



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:42 PM UTC

PDB ID : 5UW7 / pdb_00005uw7
Title : PCY1 Y481F Variant in Complex with Follower Peptide
Authors : Chekan, J.R.; Nair, S.K.
Deposited on : 2017-02-20
Resolution : 2.37 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
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

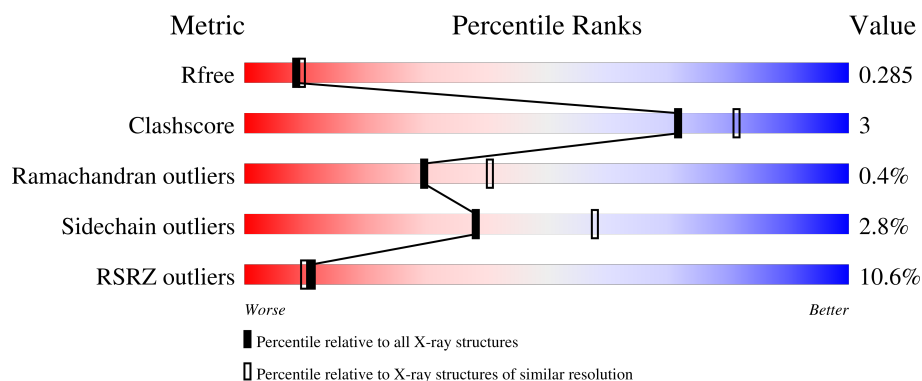
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	750	7% 80% 8% 11%
1	B	750	11% 78% 9% 13%
2	C	19	32% 68%
2	D	19	32% 68%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10789 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 Peptide cyclase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	666	Total	C	N	O	S	0	2	0
			5369	3433	910	999	27			
1	B	656	Total	C	N	O	S	0	3	0
			5308	3405	901	976	26			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	-	initiating methionine	UNP R4P353
A	-24	SER	-	expression tag	UNP R4P353
A	-23	TYR	-	expression tag	UNP R4P353
A	-22	TYR	-	expression tag	UNP R4P353
A	-21	HIS	-	expression tag	UNP R4P353
A	-20	HIS	-	expression tag	UNP R4P353
A	-19	HIS	-	expression tag	UNP R4P353
A	-18	HIS	-	expression tag	UNP R4P353
A	-17	HIS	-	expression tag	UNP R4P353
A	-16	HIS	-	expression tag	UNP R4P353
A	-15	LEU	-	expression tag	UNP R4P353
A	-14	GLU	-	expression tag	UNP R4P353
A	-13	SER	-	expression tag	UNP R4P353
A	-12	THR	-	expression tag	UNP R4P353
A	-11	SER	-	expression tag	UNP R4P353
A	-10	LEU	-	expression tag	UNP R4P353
A	-9	TYR	-	expression tag	UNP R4P353
A	-8	LYS	-	expression tag	UNP R4P353
A	-7	LYS	-	expression tag	UNP R4P353
A	-6	ALA	-	expression tag	UNP R4P353
A	-5	GLY	-	expression tag	UNP R4P353
A	-4	SER	-	expression tag	UNP R4P353
A	-3	GLU	-	expression tag	UNP R4P353
A	-2	PHE	-	expression tag	UNP R4P353
A	-1	ALA	-	expression tag	UNP R4P353

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	LEU	-	expression tag	UNP R4P353
A	481	PHE	TYR	conflict	UNP R4P353
B	-25	MET	-	initiating methionine	UNP R4P353
B	-24	SER	-	expression tag	UNP R4P353
B	-23	TYR	-	expression tag	UNP R4P353
B	-22	TYR	-	expression tag	UNP R4P353
B	-21	HIS	-	expression tag	UNP R4P353
B	-20	HIS	-	expression tag	UNP R4P353
B	-19	HIS	-	expression tag	UNP R4P353
B	-18	HIS	-	expression tag	UNP R4P353
B	-17	HIS	-	expression tag	UNP R4P353
B	-16	HIS	-	expression tag	UNP R4P353
B	-15	LEU	-	expression tag	UNP R4P353
B	-14	GLU	-	expression tag	UNP R4P353
B	-13	SER	-	expression tag	UNP R4P353
B	-12	THR	-	expression tag	UNP R4P353
B	-11	SER	-	expression tag	UNP R4P353
B	-10	LEU	-	expression tag	UNP R4P353
B	-9	TYR	-	expression tag	UNP R4P353
B	-8	LYS	-	expression tag	UNP R4P353
B	-7	LYS	-	expression tag	UNP R4P353
B	-6	ALA	-	expression tag	UNP R4P353
B	-5	GLY	-	expression tag	UNP R4P353
B	-4	SER	-	expression tag	UNP R4P353
B	-3	GLU	-	expression tag	UNP R4P353
B	-2	PHE	-	expression tag	UNP R4P353
B	-1	ALA	-	expression tag	UNP R4P353
B	0	LEU	-	expression tag	UNP R4P353
B	481	PHE	TYR	conflict	UNP R4P353

