



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2025 – 10:11 am BST

PDB ID : 9HPQ / pdb_00009hpq
Title : Peptide-substrate-binding (PSB) domain of human type I collagen prolyl 4-hydroxylase complexed with Pro-Pro-Gly-Pro-Arg-Gly-Pro-Pro-Gly.
Authors : Sulu, R.; Rahman, M.M.; Wierenga, R.K.; Koski, M.K.
Deposited on : 2024-12-16
Resolution : 2.17 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:

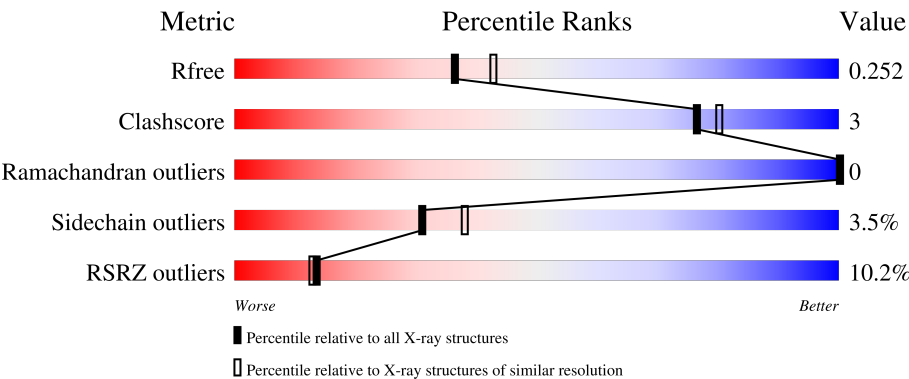
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

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 2.17 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}	164625	8336 (2.20-2.16)
Clashscore	180529	9404 (2.20-2.16)
Ramachandran outliers	177936	9297 (2.20-2.16)
Sidechain outliers	177891	9297 (2.20-2.16)
RSRZ outliers	164620	8337 (2.20-2.16)

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	105	<div><div>6%</div><div>90%6% . .</div></div>
1	B	105	<div><div>7%</div><div>89%6% . .</div></div>
1	C	105	<div><div>20%</div><div>82%7% . . 9%</div></div>
1	D	105	<div><div>3%</div><div>90%6% . .</div></div>
2	E	9	<div><div>22%</div><div>56%11%33%</div></div>

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Mol	Chain	Length	Quality of chain
2	F	9	<div><div>22%</div><div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div></div><div>78%</div><div>11%</div><div>11%</div></div>
2	G	9	<div><div>22%</div><div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div></div><div>56%</div><div>11%</div><div>33%</div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7309 atoms, of which 3555 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 Prolyl 4-hydroxylase subunit alpha-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	102	Total	C	H	N	O	S	31	1	0
			1673	547	819	137	167	3			
1	B	101	Total	C	H	N	O	S	28	0	0
			1639	535	804	132	165	3			
1	C	96	Total	C	H	N	O	S	21	2	0
			1594	518	790	125	158	3			
1	D	102	Total	C	H	N	O	S	31	1	0
			1665	543	817	135	167	3			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	MET	-	initiating methionine	UNP P13674
A	239	LEU	-	expression tag	UNP P13674
A	240	GLU	-	expression tag	UNP P13674
A	241	HIS	-	expression tag	UNP P13674
A	242	HIS	-	expression tag	UNP P13674
A	243	HIS	-	expression tag	UNP P13674
A	244	HIS	-	expression tag	UNP P13674
A	245	HIS	-	expression tag	UNP P13674
A	246	HIS	-	expression tag	UNP P13674
B	142	MET	-	initiating methionine	UNP P13674
B	239	LEU	-	expression tag	UNP P13674
B	240	GLU	-	expression tag	UNP P13674
B	241	HIS	-	expression tag	UNP P13674
B	242	HIS	-	expression tag	UNP P13674
B	243	HIS	-	expression tag	UNP P13674
B	244	HIS	-	expression tag	UNP P13674
B	245	HIS	-	expression tag	UNP P13674
B	246	HIS	-	expression tag	UNP P13674
C	142	MET	-	initiating methionine	UNP P13674
C	239	LEU	-	expression tag	UNP P13674
C	240	GLU	-	expression tag	UNP P13674

