



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2025 – 10:15 am BST

PDB ID : 9HRE / pdb_00009hre
Title : Peptide-substrate-binding (PSB) domain of human type I collagen prolyl 4-hydroxylase complexed with Pro-Hyp-Gly-Pro-Ala-Gly-Pro-Hyp-Gly.
Authors : Sulu, R.; Rahman, M.M.; Wierenga, R.K.; Koski, M.K.
Deposited on : 2024-12-18
Resolution : 2.05 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

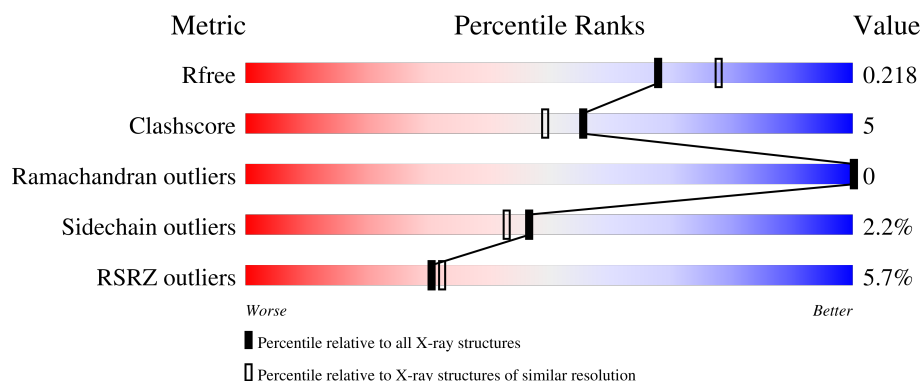
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2096 (2.04-2.04)
Clashscore	180529	2229 (2.04-2.04)
Ramachandran outliers	177936	2217 (2.04-2.04)
Sidechain outliers	177891	2217 (2.04-2.04)
RSRZ outliers	164620	2096 (2.04-2.04)

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>5%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div>.</div> </div> </div>
1	B	105	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>5%</div> </div> </div>
1	C	105	<div> <div>6%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>6%</div> </div> </div>
1	D	105	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>.</div> </div> </div>
2	E	9	<div> <div>11%</div> <div> <div></div> <div>44%</div> <div>11%</div> <div>44%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	9	<div><div></div><div>11%</div><div>89%</div><div>11%</div></div>
2	G	9	<div><div></div><div>22%</div><div>67%</div><div>11%</div><div>22%</div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7290 atoms, of which 3537 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	103	Total	C	H	N	O	S	32	0	0
			1675	547	820	138	167	3			
1	B	100	Total	C	H	N	O	S	27	0	0
			1628	532	799	131	163	3			
1	C	99	Total	C	H	N	O	S	24	1	0
			1622	528	801	127	163	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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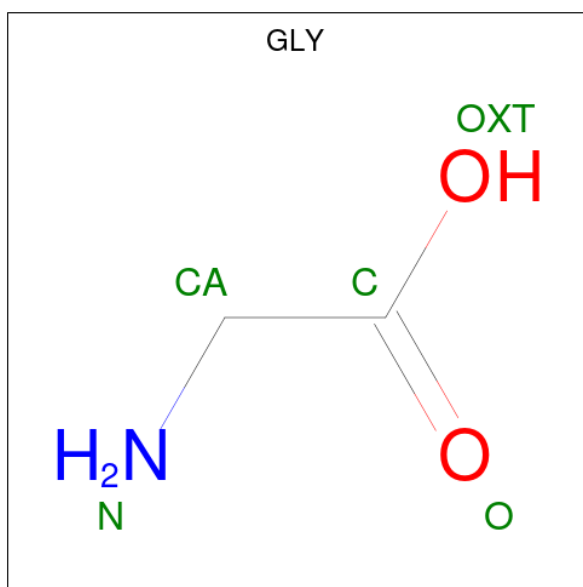
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Chain	Residue	Modelled	Actual	Comment	Reference
C	241	HIS	-	expression tag	UNP P13674
C	242	HIS	-	expression tag	UNP P13674
C	243	HIS	-	expression tag	UNP P13674
C	244	HIS	-	expression tag	UNP P13674
C	245	HIS	-	expression tag	UNP P13674
C	246	HIS	-	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-HYP-GLY-PRO-ALA-GLY-PRO-HY P-GLY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	5	Total	C	H	N	O	0	0	0
			52	17	25	5	5			
2	F	9	Total	C	H	N	O	2	0	0
			106	34	51	9	12			
2	G	7	Total	C	H	N	O	1	0	0
			75	24	35	7	9			