- Molecule 2 is a protein called Presegetalin A1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	0	0	0
			38	23	7	8			
2	D	6	Total	C	N	O	0	0	0
			38	23	7	8			

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

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

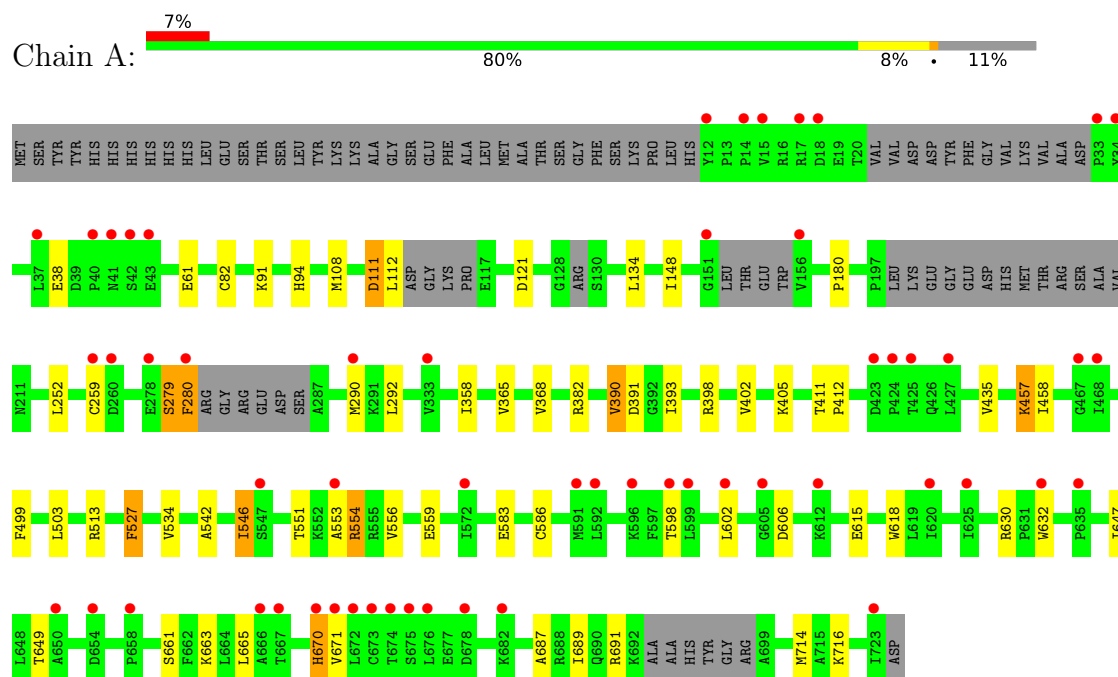
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	19	Total 19	O 19	0	0
4	B	16	Total 16	O 16	0	0