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Chain	Residue	Modelled	Actual	Comment	Reference
C	241	HIS	-	expression tag	UNP P13674
C	242	HIS	-	expression tag	UNP P13674
C	243	HIS	-	expression tag	UNP P13674
C	244	HIS	-	expression tag	UNP P13674
C	245	HIS	-	expression tag	UNP P13674
C	246	HIS	-	expression tag	UNP P13674
D	142	MET	-	initiating methionine	UNP P13674
D	239	LEU	-	expression tag	UNP P13674
D	240	GLU	-	expression tag	UNP P13674
D	241	HIS	-	expression tag	UNP P13674
D	242	HIS	-	expression tag	UNP P13674
D	243	HIS	-	expression tag	UNP P13674
D	244	HIS	-	expression tag	UNP P13674
D	245	HIS	-	expression tag	UNP P13674
D	246	HIS	-	expression tag	UNP P13674

- Molecule 2 is a protein called Synthetic peptide PRO-PRO-GLY-PRO-ARG-GLY-PRO-P RO-GLY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	6	Total	C	H	N	O	0	0	0
			80	25	40	9	6			
2	F	8	Total	C	H	N	O	0	0	0
			110	35	56	11	8			
2	G	6	Total	C	H	N	O	0	0	0
			80	25	40	9	6			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

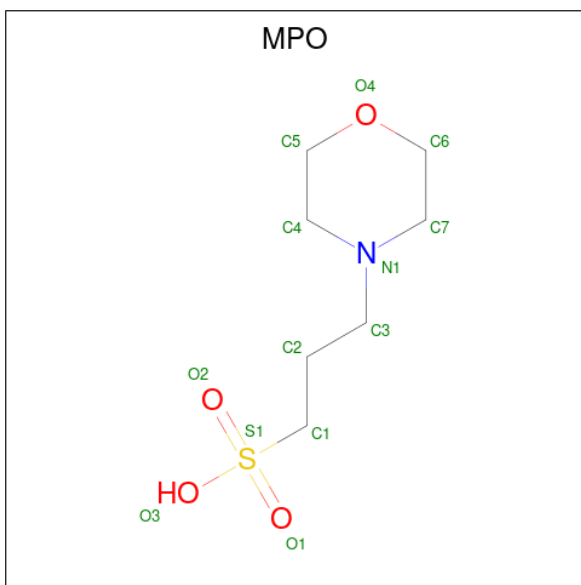
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



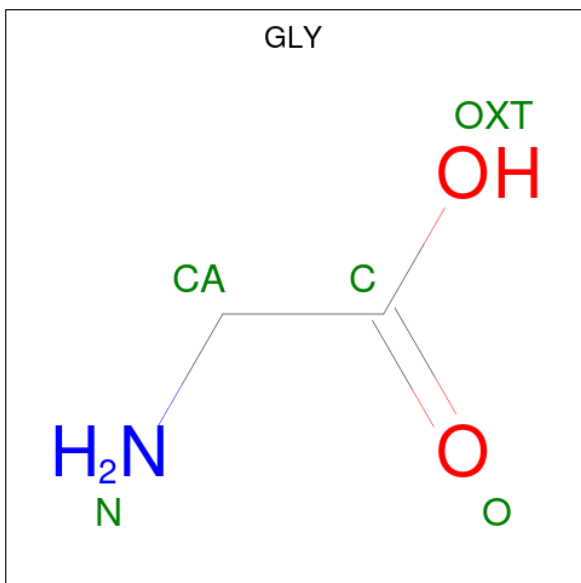
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	2	0
			22	6	14	2		
4	A	1	Total	C	H	O	2	0
			22	6	14	2		
4	B	1	Total	C	H	O	2	0
			22	6	14	2		
4	C	1	Total	C	H	O	2	0
			22	6	14	2		
4	D	1	Total	C	H	O	2	0
			22	6	14	2		
4	D	1	Total	C	H	O	2	0
			22	6	14	2		

- Molecule 5 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (CCD ID: MPO) (formula: $C_7H_{15}NO_4S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 28	C 7	H 15	N 1	O 4	S 1	1	0
5	C	1	Total 28	C 7	H 15	N 1	O 4	S 1	1	0
5	D	1	Total 28	C 7	H 15	N 1	O 4	S 1	1	0
5	F	1	Total 28	C 7	H 15	N 1	O 4	S 1	1	0