- Molecule 3 is GLYCINE (CCD ID: GLY) (formula: C₂H₅NO₂).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

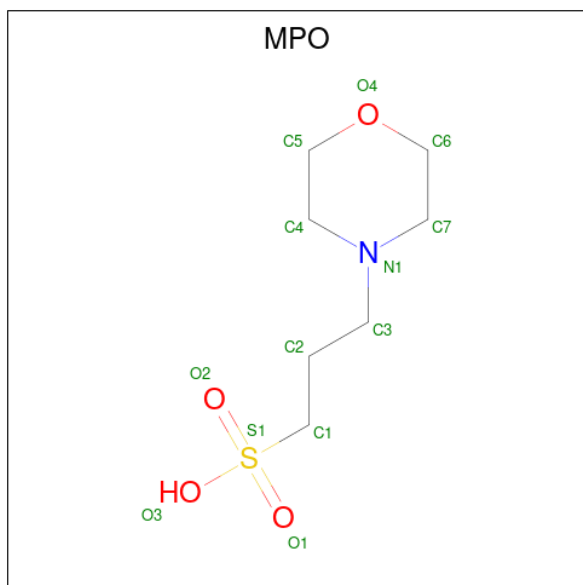
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

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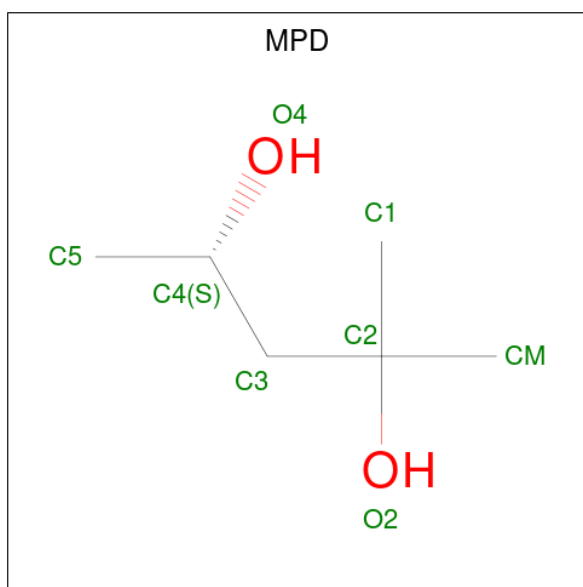
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Mg	0	0
			1	1		

- 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	C	H	N	O	S	1	0
			28	7	15	1	4	1		
5	B	1	Total	C	H	N	O	S	1	0
			28	7	15	1	4	1		
5	C	1	Total	C	H	N	O	S	1	0
			28	7	15	1	4	1		
5	D	1	Total	C	H	N	O	S	1	0
			28	7	15	1	4	1		

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	31	Total	O	0	0
			31	31		
7	B	30	Total	O	0	0
			30	30		
7	C	31	Total	O	0	0
			31	31		
7	D	32	Total	O	0	0
			32	32		
7	E	1	Total	O	0	0
			1	1		
7	F	2	Total	O	0	0
			2	2		

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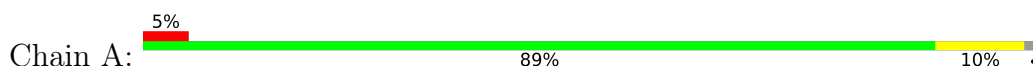
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	2	Total	O	0	0
			2	2		

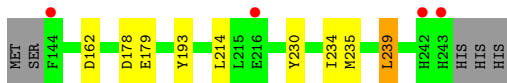
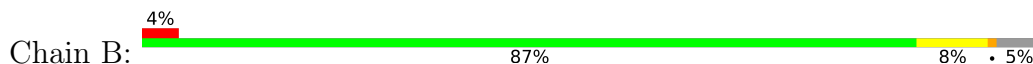
3 Residue-property plots [i](#)

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.

