Full wwPDB X-ray Structure Validation Report (i)

Feb 29, 2024 – 08:33 AM EST

PDB ID	:	5UW5
Title	:	PCY1 H695A Variant in Complex with Follower Peptide
Authors	:	Chekan, J.R.; Nair, S.K.
Deposited on	:	2017-02-20
Resolution	:	2.94 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 (i) 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 (i)) were used in the production of this report:

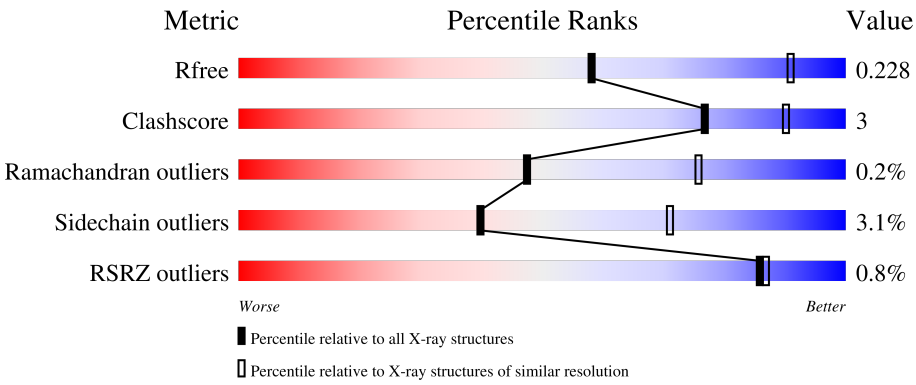
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.94 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}	130704	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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	750	2%; 83%; 8%; • ; 7%
1	B	750	86%; 8%; 6%
1	C	750	86%; 7%; • ; 6%
1	D	750	%; 86%; 7%; 7%
2	E	19	32%; 68%

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Mol	Chain	Length	Quality of chain
2	F	19	32% 68%
2	G	19	26% 5% 68%
2	H	19	32% 68%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 22798 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
			Total	C	N	O	S			
1	A	696	5639	3605	957	1051	26	0	6	0
1	B	705	5659	3616	960	1058	25	0	1	0
1	C	702	5660	3620	964	1050	26	0	2	0
1	D	697	5596	3579	951	1041	25	0	0	0

There are 108 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
A	0	LEU	-	expression tag	UNP R4P353
A	695	ALA	HIS	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	695	ALA	HIS	conflict	UNP R4P353
C	-25	MET	-	initiating methionine	UNP R4P353
C	-24	SER	-	expression tag	UNP R4P353
C	-23	TYR	-	expression tag	UNP R4P353
C	-22	TYR	-	expression tag	UNP R4P353
C	-21	HIS	-	expression tag	UNP R4P353
C	-20	HIS	-	expression tag	UNP R4P353
C	-19	HIS	-	expression tag	UNP R4P353
C	-18	HIS	-	expression tag	UNP R4P353
C	-17	HIS	-	expression tag	UNP R4P353

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	HIS	-	expression tag	UNP R4P353
C	-15	LEU	-	expression tag	UNP R4P353
C	-14	GLU	-	expression tag	UNP R4P353
C	-13	SER	-	expression tag	UNP R4P353
C	-12	THR	-	expression tag	UNP R4P353
C	-11	SER	-	expression tag	UNP R4P353
C	-10	LEU	-	expression tag	UNP R4P353
C	-9	TYR	-	expression tag	UNP R4P353
C	-8	LYS	-	expression tag	UNP R4P353
C	-7	LYS	-	expression tag	UNP R4P353
C	-6	ALA	-	expression tag	UNP R4P353
C	-5	GLY	-	expression tag	UNP R4P353
C	-4	SER	-	expression tag	UNP R4P353
C	-3	GLU	-	expression tag	UNP R4P353
C	-2	PHE	-	expression tag	UNP R4P353
C	-1	ALA	-	expression tag	UNP R4P353
C	0	LEU	-	expression tag	UNP R4P353
C	695	ALA	HIS	conflict	UNP R4P353
D	-25	MET	-	initiating methionine	UNP R4P353
D	-24	SER	-	expression tag	UNP R4P353
D	-23	TYR	-	expression tag	UNP R4P353
D	-22	TYR	-	expression tag	UNP R4P353
D	-21	HIS	-	expression tag	UNP R4P353
D	-20	HIS	-	expression tag	UNP R4P353
D	-19	HIS	-	expression tag	UNP R4P353
D	-18	HIS	-	expression tag	UNP R4P353
D	-17	HIS	-	expression tag	UNP R4P353
D	-16	HIS	-	expression tag	UNP R4P353
D	-15	LEU	-	expression tag	UNP R4P353
D	-14	GLU	-	expression tag	UNP R4P353
D	-13	SER	-	expression tag	UNP R4P353
D	-12	THR	-	expression tag	UNP R4P353
D	-11	SER	-	expression tag	UNP R4P353
D	-10	LEU	-	expression tag	UNP R4P353
D	-9	TYR	-	expression tag	UNP R4P353
D	-8	LYS	-	expression tag	UNP R4P353
D	-7	LYS	-	expression tag	UNP R4P353
D	-6	ALA	-	expression tag	UNP R4P353
D	-5	GLY	-	expression tag	UNP R4P353
D	-4	SER	-	expression tag	UNP R4P353
D	-3	GLU	-	expression tag	UNP R4P353
D	-2	PHE	-	expression tag	UNP R4P353