- Molecule 6 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
6	B	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
6	B	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
6	B	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
6	C	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
6	D	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
6	D	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
6	D	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
6	D	1	Total	C	H	N	O	0	0
			10	2	5	1	2		

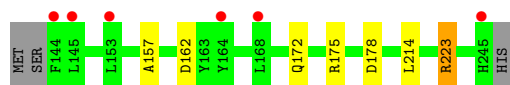
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	35	Total	O	0	0
			35	35		
7	B	31	Total	O	0	0
			31	31		
7	C	17	Total	O	0	0
			17	17		
7	D	43	Total	O	0	0
			43	43		
7	F	3	Total	O	0	0
			3	3		
7	G	1	Total	O	0	0
			1	1		

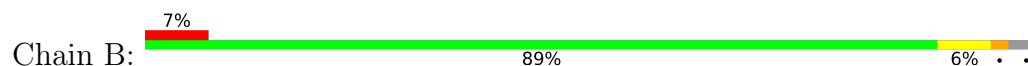
3 Residue-property plots [i](#)

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.

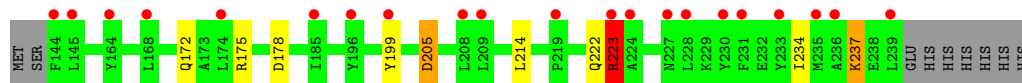
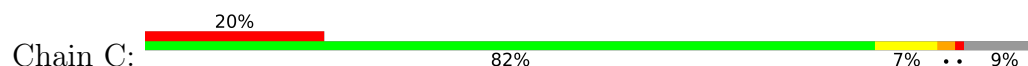
- Molecule 1: Prolyl 4-hydroxylase subunit alpha-1



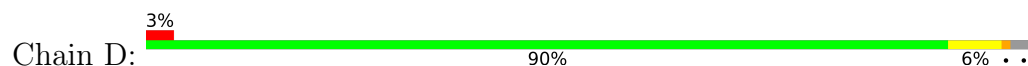
- Molecule 1: Prolyl 4-hydroxylase subunit alpha-1



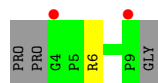
- Molecule 1: Prolyl 4-hydroxylase subunit alpha-1



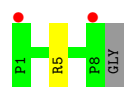
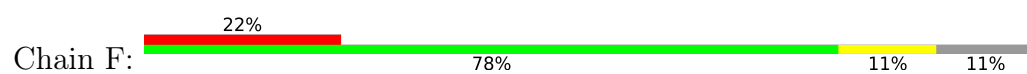
- Molecule 1: Prolyl 4-hydroxylase subunit alpha-1



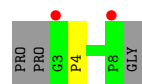
- Molecule 2: Synthetic peptide PRO-PRO-GLY-PRO-ARG-GLY-PRO-PRO-GLY



- Molecule 2: Synthetic peptide PRO-PRO-GLY-PRO-ARG-GLY-PRO-PRO-GLY



- Molecule 2: Synthetic peptide PRO-PRO-GLY-PRO-ARG-GLY-PRO-PRO-GLY



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	82.42Å 86.31Å 91.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.88 – 2.17 49.88 – 2.17	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.88-2.17) 99.4 (49.88-2.17)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.225 , 0.250 0.228 , 0.252	Depositor DCC
R_{free} test set	1726 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.116 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7309	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% 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: MG, MPO, MPD

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	0.57	0/877	0.99	1/1186 (0.1%)
1	B	0.60	0/853	1.00	2/1153 (0.2%)
1	C	0.57	0/825	1.02	1/1114 (0.1%)
1	D	0.62	0/870	1.02	2/1176 (0.2%)
2	E	0.74	0/42	1.15	0/57
2	F	0.83	0/58	1.03	0/80
2	G	0.76	0/42	1.39	1/57 (1.8%)
All	All	0.60	0/3567	1.01	7/4823 (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	B	0	1
1	C	0	2
2	F	0	1
All	All	0	4

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	205	ASP	CA-CB-CG	7.53	120.12	112.60
1	B	162	ASP	CA-CB-CG	5.94	118.54	112.60
2	G	4	PRO	CB-CA-C	-5.58	103.92	111.12
1	A	162	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	203	ASP	CA-CB-CG	5.15	117.75	112.60
1	D	192	ASP	CA-CB-CG	5.05	117.65	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	162	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	223	ARG	Sidechain
1	C	223[A]	ARG	Sidechain
1	C	223[B]	ARG	Sidechain
2	F	5	ARG	Sidechain