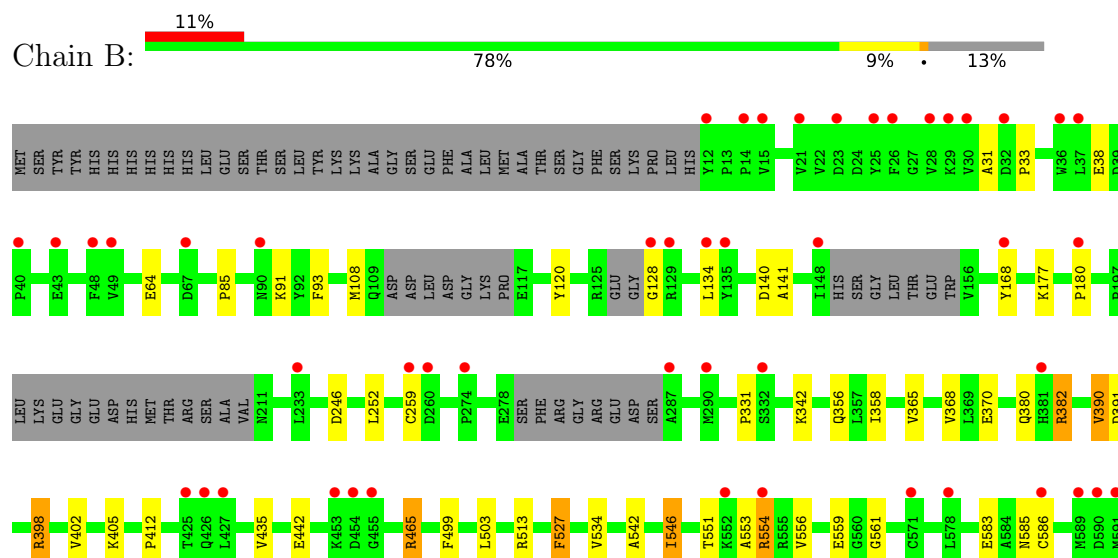
3 Residue-property plots [i](#)

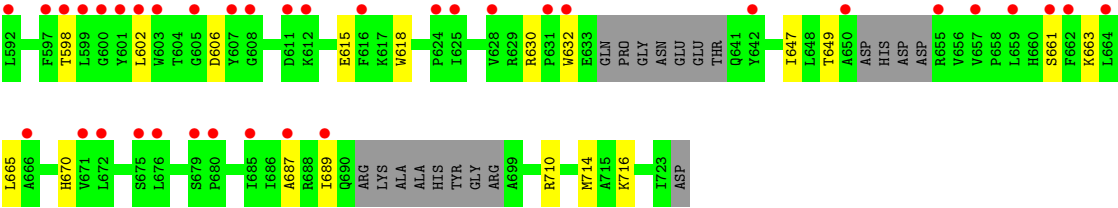
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Peptide cyclase 1

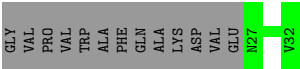


• Molecule 1: Peptide cyclase 1





● Molecule 2: Presegetalin A1



● Molecule 2: Presegetalin A1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	86.95Å 59.63Å 134.16Å 90.00° 93.12° 90.00°	Depositor
Resolution (Å)	86.80 – 2.37 86.80 – 2.37	Depositor EDS
% Data completeness (in resolution range)	99.2 (86.80-2.37) 99.2 (86.80-2.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.236 , 0.284 0.240 , 0.285	Depositor DCC
R_{free} test set	2744 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	42.4	Xtriage
Anisotropy	0.633	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10789	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.75	2/5501 (0.0%)	0.85	2/7438 (0.0%)
1	B	0.73	0/5437	0.85	2/7351 (0.0%)
2	C	0.85	0/38	0.74	0/52
2	D	0.83	0/38	0.61	0/52
All	All	0.74	2/11014 (0.0%)	0.85	4/14893 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	ASP	C-O	-5.25	1.20	1.25
1	A	411	THR	C-O	-5.09	1.21	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	546	ILE	CB-CA-C	-6.04	104.26	111.81
1	A	546	ILE	CB-CA-C	-5.70	104.68	111.81
1	B	331	PRO	N-CA-C	5.18	120.67	113.98
1	A	393	ILE	CB-CA-C	-5.03	106.47	111.80

There are no chirality outliers.

There are no planarity outliers.

