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	464	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	GLN
1	A	358	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 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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	GOL	A	503	-	5,5,5	0.89	0	5,5,5	1.07	0
5	GLY	A	506	3,2	3,3,4	0.82	0	1,2,4	0.95	0
4	GOL	B	506	-	5,5,5	0.87	0	5,5,5	1.10	1 (20%)
4	GOL	B	508	-	5,5,5	0.73	0	5,5,5	0.81	0
4	GOL	B	507	-	5,5,5	1.00	0	5,5,5	0.63	0
3	MH2	B	500	1,2	0,1,1	-	-	-		
3	MH2	A	500	5,1,2	0,1,1	-	-	-		
4	GOL	B	503	-	5,5,5	0.80	0	5,5,5	1.18	1 (20%)
4	GOL	A	505	-	5,5,5	0.86	0	5,5,5	0.97	0
6	PRO	A	507	-	8,8,8	0.64	0	10,10,10	1.45	3 (30%)
4	GOL	B	504	-	5,5,5	0.79	0	5,5,5	1.11	0
6	PRO	B	510	-	8,8,8	0.75	0	10,10,10	1.36	1 (10%)
4	GOL	A	504	-	5,5,5	0.86	0	5,5,5	1.04	0
4	GOL	B	505	-	5,5,5	0.91	0	5,5,5	1.08	0
5	GLY	B	509	2	3,3,4	0.93	0	1,2,4	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	503	-	-	0/4/4/4	-
5	GLY	A	506	3,2	-	0/0/1/2	-
4	GOL	B	506	-	-	4/4/4/4	-
4	GOL	B	508	-	-	2/4/4/4	-
4	GOL	B	507	-	-	0/4/4/4	-
4	GOL	B	503	-	-	1/4/4/4	-
4	GOL	A	505	-	-	2/4/4/4	-
6	PRO	A	507	-	-	0/4/11/11	0/1/1/1
4	GOL	B	504	-	-	2/4/4/4	-
6	PRO	B	510	-	-	0/4/11/11	0/1/1/1
4	GOL	A	504	-	-	0/4/4/4	-
4	GOL	B	505	-	-	1/4/4/4	-
5	GLY	B	509	2	-	0/0/1/2	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	510	PRO	OXT-C-CA	2.32	121.38	113.51
6	A	507	PRO	CD-N-CA	2.31	113.18	107.22
6	A	507	PRO	OXT-C-O	-2.26	118.95	124.08
4	B	503	GOL	C3-C2-C1	-2.16	103.87	111.80
4	B	506	GOL	C3-C2-C1	-2.16	103.89	111.80
6	A	507	PRO	OXT-C-CA	2.05	120.44	113.51

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	504	GOL	C1-C2-C3-O3
4	B	506	GOL	C1-C2-C3-O3
4	B	508	GOL	C1-C2-C3-O3
4	B	508	GOL	O2-C2-C3-O3
4	A	505	GOL	C1-C2-C3-O3
4	B	506	GOL	O1-C1-C2-C3
4	B	506	GOL	O1-C1-C2-O2
4	B	506	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	B	504	GOL	O2-C2-C3-O3
4	A	505	GOL	O2-C2-C3-O3
4	B	503	GOL	O1-C1-C2-O2
4	B	505	GOL	O2-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	GOL	1	0
5	A	506	GLY	1	0
4	B	506	GOL	2	0
3	B	500	MH2	1	0
3	A	500	MH2	2	0
4	A	504	GOL	4	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, 95^{th} 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	477/493 (96%)	-0.45	4 (0%)	82	87	11, 26, 58, 110	19 (3%)
1	B	483/493 (97%)	-0.36	7 (1%)	73	80	12, 27, 63, 127	14 (2%)
All	All	960/986 (97%)	-0.41	11 (1%)	78	84	11, 26, 62, 127	33 (3%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	482	CYS	6.3
1	B	464	LEU	4.5
1	B	488	PRO	3.5
1	B	487	THR	3.2
1	B	486	PHE	2.4
1	B	485	ALA	2.4
1	B	159	ARG	2.3
1	A	233	ARG	2.2
1	A	480	ALA	2.1
1	B	297	LYS	2.1
1	A	158	CYS	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, 95^{th} 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
4	GOL	B	506	6/6	0.77	0.21	35,60,84,84	0
4	GOL	B	508	6/6	0.81	0.23	63,76,89,92	14
3	MH2	A	500	2/2	0.83	0.17	30,30,30,95	2
4	GOL	B	503	6/6	0.83	0.14	34,49,63,67	3
4	GOL	A	504	6/6	0.84	0.20	33,82,110,117	0
4	GOL	B	505	6/6	0.86	0.14	53,68,82,85	0
4	GOL	B	504	6/6	0.87	0.15	41,58,66,72	0
3	MH2	B	500	2/2	0.89	0.15	25,25,25,90	2
4	GOL	A	503	6/6	0.89	0.12	37,48,70,77	0
4	GOL	A	505	6/6	0.91	0.12	44,59,70,77	0
4	GOL	B	507	6/6	0.95	0.10	24,30,35,39	11
5	GLY	A	506	4/5	0.95	0.08	21,27,32,32	0
5	GLY	B	509	4/5	0.97	0.05	23,30,36,36	0
6	PRO	A	507	8/8	0.98	0.05	21,28,35,35	0
6	PRO	B	510	8/8	0.98	0.04	23,28,35,35	0
2	MN	B	499	1/1	0.99	0.03	26,26,26,26	1
2	MN	A	499	1/1	0.99	0.04	24,24,24,24	1

6.5 Other polymers (i)

There are no such residues in this entry.