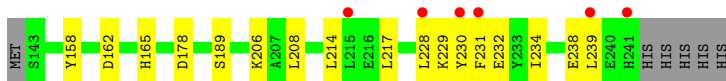
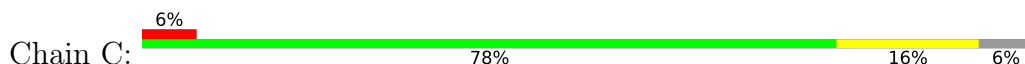
- Molecule 1: Prolyl 4-hydroxylase subunit alpha-1



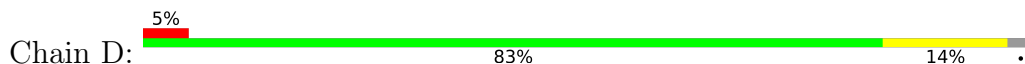
- Molecule 1: Prolyl 4-hydroxylase subunit alpha-1



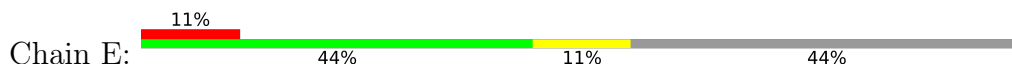
- Molecule 1: Prolyl 4-hydroxylase subunit alpha-1



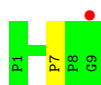
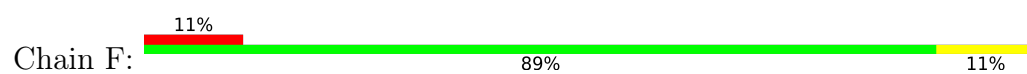
- Molecule 1: Prolyl 4-hydroxylase subunit alpha-1



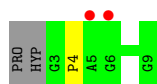
- Molecule 2: Synthetic peptide PRO-HYP-GLY-PRO-ALA-GLY-PRO-HYP-GLY



- Molecule 2: Synthetic peptide PRO-HYP-GLY-PRO-ALA-GLY-PRO-HYP-GLY



- Molecule 2: Synthetic peptide PRO-HYP-GLY-PRO-ALA-GLY-PRO-HYP-GLY



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	81.04Å 85.56Å 92.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.89 – 2.05 62.89 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.5 (62.89-2.05) 98.5 (62.89-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.88)	Depositor
R, R_{free}	0.197 , 0.218 0.197 , 0.218	Depositor DCC
R_{free} test set	1965 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.9	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	0.96	EDS
Total number of atoms	7290	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.00% 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: MPO, HYP, MG, 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	0.62	0/875	0.99	0/1183
1	B	0.61	0/847	1.05	2/1145 (0.2%)
1	C	0.64	0/840	1.04	2/1134 (0.2%)
1	D	0.63	0/870	1.01	2/1176 (0.2%)
2	E	0.70	0/28	1.11	0/38
2	F	0.77	0/39	0.93	0/48
2	G	0.76	0/32	1.02	0/40
All	All	0.63	0/3531	1.02	6/4764 (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	D	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	235	MET	CG-SD-CE	6.42	115.02	100.90
1	B	178	ASP	CA-CB-CG	5.68	118.28	112.60
1	C	238	GLU	CB-CG-CD	5.36	121.72	112.60
1	D	192	ASP	CA-CB-CG	5.28	117.88	112.60
1	C	206	LYS	CB-CG-CD	5.23	123.34	111.30
1	D	149	ASP	CA-CB-CG	5.14	117.74	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	175	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	855	820	812	7	0
1	B	829	799	793	5	0
1	C	821	801	797	10	0
1	D	848	817	810	13	0
2	E	27	25	24	1	0
2	F	55	51	51	1	0
2	G	40	35	34	3	0
3	A	5	5	2	0	0
3	B	10	10	4	0	0
3	C	5	5	2	0	0
3	D	25	25	10	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	13	15	15	0	0
5	B	13	15	15	1	0
5	C	13	15	15	1	0
5	D	13	15	15	0	0
6	A	16	28	28	0	0
6	B	8	14	14	0	0
6	C	8	14	14	0	0
6	D	16	28	28	1	0
7	A	31	0	0	2	0
7	B	30	0	0	0	0
7	C	31	0	0	0	0
7	D	32	0	0	1	0
7	E	1	0	0	0	0
7	F	2	0	0	1	0
7	G	2	0	0	0	0
All	All	3753	3537	3483	33	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 5.