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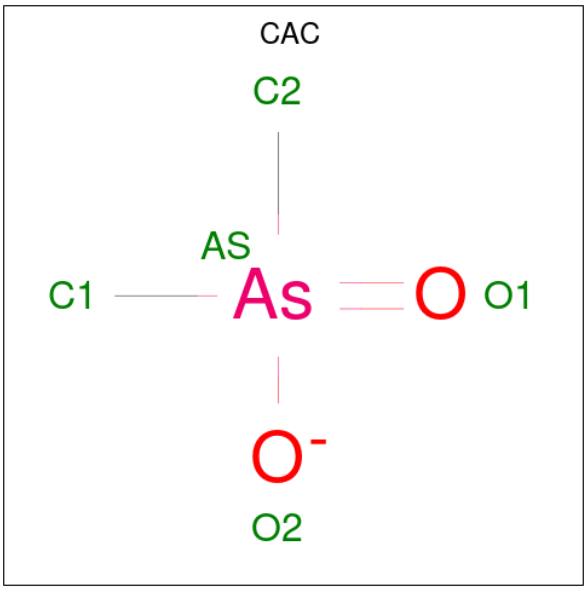
Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	ALA	-	expression tag	UNP R4P353
D	0	LEU	-	expression tag	UNP R4P353
D	695	ALA	HIS	conflict	UNP R4P353

- Molecule 2 is a protein called Presegetalin A1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	6	38	23	7	8	0	0	0
2	F	6	39	23	7	9	0	0	0
2	G	6	38	23	7	8	0	0	0
2	H	6	39	23	7	9	0	0	0

- Molecule 3 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	2	2	2	0	0
4	B	2	2	2	0	0
4	C	2	2	2	0	0

- Molecule 5 is water.

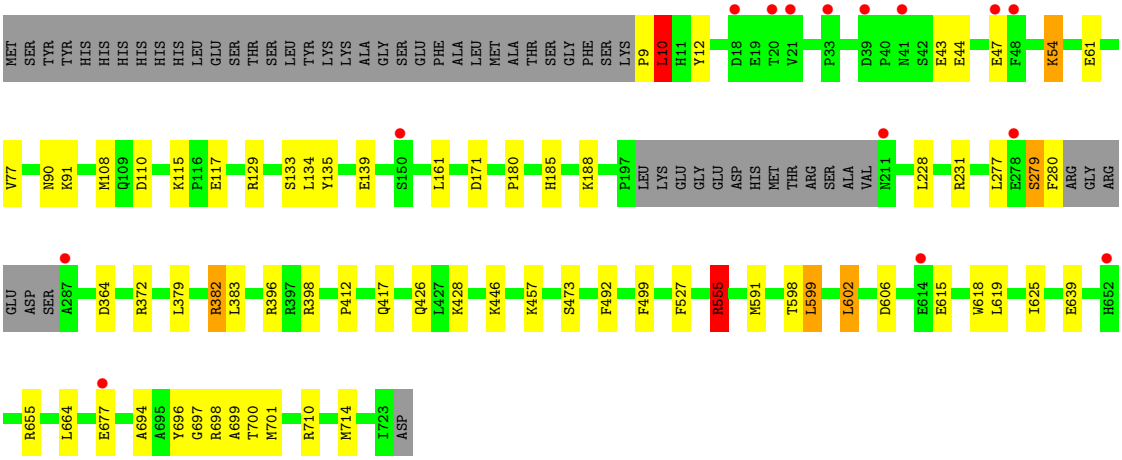
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	19	19	19	0	0
5	B	13	13	13	0	0
5	C	17	17	17	0	0
5	D	15	15	15	0	0

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.