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	5369	0	5222	35	0
1	B	5308	0	5195	37	0
2	C	38	0	36	0	0
2	D	38	0	36	0	0
3	A	1	0	0	0	0
4	A	19	0	0	0	0
4	B	16	0	0	1	0
All	All	10789	0	10489	71	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 (71) 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:290[B]:MET:HE1	1:A:292:LEU:HA	1.69	0.74
1:A:457:LYS:HG2	1:A:457:LYS:O	1.89	0.70
1:A:457:LYS:O	1:A:458:ILE:HD13	1.91	0.70
1:B:134:LEU:CD1	1:B:180:PRO:HA	2.25	0.67
1:A:290[B]:MET:HE1	1:A:292:LEU:CA	2.30	0.62
1:B:390:VAL:HA	1:B:405:LYS:O	2.02	0.60
1:A:134:LEU:CD1	1:A:180:PRO:HA	2.33	0.59
1:A:111:ASP:CG	1:A:112:LEU:N	2.62	0.58
1:B:368:VAL:CG1	1:B:382:ARG:HD3	2.33	0.58
1:A:290[B]:MET:HE2	1:A:290[B]:MET:C	2.30	0.57
1:A:390:VAL:HA	1:A:405:LYS:O	2.05	0.57
1:A:279:SER:O	1:A:280:PHE:CD1	2.60	0.55
1:B:134:LEU:HD13	1:B:180:PRO:HA	1.90	0.52
1:A:358:ILE:HD11	1:A:402:VAL:HG21	1.92	0.52
1:A:412:PRO:HG3	1:A:435:VAL:HG23	1.93	0.51
1:A:457:LYS:O	1:A:457:LYS:CG	2.51	0.51
1:B:370:GLU:HG2	1:B:382:ARG:HG2	1.94	0.50
1:A:82[B]:CYS:SG	1:A:94:HIS:CD2	3.05	0.50
1:B:559:GLU:HA	1:B:583:GLU:O	2.12	0.49
1:B:412:PRO:HG3	1:B:435:VAL:HG23	1.93	0.49
1:B:665:LEU:HD22	1:B:687:ALA:HB2	1.95	0.48
1:A:38:GLU:OE2	1:A:663:LYS:NZ	2.44	0.48
1:A:358:ILE:CD1	1:A:402:VAL:HG11	2.44	0.48
1:B:442:GLU:OE1	1:B:465[B]:ARG:NH2	2.47	0.48
1:A:559:GLU:HA	1:A:583:GLU:O	2.14	0.47
1:B:128:GLY:HA2	4:B:803:HOH:O	2.14	0.47
1:B:513:ARG:O	1:B:534:VAL:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ILE:HD11	1:B:402:VAL:HG21	1.96	0.47
1:B:91:LYS:HD3	1:B:108[A]:MET:CE	2.44	0.47
1:A:630:ARG:HB3	1:A:632:TRP:CE2	2.50	0.47
1:A:91:LYS:HD3	1:A:108:MET:CE	2.45	0.47
1:A:665:LEU:HD22	1:A:687:ALA:HB2	1.96	0.47
1:B:358:ILE:CD1	1:B:402:VAL:HG11	2.46	0.46
1:B:542:ALA:O	1:B:546:ILE:HG12	2.15	0.46
1:A:649:THR:O	1:A:689:ILE:HA	2.15	0.46
1:B:134:LEU:HD11	1:B:180:PRO:HA	1.95	0.46
1:B:615:GLU:HG2	1:B:618:TRP:CH2	2.51	0.46
1:A:551:THR:HG21	1:A:556:VAL:HG22	1.98	0.46
1:B:551:THR:HG21	1:B:556:VAL:HG22	1.98	0.46
1:B:38:GLU:OE2	1:B:663:LYS:NZ	2.44	0.46
1:A:513:ARG:O	1:A:534:VAL:HG22	2.16	0.45
1:B:630:ARG:HB3	1:B:632:TRP:CE2	2.50	0.45
1:A:391:ASP:OD1	1:A:391:ASP:C	2.58	0.45
1:B:31:ALA:C	1:B:33:PRO:HD3	2.41	0.45
1:A:499:PHE:CE1	1:A:714:MET:CE	3.01	0.44
1:A:615:GLU:HG2	1:A:618:TRP:CH2	2.52	0.44
1:A:542:ALA:O	1:A:546:ILE:HG12	2.18	0.44
1:B:120:TYR:HE1	1:B:168:TYR:HH	1.63	0.44
1:B:391:ASP:OD1	1:B:391:ASP:C	2.60	0.43
1:B:85:PRO:HA	1:B:93:PHE:O	2.17	0.43
1:A:290[B]:MET:CE	1:A:292:LEU:N	2.81	0.43
1:B:546:ILE:HD12	1:B:553:ALA:N	2.34	0.43
1:B:649:THR:O	1:B:689:ILE:HA	2.18	0.43
1:B:499:PHE:CE1	1:B:714:MET:CE	3.02	0.43
1:A:134:LEU:HD13	1:A:180:PRO:HA	2.00	0.43
1:B:140:ASP:O	1:B:141:ALA:HB3	2.19	0.43
1:A:553:ALA:O	1:A:554:ARG:HB2	2.19	0.42
1:B:356:GLN:NE2	1:B:380:GLN:OE1	2.48	0.42
1:B:553:ALA:O	1:B:554:ARG:HB2	2.19	0.42
1:A:670:HIS:O	1:A:671:VAL:C	2.63	0.42
1:B:647:ILE:CG2	1:B:661:SER:HB3	2.50	0.42
1:B:91:LYS:HD3	1:B:108[B]:MET:SD	2.59	0.41
1:B:710[B]:ARG:HE	1:B:710[B]:ARG:HB3	1.52	0.41
1:B:527:PHE:CD1	1:B:527:PHE:C	2.97	0.41
1:A:647:ILE:CG2	1:A:661:SER:HB3	2.50	0.41
1:B:246:ASP:OD1	1:B:398:ARG:NH2	2.51	0.41
1:A:546:ILE:HD12	1:A:553:ALA:N	2.36	0.40
1:A:61:GLU:HG3	1:B:64:GLU:OE2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:561:GLY:HA2	1:B:585:ASN:O	2.22	0.40
1:A:368:VAL:HG11	1:A:382:ARG:CZ	2.52	0.40
1:A:527:PHE:CD1	1:A:527:PHE:C	2.99	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	652/750 (87%)	615 (94%)	34 (5%)	3 (0%)	24	34
1	B	641/750 (86%)	609 (95%)	30 (5%)	2 (0%)	36	48
2	C	4/19 (21%)	3 (75%)	1 (25%)	0	100	100
2	D	4/19 (21%)	3 (75%)	1 (25%)	0	100	100
All	All	1301/1538 (85%)	1230 (94%)	66 (5%)	5 (0%)	30	40