All (33) 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:230:TYR:CZ	1:B:234:ILE:HD11	2.31	0.66
1:D:230:TYR:CZ	1:D:234:ILE:HD11	2.33	0.63
1:A:241:HIS:ND1	7:A:401:HOH:O	2.31	0.63
1:C:208:LEU:HD13	1:C:231:PHE:CD2	2.35	0.62
5:B:304:MPO:H61	7:F:102:HOH:O	2.00	0.61
1:A:184:THR:HA	1:C:229[B]:LYS:HD3	1.83	0.60
1:A:199:TYR:CE1	2:E:5:PRO:HG2	2.41	0.55
1:D:199:TYR:CE2	2:G:4:PRO:HD2	2.43	0.53
1:D:230:TYR:OH	1:D:234:ILE:HD11	2.09	0.52
1:B:230:TYR:OH	1:B:234:ILE:HD11	2.10	0.52
1:D:199:TYR:CE2	2:G:4:PRO:CD	2.94	0.50
1:C:214:LEU:C	1:C:214:LEU:HD23	2.37	0.49
1:C:230:TYR:O	1:C:234:ILE:HG12	2.11	0.49
1:C:217:LEU:HD22	1:D:216:GLU:HB3	1.96	0.47
1:A:143:SER:OG	1:A:144:PHE:N	2.45	0.47
1:C:228:LEU:O	1:C:232:GLU:HG3	2.14	0.47
1:D:158:TYR:HE2	1:D:196:TYR:HD2	1.63	0.46
1:A:214:LEU:HD23	1:A:214:LEU:C	2.41	0.46
1:C:214:LEU:HD23	1:C:214:LEU:O	2.16	0.46
1:D:229:LYS:HE3	7:D:402:HOH:O	2.16	0.45
1:D:158:TYR:HE2	1:D:196:TYR:CD2	2.34	0.45
1:B:193:TYR:CD1	2:F:7:PRO:HG2	2.51	0.45
1:A:162:ASP:OD2	1:A:165:HIS:ND1	2.44	0.44
1:D:144:PHE:O	3:D:305:GLY:CA	2.65	0.44
1:D:214:LEU:C	1:D:214:LEU:HD23	2.42	0.44
1:C:162:ASP:OD2	1:C:165:HIS:ND1	2.45	0.44
1:B:214:LEU:C	1:B:214:LEU:HD23	2.43	0.43
1:D:157:ALA:HA	6:D:308:MPD:H53	2.01	0.42
1:B:239:LEU:CD1	1:C:239:LEU:HG	2.50	0.42
1:D:199:TYR:CZ	2:G:4:PRO:HD3	2.55	0.42
1:D:144:PHE:O	3:D:305:GLY:HA3	2.21	0.41
1:C:158:TYR:CZ	5:C:303:MPO:H31	2.56	0.41
1:A:200:GLN:NE2	7:A:403:HOH:O	2.53	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	98/105 (93%)	98 (100%)	0	0	100	100
1	C	98/105 (93%)	98 (100%)	0	0	100	100
1	D	101/105 (96%)	100 (99%)	1 (1%)	0	100	100
2	E	3/9 (33%)	3 (100%)	0	0	100	100
2	F	5/9 (56%)	5 (100%)	0	0	100	100
2	G	4/9 (44%)	4 (100%)	0	0	100	100
All	All	410/447 (92%)	409 (100%)	1 (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%)	90 (99%)	1 (1%)	70	71
1	B	88/93 (95%)	85 (97%)	3 (3%)	32	26
1	C	88/93 (95%)	86 (98%)	2 (2%)	45	41
1	D	91/93 (98%)	89 (98%)	2 (2%)	47	43
2	E	2/3 (67%)	2 (100%)	0	100	100
2	F	3/3 (100%)	3 (100%)	0	100	100
2	G	2/3 (67%)	2 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	365/381 (96%)	357 (98%)	8 (2%)	47 43