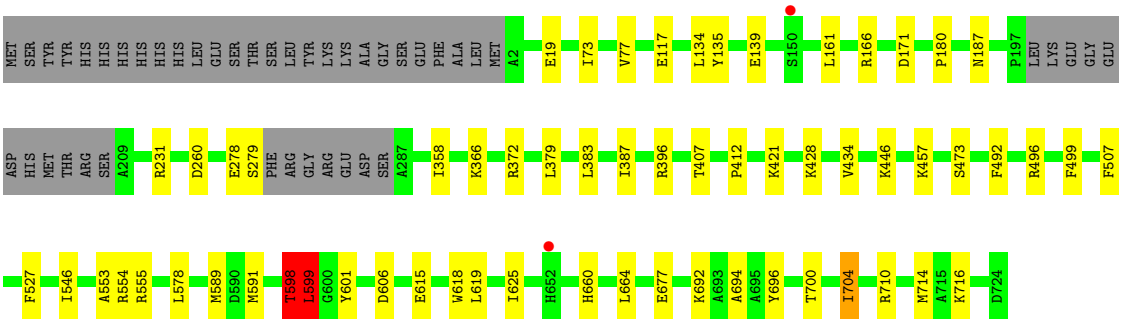
• Molecule 1: Peptide cyclase 1

Chain A: 2% 83% 8% • 7%



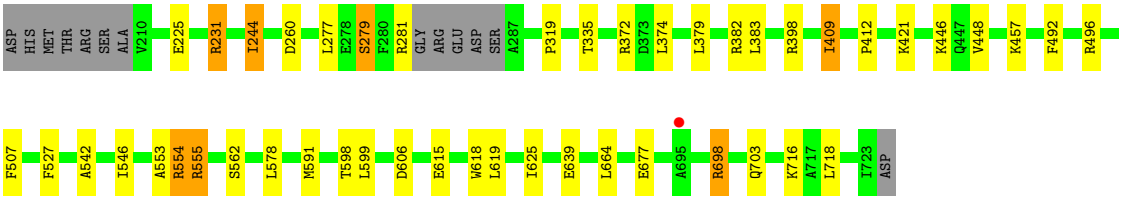
• Molecule 1: Peptide cyclase 1

Chain B: 86% 8% 6%



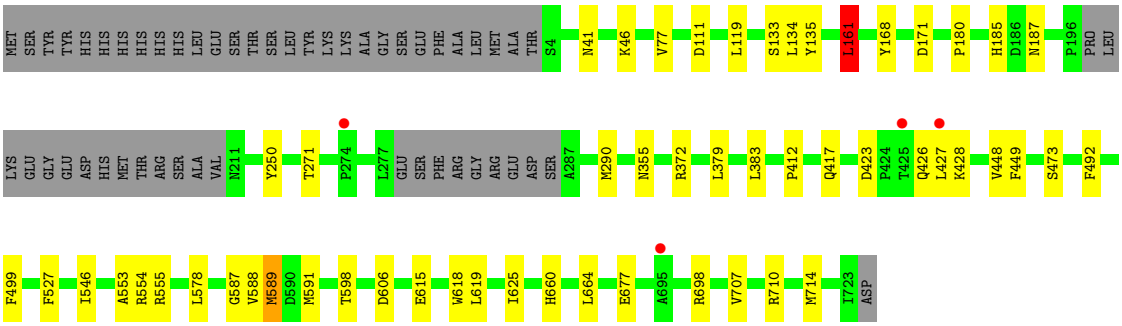
• Molecule 1: Peptide cyclase 1

Chain C: 86% 7% • 6%



• Molecule 1: Peptide cyclase 1

Chain D:



• Molecule 2: Presegetalin A1

Chain E:

• Molecule 2: Presegetalin A1

Chain F:

• Molecule 2: Presegetalin A1

Chain G:

• Molecule 2: Presegetalin A1

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	65.02Å 85.61Å 137.87Å 87.49° 78.51° 89.44°	Depositor
Resolution (Å)	44.90 – 2.94 44.99 – 2.94	Depositor EDS
% Data completeness (in resolution range)	98.8 (44.90-2.94) 98.8 (44.99-2.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	3.08 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.186 , 0.227 0.190 , 0.228	Depositor DCC
R_{free} test set	3094 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	34.1	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 34.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.043 for h,-k,h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	22798	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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 (i)

5.1 Standard geometry (i)

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

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	0.52	0/5784	0.73	6/7833 (0.1%)
1	B	0.55	0/5804	0.73	4/7862 (0.1%)
1	C	0.54	0/5806	0.73	6/7861 (0.1%)
1	D	0.54	0/5740	0.71	2/7773 (0.0%)
2	E	0.52	0/38	0.44	0/52
2	F	0.65	0/39	0.49	0/52
2	G	0.58	0/38	0.55	0/52
2	H	0.60	0/39	0.45	0/52
All	All	0.54	0/23288	0.72	18/31537 (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	A	0	2

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	134	LEU	CA-CB-CG	9.67	137.54	115.30
1	C	599	LEU	CA-CB-CG	7.14	131.72	115.30
1	C	554	ARG	CA-CB-CG	6.58	127.88	113.40
1	A	602	LEU	CA-CB-CG	6.58	130.42	115.30
1	B	598	THR	CB-CA-C	-6.50	94.04	111.60
1	A	161	LEU	CB-CG-CD1	-6.43	100.07	111.00
1	B	599	LEU	CA-CB-CG	6.38	129.98	115.30
1	B	704	ILE	CA-CB-CG1	6.20	122.79	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	10	LEU	CA-CB-CG	5.80	128.65	115.30
1	A	161	LEU	CA-CB-CG	5.73	128.49	115.30
1	A	555	ARG	CG-CD-NE	-5.55	100.15	111.80
1	B	161	LEU	CB-CA-C	-5.51	99.72	110.20
1	C	231	ARG	N-CA-C	5.49	125.82	111.00
1	A	382	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	C	161	LEU	CB-CA-C	-5.25	100.23	110.20
1	D	161	LEU	CB-CA-C	-5.09	100.52	110.20
1	C	134	LEU	CB-CG-CD2	5.06	119.60	111.00
1	D	589	MET	N-CA-C	-5.02	97.44	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	697	GLY	Peptide
1	A	9	PRO	Peptide

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	5639	0	5481	48	0
1	B	5659	0	5501	29	0
1	C	5660	0	5512	30	1
1	D	5596	0	5448	34	1
2	E	38	0	36	0	0
2	F	39	0	36	0	0
2	G	38	0	36	1	0
2	H	39	0	36	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	2	0
3	D	5	0	0	0	0
4	A	2	0	0	0	1
4	B	2	0	0	0	0
4	C	2	0	0	1	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	19	0	0	5	0
5	B	13	0	0	1	0
5	C	17	0	0	1	0
5	D	15	0	0	1	0
All	All	22798	0	22086	133	2