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	854	819	811	5	0
1	B	835	804	798	4	0
1	C	804	790	787	7	0
1	D	848	817	810	3	0
2	E	40	40	39	1	0
2	F	54	56	56	0	0
2	G	40	40	39	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	16	28	28	1	0
4	B	8	14	14	0	0
4	C	8	14	14	0	0
4	D	16	28	28	0	0
5	A	13	15	15	0	0
5	C	13	15	15	0	0
5	D	13	15	15	1	0
5	F	13	15	15	0	0
6	B	20	20	8	0	0
6	C	5	5	2	0	0
6	D	20	20	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	35	0	0	0	0
7	B	31	0	0	2	0
7	C	17	0	0	0	0
7	D	43	0	0	1	0
7	F	3	0	0	0	0
7	G	1	0	0	0	0
All	All	3754	3555	3502	20	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 (20) 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:172[A]:GLN:OE1	1:C:175:ARG:NH1	2.29	0.66
1:B:229:LYS:NZ	7:B:403:HOH:O	2.33	0.60
1:C:234:ILE:O	1:C:237:LYS:HG3	2.07	0.55
1:C:214:LEU:C	1:C:214:LEU:HD23	2.32	0.54
1:A:172:GLN:OE1	1:A:175:ARG:NH1	2.41	0.54
2:E:6:ARG:HH11	2:E:6:ARG:HG2	1.74	0.52
5:D:308:MPO:H22	7:D:402:HOH:O	2.10	0.51
1:D:214:LEU:HD23	1:D:214:LEU:C	2.37	0.50
1:A:214:LEU:C	1:A:214:LEU:HD23	2.38	0.49
1:B:214:LEU:C	1:B:214:LEU:HD23	2.39	0.46
1:A:157:ALA:HA	4:A:302:MPD:HM1	1.96	0.46
1:B:229:LYS:NZ	1:D:186:ASP:HB3	2.30	0.46
1:C:214:LEU:HD23	1:C:214:LEU:O	2.17	0.45
1:C:199:TYR:CD1	1:C:199:TYR:C	2.96	0.44
1:C:234:ILE:HD12	1:C:234:ILE:N	2.33	0.44
1:A:223:ARG:HH11	1:A:223:ARG:CG	2.30	0.44
1:A:223:ARG:HH11	1:A:223:ARG:HG2	1.81	0.43
1:C:223[B]:ARG:HH11	1:C:223[B]:ARG:HG3	1.83	0.42
1:D:231:PHE:O	1:D:235:MET:HG3	2.19	0.42
1:B:186:ASP:HA	7:B:421:HOH:O	2.20	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	101/105 (96%)	101 (100%)	0	0	100	100
1	B	99/105 (94%)	99 (100%)	0	0	100	100
1	C	96/105 (91%)	96 (100%)	0	0	100	100
1	D	101/105 (96%)	101 (100%)	0	0	100	100
2	E	4/9 (44%)	4 (100%)	0	0	100	100
2	F	6/9 (67%)	6 (100%)	0	0	100	100
2	G	4/9 (44%)	4 (100%)	0	0	100	100
All	All	411/447 (92%)	411 (100%)	0	0	100	100

There are no Ramachandran outliers to report.

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	91/93 (98%)	89 (98%)	2 (2%)	47	58
1	B	89/93 (96%)	85 (96%)	4 (4%)	23	27
1	C	86/93 (92%)	80 (93%)	6 (7%)	12	12
1	D	91/93 (98%)	89 (98%)	2 (2%)	47	58
2	E	4/6 (67%)	4 (100%)	0	100	100
2	F	6/6 (100%)	6 (100%)	0	100	100
2	G	4/6 (67%)	4 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	371/390 (95%)	357 (96%)	14 (4%)	31	34