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	SER
1	B	162	ASP
1	B	179	GLU
1	B	239	LEU
1	C	178	ASP
1	C	189	SER
1	D	162	ASP
1	D	178	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	GLN
1	A	200	GLN
1	B	200	GLN
1	C	172	GLN
1	C	200	GLN
1	D	200	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HYP	F	8	2	6,8,9	0.62	0	5,10,12	1.26	0
2	HYP	G	8	2	6,8,9	0.49	0	5,10,12	1.03	0
2	HYP	F	2	2	6,8,9	0.55	0	5,10,12	1.20	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
2	HYP	F	8	2	-	0/0/11/13	0/1/1/1
2	HYP	G	8	2	-	0/0/11/13	0/1/1/1
2	HYP	F	2	2	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
5	MPO	B	304	-	13,13,13	0.65	1 (7%)	17,17,17	0.99	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MPD	A	305	-	7,7,7	0.26	0	9,10,10	0.68	0
6	MPD	B	305	-	7,7,7	0.35	0	9,10,10	0.52	0
5	MPO	A	303	-	13,13,13	0.68	1 (7%)	17,17,17	0.93	1 (5%)
3	GLY	D	302	-	4,4,4	0.88	0	3,4,4	1.21	0
3	GLY	D	305	-	4,4,4	0.96	0	3,4,4	1.17	0
3	GLY	B	301	-	4,4,4	0.92	0	3,4,4	1.12	0
6	MPD	D	308	-	7,7,7	0.21	0	9,10,10	0.78	0
3	GLY	D	301	-	4,4,4	1.01	0	3,4,4	1.09	0
5	MPO	C	303	-	13,13,13	0.49	0	17,17,17	1.18	2 (11%)
6	MPD	D	309	-	7,7,7	0.27	0	9,10,10	0.49	0
3	GLY	A	301	-	4,4,4	0.98	0	3,4,4	1.22	0
3	GLY	D	304	-	4,4,4	0.95	0	3,4,4	1.10	0
3	GLY	B	302	-	4,4,4	1.01	0	3,4,4	1.15	0
6	MPD	C	304	-	7,7,7	0.37	0	9,10,10	0.69	0
5	MPO	D	307	-	13,13,13	0.50	0	17,17,17	1.11	2 (11%)
6	MPD	A	304	-	7,7,7	0.47	0	9,10,10	0.63	0
3	GLY	C	301	-	4,4,4	1.11	0	3,4,4	1.03	0
3	GLY	D	303	-	4,4,4	0.97	0	3,4,4	1.15	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
5	MPO	B	304	-	-	3/7/15/15	0/1/1/1
6	MPD	A	305	-	-	1/5/5/5	-
6	MPD	B	305	-	-	0/5/5/5	-
5	MPO	A	303	-	-	4/7/15/15	0/1/1/1
3	GLY	D	302	-	-	2/2/2/2	-
3	GLY	D	305	-	-	0/2/2/2	-
3	GLY	B	301	-	-	2/2/2/2	-
6	MPD	D	308	-	-	0/5/5/5	-
3	GLY	D	301	-	-	0/2/2/2	-
5	MPO	C	303	-	-	1/7/15/15	0/1/1/1
6	MPD	D	309	-	-	2/5/5/5	-
3	GLY	A	301	-	-	0/2/2/2	-
3	GLY	D	304	-	-	0/2/2/2	-
3	GLY	B	302	-	-	2/2/2/2	-
6	MPD	C	304	-	-	4/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MPO	D	307	-	-	1/7/15/15	0/1/1/1
6	MPD	A	304	-	-	3/5/5/5	-
3	GLY	C	301	-	-	2/2/2/2	-
3	GLY	D	303	-	-	2/2/2/2	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	303	MPO	O3-S1	2.27	1.55	1.47
5	B	304	MPO	O3-S1	2.15	1.55	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	303	MPO	O3-S1-C1	-3.80	99.61	105.77
5	B	304	MPO	O3-S1-C1	-3.31	100.42	105.77
5	D	307	MPO	O3-S1-C1	-2.81	101.23	105.77
5	A	303	MPO	O3-S1-C1	-2.55	101.64	105.77
5	C	303	MPO	O2-S1-O1	2.13	121.31	113.95
5	D	307	MPO	O3-S1-O1	-2.08	106.18	111.27

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	301	GLY	O-C-CA-N
3	B	302	GLY	O-C-CA-N
3	B	302	GLY	OXT-C-CA-N
3	C	301	GLY	O-C-CA-N
3	C	301	GLY	OXT-C-CA-N
3	D	302	GLY	O-C-CA-N
3	D	302	GLY	OXT-C-CA-N
5	C	303	MPO	S1-C1-C2-C3
6	D	309	MPD	C2-C3-C4-O4
5	A	303	MPO	C2-C1-S1-O3
3	B	301	GLY	OXT-C-CA-N
3	D	303	GLY	OXT-C-CA-N
3	D	303	GLY	O-C-CA-N
5	B	304	MPO	C2-C3-N1-C4
5	A	303	MPO	C2-C1-S1-O1