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 (133) 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:639:GLU:O	5:A:901:HOH:O	1.79	1.00
1:D:383:LEU:HD21	1:D:427:LEU:HD11	1.62	0.79
1:D:383:LEU:CD2	1:D:427:LEU:HD11	2.18	0.73
1:D:587:GLY:C	1:D:589:MET:HE2	2.10	0.72
1:D:473:SER:O	1:D:555:ARG:NH2	2.24	0.71
1:D:588:VAL:N	1:D:589:MET:HE2	2.07	0.70
1:A:115:LYS:HD3	5:A:919:HOH:O	1.90	0.70
1:A:90[B]:ASN:ND2	1:D:250:TYR:OH	2.25	0.69
1:B:589:MET:O	1:B:660:HIS:ND1	2.23	0.69
1:D:589:MET:O	1:D:660:HIS:ND1	2.23	0.69
1:B:598:THR:O	1:B:598:THR:OG1	2.03	0.69
1:A:44:GLU:HA	1:A:47:GLU:HG2	1.75	0.68
1:A:91:LYS:HD3	1:A:108:MET:CE	2.24	0.68
1:A:129:ARG:HD3	5:A:913:HOH:O	1.94	0.66
1:B:407:THR:CG2	1:B:492:PHE:H	2.09	0.66
1:A:188:LYS:HE2	1:D:355:ASN:CG	2.16	0.66
1:D:161:LEU:HD11	1:D:168:TYR:CE1	2.31	0.65
1:D:587:GLY:HA3	1:D:589:MET:HE3	1.81	0.62
1:C:62:GLU:OE1	1:C:716:LYS:NZ	2.28	0.61
1:B:555:ARG:HD3	5:B:910:HOH:O	2.01	0.60
1:C:639:GLU:OE1	4:C:803:CA:CA	1.78	0.60
1:A:43:GLU:O	1:A:47:GLU:HG2	2.01	0.60
1:B:553:ALA:O	1:B:578:LEU:O	2.20	0.59
1:B:73:ILE:HG22	1:B:704:ILE:HD12	1.84	0.59
1:D:423:ASP:OD2	1:D:426:GLN:NE2	2.35	0.58
1:D:134:LEU:HD13	1:D:180:PRO:HA	1.86	0.58
1:D:553:ALA:O	1:D:578:LEU:O	2.22	0.58
1:A:134:LEU:HD13	1:A:180:PRO:HA	1.86	0.57
1:B:134:LEU:HD13	1:B:180:PRO:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:446:LYS:HE3	1:C:448:VAL:CG1	2.33	0.57
1:A:44:GLU:O	1:A:47:GLU:HG3	2.04	0.57
1:C:553:ALA:O	1:C:578:LEU:O	2.23	0.57
1:D:383:LEU:HD21	1:D:427:LEU:CD1	2.33	0.57
1:A:44:GLU:HA	1:A:47:GLU:CG	2.35	0.56
1:B:117:GLU:OE1	1:B:166:ARG:NH2	2.40	0.55
1:D:372:ARG:HG2	1:D:379:LEU:HA	1.88	0.55
1:A:54:LYS:HD2	1:A:54:LYS:O	2.07	0.55
1:B:372:ARG:HG2	1:B:379:LEU:HA	1.90	0.54
1:A:372:ARG:HG2	1:A:379:LEU:HA	1.90	0.54
1:B:187:ASN:O	1:C:421:LYS:NZ	2.40	0.53
1:A:139:GLU:OE2	1:A:396:ARG:NH1	2.42	0.53
1:C:625:ILE:HG22	1:C:664:LEU:HA	1.90	0.53
1:B:694:ALA:HB1	1:B:696:TYR:CE2	2.44	0.53
1:C:372:ARG:HG2	1:C:379:LEU:HA	1.91	0.53
1:C:409:ILE:HD12	1:C:496:ARG:NH1	2.24	0.52
1:A:625:ILE:HG22	1:A:664:LEU:HA	1.91	0.52
1:A:117:GLU:HG3	5:A:919:HOH:O	2.09	0.51
1:A:473:SER:O	1:A:555:ARG:NH1	2.44	0.51
1:C:87[A]:ARG:HD3	1:C:92:TYR:CZ	2.46	0.51
1:B:139:GLU:OE2	1:B:396:ARG:NH1	2.44	0.51
1:B:599:LEU:HA	1:B:601:TYR:CE1	2.46	0.51
1:C:446:LYS:HE3	1:C:448:VAL:HG12	1.94	0.50
1:B:625:ILE:HG22	1:B:664:LEU:HA	1.92	0.50
1:D:625:ILE:HG22	1:D:664:LEU:HA	1.93	0.50
1:A:382:ARG:HH22	1:C:382:ARG:NH2	2.10	0.50
1:D:588:VAL:C	1:D:589:MET:HE2	2.33	0.50
1:C:191:PHE:HE2	1:C:244:ILE:HD11	1.78	0.49
1:A:91:LYS:HD3	1:A:108:MET:HE1	1.94	0.49
1:A:277:LEU:O	1:A:279:SER:O	2.30	0.49
1:B:694:ALA:CB	1:B:696:TYR:CE2	2.96	0.49
1:A:110:ASP:HB3	1:D:271:THR:HB	1.94	0.48
1:A:457:LYS:O	1:A:457:LYS:HG3	2.12	0.48
1:C:562:SER:HB3	3:C:801:CAC:O1	2.12	0.48
1:D:412:PRO:HA	1:D:492:PHE:CG	2.48	0.48
1:C:555:ARG:NH1	1:C:718:LEU:O	2.46	0.48
1:A:700:THR:O	1:A:701:MET:HB2	2.14	0.47
1:B:473:SER:O	1:B:555:ARG:NH1	2.47	0.47