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	598	THR
1	B	598	THR
1	A	670	HIS
1	A	691	ARG
1	B	670	HIS

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	584/652 (90%)	567 (97%)	17 (3%)	37	57
1	B	576/652 (88%)	559 (97%)	17 (3%)	36	56
2	C	4/14 (29%)	4 (100%)	0	100	100
2	D	4/14 (29%)	4 (100%)	0	100	100
All	All	1168/1332 (88%)	1134 (97%)	34 (3%)	38	57

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	ASP
1	A	148	ILE
1	A	252	LEU
1	A	259	CYS
1	A	279	SER
1	A	280	PHE
1	A	365	VAL
1	A	390	VAL
1	A	398	ARG
1	A	457	LYS
1	A	503	LEU
1	A	527	PHE
1	A	554	ARG
1	A	586	CYS
1	A	602	LEU
1	A	606	ASP
1	A	716	LYS
1	B	177	LYS
1	B	252	LEU
1	B	259	CYS
1	B	342	LYS
1	B	365	VAL
1	B	382	ARG
1	B	390	VAL
1	B	398	ARG
1	B	465[A]	ARG
1	B	465[B]	ARG
1	B	503	LEU
1	B	527	PHE
1	B	554	ARG

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Mol	Chain	Res	Type
1	B	586	CYS
1	B	602	LEU
1	B	606	ASP
1	B	716	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	107	GLN
1	A	149	HIS
1	A	211	ASN
1	A	353	ASN
1	A	356	GLN
1	A	380	GLN
1	A	670	HIS
1	B	41	ASN
1	B	107	GLN
1	B	211	ASN
1	B	275	ASN
1	B	353	ASN
1	B	356	GLN
1	B	380	GLN
1	B	447	GLN
1	B	532	GLN
1	B	574	GLN
1	B	595	HIS
1	B	670	HIS

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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	666/750 (88%)	0.56	56 (8%) 17 15	18, 46, 88, 123	2 (0%)
1	B	656/750 (87%)	0.76	85 (12%) 7 6	20, 48, 86, 111	3 (0%)
2	C	6/19 (31%)	0.30	0 100 100	35, 41, 46, 46	0
2	D	6/19 (31%)	0.36	0 100 100	36, 40, 47, 52	0
All	All	1334/1538 (86%)	0.66	141 (10%) 11 10	18, 47, 87, 123	5 (0%)