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	ASP
1	A	223	ARG
1	B	143	SER
1	B	162	ASP
1	B	178	ASP
1	B	229	LYS
1	C	178	ASP
1	C	205	ASP
1	C	222	GLN
1	C	223[A]	ARG
1	C	223[B]	ARG
1	C	237	LYS
1	D	162	ASP
1	D	178	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	176	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 23 ligands modelled in this entry, 4 are monoatomic - leaving 19 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	MPD	D	307	-	7,7,7	0.24	0	9,10,10	0.64	0
5	MPO	A	304	-	13,13,13	0.62	1 (7%)	17,17,17	0.90	1 (5%)
6	GLY	B	302	-	4,4,4	0.87	0	3,4,4	1.23	0
5	MPO	C	304	-	13,13,13	0.69	1 (7%)	17,17,17	0.62	0
5	MPO	D	308	-	13,13,13	0.43	0	17,17,17	1.05	1 (5%)
4	MPD	B	306	-	7,7,7	0.15	0	9,10,10	0.36	0
4	MPD	C	303	-	7,7,7	0.23	0	9,10,10	0.26	0
4	MPD	A	303	-	7,7,7	0.20	0	9,10,10	0.42	0
6	GLY	B	301	-	4,4,4	0.98	0	3,4,4	1.15	0
6	GLY	D	303	-	4,4,4	1.07	0	3,4,4	1.09	0
6	GLY	D	301	-	4,4,4	0.91	0	3,4,4	1.18	0
4	MPD	A	302	-	7,7,7	0.20	0	9,10,10	0.39	0
6	GLY	B	303	-	4,4,4	0.94	0	3,4,4	1.27	0
5	MPO	F	101	-	13,13,13	0.48	0	17,17,17	1.04	1 (5%)
6	GLY	B	304	-	4,4,4	0.94	0	3,4,4	1.11	0
6	GLY	C	301	-	4,4,4	1.04	0	3,4,4	1.05	0
6	GLY	D	304	-	4,4,4	0.96	0	3,4,4	1.11	0
6	GLY	D	302	-	4,4,4	0.94	0	3,4,4	1.18	0
4	MPD	D	306	-	7,7,7	0.47	0	9,10,10	0.51	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	MPD	D	307	-	-	0/5/5/5	-
5	MPO	A	304	-	-	3/7/15/15	0/1/1/1
6	GLY	B	302	-	-	2/2/2/2	-
5	MPO	C	304	-	-	0/7/15/15	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MPO	D	308	-	-	1/7/15/15	0/1/1/1
4	MPD	B	306	-	-	0/5/5/5	-
4	MPD	C	303	-	-	3/5/5/5	-
4	MPD	A	303	-	-	2/5/5/5	-
6	GLY	B	301	-	-	0/2/2/2	-
6	GLY	D	303	-	-	2/2/2/2	-
6	GLY	D	301	-	-	2/2/2/2	-
4	MPD	A	302	-	-	1/5/5/5	-
6	GLY	B	303	-	-	2/2/2/2	-
5	MPO	F	101	-	-	1/7/15/15	0/1/1/1
6	GLY	B	304	-	-	0/2/2/2	-
6	GLY	C	301	-	-	0/2/2/2	-
6	GLY	D	304	-	-	2/2/2/2	-
6	GLY	D	302	-	-	0/2/2/2	-
4	MPD	D	306	-	-	0/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	304	MPO	O3-S1	2.18	1.55	1.47
5	A	304	MPO	O3-S1	2.02	1.54	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	308	MPO	O3-S1-C1	-3.68	99.81	105.77
5	F	101	MPO	O3-S1-C1	-3.47	100.16	105.77
5	A	304	MPO	O2-S1-O1	2.19	121.52	113.95

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	303	MPD	C2-C3-C4-O4
5	A	304	MPO	C2-C1-S1-O1
5	A	304	MPO	C2-C1-S1-O2
6	D	301	GLY	O-C-CA-N
6	D	301	GLY	OXT-C-CA-N
6	D	303	GLY	O-C-CA-N
6	D	303	GLY	OXT-C-CA-N

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Mol	Chain	Res	Type	Atoms
6	D	304	GLY	O-C-CA-N
6	D	304	GLY	OXT-C-CA-N
5	A	304	MPO	C2-C1-S1-O3
6	B	303	GLY	OXT-C-CA-N
5	F	101	MPO	C2-C3-N1-C4
5	D	308	MPO	C2-C3-N1-C4
4	C	303	MPD	O2-C2-C3-C4
6	B	302	GLY	O-C-CA-N
6	B	303	GLY	O-C-CA-N
4	A	303	MPD	C2-C3-C4-C5
4	C	303	MPD	C1-C2-C3-C4
4	C	303	MPD	CM-C2-C3-C4
4	A	302	MPD	O2-C2-C3-C4
6	B	302	GLY	OXT-C-CA-N