1:C:277:LEU:O	1:C:279:SER:O	2.32	0.47
1:C:412:PRO:HA	1:C:492:PHE:CG	2.49	0.47
1:A:599:LEU:O	1:A:602:LEU:HD23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:LYS:HG3	1:B:457:LYS:O	2.12	0.47
1:C:225:GLU:O	1:C:281:ARG:NH1	2.48	0.47
1:B:499:PHE:CE1	1:B:714:MET:HE1	2.50	0.46
1:A:412:PRO:HA	1:A:492:PHE:CG	2.49	0.46
1:D:41:ASN:O	1:D:46:LYS:HE3	2.15	0.46
1:A:457:LYS:O	1:A:457:LYS:CG	2.64	0.46
1:C:615:GLU:HG2	1:C:618:TRP:CH2	2.50	0.46
1:C:698:ARG:HD2	1:C:698:ARG:N	2.31	0.46
1:D:134:LEU:HD12	1:D:135:TYR:N	2.31	0.46
1:A:364:ASP:OD2	1:C:457:LYS:HE2	2.16	0.46
1:A:591:MET:HB3	1:A:619:LEU:HD22	1.97	0.46
1:B:615:GLU:HG2	1:B:618:TRP:CH2	2.51	0.45
1:C:703:GLN:HG3	2:G:32:VAL:HG21	1.99	0.45
1:D:448:VAL:HG22	1:D:449:PHE:N	2.30	0.45
1:A:599:LEU:HB2	1:A:602:LEU:HD21	1.97	0.45
1:C:591:MET:HB3	1:C:619:LEU:HD22	1.97	0.45
1:A:599:LEU:HB2	1:A:602:LEU:CD2	2.46	0.45
1:A:699:ALA:C	1:A:700:THR:O	2.51	0.45
1:A:54:LYS:O	1:A:54:LYS:CD	2.65	0.45
1:C:698:ARG:CG	1:C:698:ARG:HH11	2.30	0.45
1:A:10:LEU:HD11	1:A:12:TYR:CE1	2.52	0.45
1:B:412:PRO:HA	1:B:492:PHE:CG	2.52	0.45
1:D:615:GLU:HG2	1:D:618:TRP:CH2	2.51	0.45
1:A:228:LEU:HD11	1:A:231:ARG:HG2	1.98	0.45
1:B:457:LYS:O	1:B:457:LYS:CG	2.65	0.45
1:B:591:MET:HB3	1:B:619:LEU:HD22	1.98	0.45
1:D:499:PHE:CE1	1:D:714:MET:HE1	2.52	0.45
1:B:700:THR:O	1:B:704:ILE:HG12	2.17	0.44
1:C:698:ARG:HH11	1:C:698:ARG:HG3	1.83	0.44
1:A:499:PHE:CE1	1:A:714:MET:HE1	2.53	0.44
1:A:599:LEU:HD21	1:A:655:ARG:HA	1.99	0.44
1:D:591:MET:HB3	1:D:619:LEU:HD22	1.98	0.44
1:D:588:VAL:N	1:D:589:MET:CE	2.79	0.44
1:B:134:LEU:HD12	1:B:135:TYR:N	2.33	0.43
1:A:54:LYS:HD2	1:A:54:LYS:C	2.38	0.43
1:B:499:PHE:CE1	1:B:714:MET:CE	3.02	0.43
1:A:54:LYS:CD	1:A:54:LYS:C	2.87	0.43
1:C:562:SER:HB3	3:C:801:CAC:AS	2.78	0.43
1:C:87[A]:ARG:CD	1:C:92:TYR:CZ	3.02	0.43
1:A:699:ALA:O	1:A:700:THR:C	2.57	0.43
1:B:499:PHE:CD1	1:B:714:MET:HE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:LEU:HD12	1:A:135:TYR:N	2.34	0.42
1:A:188:LYS:HE2	1:D:355:ASN:OD1	2.19	0.42
1:A:44:GLU:CA	1:A:47:GLU:HG2	2.47	0.42
1:A:615:GLU:HG2	1:A:618:TRP:CH2	2.54	0.42
1:B:496:ARG:HD3	1:B:507:PHE:CD2	2.55	0.42
1:D:499:PHE:CD1	1:D:714:MET:HE1	2.55	0.42
1:C:496:ARG:HD3	1:C:507:PHE:CD2	2.55	0.42
1:D:588:VAL:C	1:D:589:MET:CE	2.88	0.42
1:D:707:VAL:HA	1:D:710:ARG:HG2	2.02	0.42
1:A:499:PHE:CD1	1:A:714:MET:HE1	2.56	0.41
1:C:542:ALA:O	1:C:546:ILE:HG12	2.21	0.41
1:A:694:ALA:HB1	1:A:696:TYR:CE2	2.56	0.41
1:A:499:PHE:CE1	1:A:714:MET:CE	3.04	0.41
1:C:319:PRO:HB2	5:C:908:HOH:O	2.20	0.41
1:A:117:GLU:CG	5:A:919:HOH:O	2.69	0.41
1:C:496:ARG:HD3	1:C:507:PHE:CG	2.56	0.40
1:D:187:ASN:HA	5:D:906:HOH:O	2.21	0.40
1:A:188:LYS:HE2	1:D:355:ASN:ND2	2.36	0.40
1:B:716:LYS:HA	1:B:716:LYS:HD2	1.92	0.40
1:B:366:LYS:NZ	1:B:387:ILE:HG13	2.36	0.40
1:D:499:PHE:CE1	1:D:714:MET:CE	3.04	0.40
1:D:587:GLY:HA3	1:D:589:MET:CE	2.47	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:802:CA:CA	4:C:802:CA:CA[1_545]	1.68	0.52
1:C:188:LYS:NZ	1:D:111:ASP:OD1[1_465]	2.19	0.01