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	134	LEU	5.5
1	A	280	PHE	4.7
1	A	15	VAL	4.2
1	B	601	TYR	4.1
1	B	36	TRP	4.0
1	B	602	LEU	3.9
1	B	128	GLY	3.9
1	A	40	PRO	3.8
1	B	591	MET	3.8
1	A	598	THR	3.6
1	B	290	MET	3.5
1	A	654	ASP	3.4
1	B	607	TYR	3.4
1	A	572	ILE	3.3
1	B	40	PRO	3.3
1	B	12	TYR	3.3
1	B	21	VAL	3.3
1	B	168	TYR	3.2
1	A	599	LEU	3.2
1	A	425	THR	3.2
1	B	25	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	599	LEU	3.1
1	B	676	LEU	3.1
1	A	290[A]	MET	3.1
1	A	672	LEU	3.0
1	B	603	TRP	3.0
1	A	591	MET	3.0
1	A	592	LEU	3.0
1	B	552	LYS	3.0
1	B	15	VAL	2.9
1	B	632	TRP	2.9
1	B	666	ALA	2.9
1	B	37	LEU	2.8
1	A	43	GLU	2.8
1	B	598	THR	2.8
1	B	680	PRO	2.8
1	B	426	GLN	2.8
1	A	14	PRO	2.8
1	A	612	LYS	2.8
1	B	589	MET	2.8
1	B	650	ALA	2.8
1	B	600	GLY	2.7
1	A	553	ALA	2.7
1	B	616	PHE	2.7
1	A	33	PRO	2.7
1	B	578	LEU	2.7
1	B	26	PHE	2.7
1	B	590	ASP	2.7
1	A	723	ILE	2.7
1	B	14	PRO	2.7
1	B	659	LEU	2.7
1	A	667	THR	2.6
1	A	424	PRO	2.6
1	B	625	ILE	2.6
1	B	655	ARG	2.6
1	A	676	LEU	2.6
1	A	682	LYS	2.6
1	B	67	ASP	2.6
1	A	674	THR	2.6
1	B	671	VAL	2.6
1	A	467	GLY	2.6
1	A	671	VAL	2.6
1	A	625	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	602	LEU	2.6
1	B	332	SER	2.6
1	A	620	ILE	2.5
1	A	17	ARG	2.5
1	A	678	ASP	2.5
1	A	596	LYS	2.5
1	B	597	PHE	2.5
1	A	260	ASP	2.5
1	A	635	PRO	2.5
1	A	547	SER	2.5
1	B	689	ILE	2.5
1	B	687	ALA	2.5
1	B	274	PRO	2.5
1	B	661	SER	2.4
1	A	666	ALA	2.4
1	A	156	VAL	2.4
1	A	468	ILE	2.4
1	B	608	GLY	2.4
1	A	650	ALA	2.4
1	B	605	GLY	2.4
1	B	679	SER	2.4
1	A	259	CYS	2.4
1	B	454	ASP	2.3
1	B	28	VAL	2.3
1	A	427	LEU	2.3
1	B	233	LEU	2.3
1	B	43	GLU	2.3
1	B	592	LEU	2.3
1	B	612	LYS	2.3
1	B	30	VAL	2.3
1	B	29	LYS	2.3
1	B	427	LEU	2.3
1	B	586	CYS	2.3
1	A	632	TRP	2.3
1	A	675	SER	2.3
1	A	37	LEU	2.2
1	B	260	ASP	2.2
1	A	151	GLY	2.2
1	B	129	ARG	2.2
1	B	48	PHE	2.2
1	B	628	VAL	2.2
1	B	180	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	18	ASP	2.2
1	B	624	PRO	2.2
1	B	259	CYS	2.2
1	B	381	HIS	2.2
1	B	642	TYR	2.2
1	B	664	LEU	2.2
1	A	670	HIS	2.2
1	A	12	TYR	2.1
1	B	453	LYS	2.1
1	A	34	TYR	2.1
1	B	135	TYR	2.1
1	B	672	LEU	2.1
1	B	685	ILE	2.1
1	A	41	ASN	2.1
1	A	278	GLU	2.1
1	B	32	ASP	2.1
1	A	333	VAL	2.1
1	B	49	VAL	2.1
1	A	605	GLY	2.1
1	B	455	GLY	2.1
1	A	42	SER	2.1
1	B	425	THR	2.1
1	B	287	ALA	2.1
1	B	23	ASP	2.1
1	B	148	ILE	2.1
1	B	554	ARG	2.1
1	A	673	CYS	2.1
1	B	611	ASP	2.1
1	B	657	VAL	2.1
1	B	662	PHE	2.1
1	B	571	CYS	2.0
1	A	658	PRO	2.0
1	B	675	SER	2.0
1	A	423	ASP	2.0
1	B	90	ASN	2.0
1	B	631	PRO	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	801	1/1	0.95	0.07	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.