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	308	MPO	1	0
4	A	302	MPD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	102/105 (97%)	0.64	6 (5%)	29 29	38, 63, 81, 119	1 (0%)
1	B	101/105 (96%)	0.17	7 (6%)	24 24	35, 50, 87, 122	0
1	C	96/105 (91%)	1.12	21 (21%)	3 3	33, 67, 111, 147	2 (2%)
1	D	102/105 (97%)	0.18	3 (2%)	54 53	23, 53, 73, 97	1 (0%)
2	E	6/9 (66%)	1.40	2 (33%)	1 1	63, 79, 86, 97	0
2	F	8/9 (88%)	0.98	2 (25%)	2 2	56, 74, 89, 93	0
2	G	6/9 (66%)	1.88	2 (33%)	1 1	65, 79, 84, 85	0
All	All	421/447 (94%)	0.56	43 (10%)	13 13	23, 61, 96, 147	4 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	239	LEU	6.6
1	A	144	PHE	6.5
1	C	144	PHE	4.9
1	C	230	TYR	4.2
1	A	245	HIS	3.8
2	E	9	PRO	3.7
1	C	223[A]	ARG	3.6
1	B	239	LEU	3.5
1	D	244	HIS	3.5
1	B	144	PHE	3.4
1	C	231	PHE	3.3
2	G	8	PRO	3.2
2	F	8	PRO	2.9
1	C	228	LEU	2.8
1	C	185	ILE	2.7
1	A	168	LEU	2.7
1	C	196	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
2	E	4	GLY	2.6
1	C	208	LEU	2.5
1	C	199	TYR	2.5
1	C	209	LEU	2.5
1	C	236	ALA	2.4
1	A	153	LEU	2.4
1	C	145	LEU	2.3
1	D	143	SER	2.3
2	G	3	GLY	2.3
1	C	235	MET	2.3
1	B	143	SER	2.3
1	B	241	HIS	2.2
1	C	219	PRO	2.2
1	C	227	ASN	2.2
1	A	145	LEU	2.1
1	C	164	TYR	2.1
2	F	1	PRO	2.1
1	C	224	ALA	2.1
1	C	233	TYR	2.1
1	C	168	LEU	2.1
1	B	235	MET	2.1
1	A	164	TYR	2.0
1	C	174	LEU	2.0
1	D	235	MET	2.0
1	B	242	HIS	2.0
1	B	243	HIS	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, 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(\AA^2)	Q<0.9
3	MG	C	302	1/1	0.75	0.34	83,83,83,83	0
6	GLY	B	302	5/5	0.81	0.17	76,79,82,83	0
5	MPO	A	304	13/13	0.83	0.14	61,75,99,131	1
3	MG	B	305	1/1	0.86	0.08	65,65,65,65	0
6	GLY	D	301	5/5	0.88	0.17	86,87,90,91	0
5	MPO	C	304	13/13	0.89	0.12	65,90,94,103	2
4	MPD	A	302	8/8	0.90	0.21	65,83,94,96	2
6	GLY	C	301	5/5	0.91	0.13	78,80,85,85	0
3	MG	A	301	1/1	0.91	0.07	77,77,77,77	0
6	GLY	B	304	5/5	0.92	0.13	91,93,95,96	0
5	MPO	D	308	13/13	0.92	0.09	51,58,65,72	3
4	MPD	C	303	8/8	0.92	0.18	57,68,88,94	2
6	GLY	D	302	5/5	0.92	0.14	90,90,91,91	0
6	GLY	D	303	5/5	0.92	0.26	90,91,93,94	0
6	GLY	B	303	5/5	0.93	0.13	72,73,74,74	0
4	MPD	D	307	8/8	0.93	0.16	65,75,82,85	2
6	GLY	B	301	5/5	0.94	0.13	87,90,93,95	0
4	MPD	D	306	8/8	0.94	0.14	42,52,60,65	2
6	GLY	D	304	5/5	0.94	0.14	83,84,85,86	0
4	MPD	A	303	8/8	0.95	0.16	65,82,87,93	2
5	MPO	F	101	13/13	0.96	0.07	50,55,62,65	2
4	MPD	B	306	8/8	0.96	0.08	44,46,49,65	2
3	MG	D	305	1/1	0.98	0.04	73,73,73,73	0

6.5 Other polymers

There are no such residues in this entry.