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	696/750 (93%)	665 (96%)	29 (4%)	2 (0%)	41	69
1	B	700/750 (93%)	667 (95%)	32 (5%)	1 (0%)	51	80
1	C	698/750 (93%)	665 (95%)	32 (5%)	1 (0%)	51	80
1	D	691/750 (92%)	658 (95%)	32 (5%)	1 (0%)	51	80
2	E	4/19 (21%)	4 (100%)	0	0	100	100
2	F	4/19 (21%)	4 (100%)	0	0	100	100
2	G	4/19 (21%)	4 (100%)	0	0	100	100
2	H	4/19 (21%)	4 (100%)	0	0	100	100
All	All	2801/3076 (91%)	2671 (95%)	125 (4%)	5 (0%)	47	76

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	598	THR
1	A	598	THR
1	C	598	THR
1	D	598	THR
1	A	698	ARG

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	611/651 (94%)	590 (97%)	21 (3%)	37	68
1	B	612/651 (94%)	591 (97%)	21 (3%)	37	68
1	C	612/651 (94%)	592 (97%)	20 (3%)	38	69
1	D	605/651 (93%)	590 (98%)	15 (2%)	47	76
2	E	4/14 (29%)	4 (100%)	0	100	100
2	F	4/14 (29%)	4 (100%)	0	100	100
2	G	4/14 (29%)	4 (100%)	0	100	100
2	H	4/14 (29%)	4 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2456/2660 (92%)	2379 (97%)	77 (3%)	40 71

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	54	LYS
1	A	61	GLU
1	A	77	VAL
1	A	133	SER
1	A	171	ASP
1	A	185	HIS
1	A	279	SER
1	A	280	PHE
1	A	383	LEU
1	A	398	ARG
1	A	417	GLN
1	A	426	GLN
1	A	428	LYS
1	A	446	LYS
1	A	527	PHE
1	A	555	ARG
1	A	599	LEU
1	A	606	ASP
1	A	677	GLU
1	A	710	ARG
1	B	19	GLU
1	B	77	VAL
1	B	171	ASP
1	B	231	ARG
1	B	260	ASP
1	B	278	GLU
1	B	279	SER
1	B	358	ILE
1	B	383	LEU
1	B	421	LYS
1	B	428	LYS
1	B	434	VAL
1	B	446	LYS
1	B	527	PHE
1	B	546	ILE
1	B	554	ARG