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Mol	Chain	Res	Type	Atoms
5	A	303	MPO	C2-C1-S1-O2
5	B	304	MPO	C2-C1-S1-O2
5	D	307	MPO	C2-C1-S1-O2
6	A	304	MPD	O2-C2-C3-C4
6	C	304	MPD	O2-C2-C3-C4
6	D	309	MPD	C2-C3-C4-C5
6	A	304	MPD	C1-C2-C3-C4
6	A	304	MPD	CM-C2-C3-C4
6	C	304	MPD	C1-C2-C3-C4
6	C	304	MPD	CM-C2-C3-C4
5	A	303	MPO	C1-C2-C3-N1
5	B	304	MPO	C2-C1-S1-O3
6	A	305	MPD	C2-C3-C4-O4
6	C	304	MPD	C2-C3-C4-O4

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	304	MPO	1	0
3	D	305	GLY	2	0
6	D	308	MPD	1	0
5	C	303	MPO	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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	103/105 (98%)	0.16	5 (4%)	36 38	36, 54, 76, 102	0
1	B	100/105 (95%)	0.23	4 (4%)	43 45	37, 54, 98, 115	0
1	C	99/105 (94%)	0.46	6 (6%)	28 29	36, 56, 108, 126	1 (1%)
1	D	102/105 (97%)	0.26	5 (4%)	36 38	25, 55, 80, 106	1 (0%)
2	E	5/9 (55%)	1.46	1 (20%)	3 2	77, 81, 92, 106	0
2	F	7/9 (77%)	0.63	1 (14%)	7 7	62, 64, 104, 111	0
2	G	6/9 (66%)	1.93	2 (33%)	1 0	84, 87, 99, 125	0
All	All	422/447 (94%)	0.32	24 (5%)	30 32	25, 55, 98, 126	2 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	178	ASP	3.8
1	D	145	LEU	3.8
2	G	5	ALA	3.7
1	C	241	HIS	3.6
1	C	230	TYR	3.4
2	E	4	GLY	3.4
1	D	244	HIS	3.2
1	B	144	PHE	3.1
1	B	242	HIS	3.1
2	G	6	GLY	2.9
1	B	243	HIS	2.9
1	A	245	HIS	2.8
1	C	239	LEU	2.8
1	D	204	LEU	2.7
1	A	144	PHE	2.7
1	A	180	GLY	2.6
1	D	203	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
2	F	9	GLY	2.4
1	C	231	PHE	2.4
1	C	215	LEU	2.3
1	C	228	LEU	2.2
1	D	235	MET	2.2
1	A	196	TYR	2.1
1	B	216	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	HYP	F	8	8/9	0.76	0.13	90,98,102,109	1
2	HYP	G	8	8/9	0.76	0.11	112,121,124,124	1
2	HYP	F	2	8/9	0.86	0.08	82,90,97,101	1

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(Å ²)	Q<0.9
3	GLY	D	305	5/5	0.73	0.16	98,107,114,116	0
3	GLY	C	301	5/5	0.84	0.16	75,82,84,84	0
3	GLY	D	302	5/5	0.85	0.13	88,98,99,108	0
5	MPO	A	303	13/13	0.88	0.11	67,81,105,135	1
5	MPO	C	303	13/13	0.88	0.13	66,82,97,103	2
5	MPO	D	307	13/13	0.88	0.13	69,85,95,98	2
3	GLY	B	301	5/5	0.89	0.15	83,93,102,104	0
3	GLY	D	304	5/5	0.89	0.14	91,93,96,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GLY	A	301	5/5	0.90	0.15	91,97,106,110	0
5	MPO	B	304	13/13	0.90	0.10	62,75,80,90	2
6	MPD	D	309	8/8	0.90	0.22	79,103,109,145	2
6	MPD	A	305	8/8	0.93	0.20	74,96,105,139	2
3	GLY	D	303	5/5	0.93	0.11	79,104,109,111	0
6	MPD	C	304	8/8	0.94	0.11	43,51,54,67	2
6	MPD	D	308	8/8	0.94	0.12	49,62,72,76	2
3	GLY	D	301	5/5	0.94	0.11	74,86,88,89	0
3	GLY	B	302	5/5	0.95	0.10	84,84,88,89	0
6	MPD	B	305	8/8	0.96	0.10	44,53,58,61	2
6	MPD	A	304	8/8	0.96	0.10	42,46,50,75	2
4	MG	D	306	1/1	0.97	0.07	90,90,90,90	0
4	MG	B	303	1/1	0.98	0.04	59,59,59,59	0
4	MG	A	302	1/1	0.98	0.07	61,61,61,61	0
4	MG	C	302	1/1	1.00	0.05	63,63,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.