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Mol	Chain	Res	Type
1	B	599	LEU
1	B	606	ASP
1	B	677	GLU
1	B	692	LYS
1	B	710	ARG
1	C	62	GLU
1	C	77	VAL
1	C	119	LEU
1	C	126	GLU
1	C	171	ASP
1	C	231	ARG
1	C	244	ILE
1	C	260	ASP
1	C	279	SER
1	C	335	THR
1	C	374	LEU
1	C	383	LEU
1	C	398	ARG
1	C	409	ILE
1	C	527	PHE
1	C	554	ARG
1	C	555	ARG
1	C	606	ASP
1	C	677	GLU
1	C	698	ARG
1	D	77	VAL
1	D	119	LEU
1	D	133	SER
1	D	161	LEU
1	D	171	ASP
1	D	185	HIS
1	D	290	MET
1	D	417	GLN
1	D	428	LYS
1	D	527	PHE
1	D	546	ILE
1	D	554	ARG
1	D	606	ASP
1	D	677	GLU
1	D	698	ARG

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	94	HIS
1	A	109	GLN
1	A	149	HIS
1	A	652	HIS
1	B	107	GLN
1	B	185	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
3	CAC	B	801	-	0,4,4	-	-	0,6,6	-	-
3	CAC	D	801	-	0,4,4	-	-	0,6,6	-	-
3	CAC	C	801	-	0,4,4	-	-	0,6,6	-	-
3	CAC	A	801	-	0,4,4	-	-	0,6,6	-	-

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	801	CAC	2	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	696/750 (92%)	-0.07	15 (2%)	62	63	15, 34, 71, 98	0
1	B	705/750 (94%)	-0.32	2 (0%)	94	94	14, 28, 56, 86	0
1	C	702/750 (93%)	-0.33	1 (0%)	95	96	13, 27, 55, 97	0
1	D	697/750 (92%)	-0.32	4 (0%)	89	90	15, 27, 57, 99	0
2	E	6/19 (31%)	-0.30	0	100	100	27, 30, 32, 33	0
2	F	6/19 (31%)	-0.45	0	100	100	18, 21, 23, 25	0
2	G	6/19 (31%)	-0.53	0	100	100	23, 25, 28, 29	0
2	H	6/19 (31%)	-0.58	0	100	100	21, 23, 27, 32	0
All	All	2824/3076 (91%)	-0.26	22 (0%)	86	87	13, 29, 62, 99	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	695	ALA	4.0
1	A	677	GLU	3.3
1	A	652	HIS	3.3
1	B	652	HIS	3.3
1	A	211	ASN	3.1
1	A	39	ASP	3.1
1	D	274	PRO	2.8
1	A	47	GLU	2.8
1	A	41	ASN	2.7
1	A	150	SER	2.5
1	D	695	ALA	2.3
1	A	18	ASP	2.3
1	A	33	PRO	2.3
1	A	21	VAL	2.2
1	A	614	GLU	2.2
1	A	48	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	427	LEU	2.1
1	D	425	THR	2.1
1	A	287	ALA	2.1
1	B	150	SER	2.1
1	A	278	GLU	2.0
1	A	20	THR	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 monosaccharides 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
4	CA	A	802	1/1	0.86	0.13	105,105,105,105	0
4	CA	A	803	1/1	0.89	0.06	41,41,41,41	0
4	CA	C	802	1/1	0.92	0.07	73,73,73,73	0
4	CA	B	802	1/1	0.94	0.08	31,31,31,31	0
4	CA	B	803	1/1	0.96	0.20	70,70,70,70	0
4	CA	C	803	1/1	0.96	0.07	44,44,44,44	0
3	CAC	A	801	5/5	0.98	0.11	44,47,48,51	0
3	CAC	B	801	5/5	0.99	0.09	33,33,34,36	0
3	CAC	C	801	5/5	0.99	0.11	37,37,38,38	0
3	CAC	D	801	5/5	0.99	0.12	32,32,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.