



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:58 PM GMT

PDB ID : 4PEL  
Title : S1C mutant of Penicillin G acylase from *Kluyvera citrophila*  
Authors : Ramasamy, S.; Chand, D.; Varshney, N.K.; Brannigan, J.A.; Wilkinson, A.J.; Suresh, C.G.  
Deposited on : 2014-04-24  
Resolution : 2.80 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

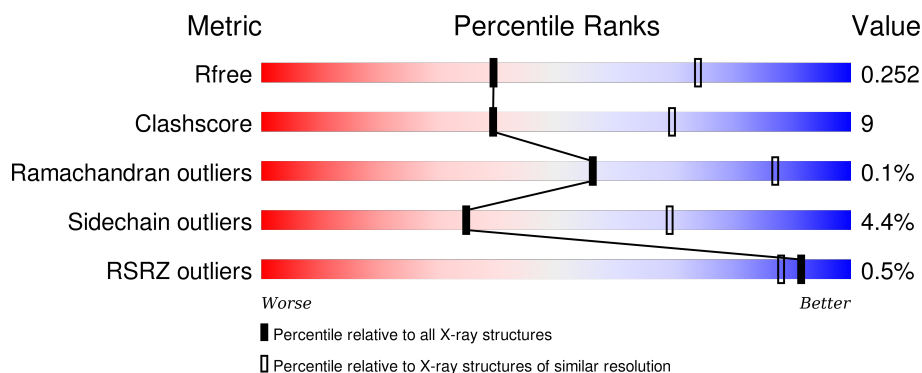
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	222	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 69%, yellow 15%, orange 4%, grey 13%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>70%</span> <span>15%</span> <span>•</span> <span>13%</span> </div> </div>
1	C	222	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 76%, yellow 10%, orange 1%, grey 13%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span></span> <span>76%</span> <span>10%</span> <span>•</span> <span>13%</span> </div> </div>
1	E	222	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 75%, yellow 12%, orange 1%, grey 13%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span></span> <span>75%</span> <span>12%</span> <span></span> <span>13%</span> </div> </div>
1	G	222	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 74%, yellow 13%, orange 1%, grey 13%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span></span> <span>74%</span> <span>13%</span> <span></span> <span>13%</span> </div> </div>
2	B	565	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 79%, yellow 17%, orange 3%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>80%</span> <span>17%</span> <span>••</span> </div> </div>

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Mol	Chain	Length	Quality of chain
2	D	565	<div><div>%</div><div><div></div><div>79%</div><div>18%</div><div>..</div></div></div>
2	F	565	<div><div></div><div>82%</div><div>15%</div><div>..</div></div>
2	H	565	<div><div>%</div><div><div></div><div>80%</div><div>17%</div><div>..</div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23734 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 Penicillin G acylase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	0
			1545	989	259	290	7			
1	C	194	Total	C	N	O	S	0	0	0
			1545	989	259	290	7			
1	E	194	Total	C	N	O	S	0	0	0
			1545	989	259	290	7			
1	G	194	Total	C	N	O	S	0	0	0
			1545	989	259	290	7			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	162	LEU	VAL	conflict	UNP P07941
A	168	LYS	ASN	conflict	UNP P07941
A	169	GLN	ASP	conflict	UNP P07941
A	170	GLN	GLU	conflict	UNP P07941
A	196	ALA	SER	conflict	UNP P07941
C	162	LEU	VAL	conflict	UNP P07941
C	168	LYS	ASN	conflict	UNP P07941
C	169	GLN	ASP	conflict	UNP P07941
C	170	GLN	GLU	conflict	UNP P07941
C	196	ALA	SER	conflict	UNP P07941
E	162	LEU	VAL	conflict	UNP P07941
E	168	LYS	ASN	conflict	UNP P07941
E	169	GLN	ASP	conflict	UNP P07941
E	170	GLN	GLU	conflict	UNP P07941
E	196	ALA	SER	conflict	UNP P07941
G	162	LEU	VAL	conflict	UNP P07941
G	168	LYS	ASN	conflict	UNP P07941
G	169	GLN	ASP	conflict	UNP P07941
G	170	GLN	GLU	conflict	UNP P07941
G	196	ALA	SER	conflict	UNP P07941

- Molecule 2 is a protein called Penicillin G acylase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	557	Total	C	N	O	S	0	0	0
			4379	2786	758	826	9			
2	D	557	Total	C	N	O	S	0	0	0
			4379	2786	758	826	9			
2	F	557	Total	C	N	O	S	0	0	0
			4379	2786	758	826	9			
2	H	557	Total	C	N	O	S	0	0	0
			4379	2786	758	826	9			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	CYS	SER	engineered mutation	UNP P07941
B	123	HIS	ASP	conflict	UNP P07941
B	132	ALA	ARG	conflict	UNP P07941
B	144	ASP	ALA	conflict	UNP P07941
B	211	GLY	-	insertion	UNP P07941
B	212	THR	ASP	conflict	UNP P07941
B	270	THR	ILE	conflict	UNP P07941
B	291	ARG	LEU	conflict	UNP P07941
B	295	ASN	-	insertion	UNP P07941
B	419	GLN	GLU	conflict	UNP P07941
B	526	ILE	LYS	conflict	UNP P07941
B	558	LEU	-	expression tag	UNP P07941
B	559	GLU	-	expression tag	UNP P07941
B	560	HIS	-	expression tag	UNP P07941
B	561	HIS	-	expression tag	UNP P07941
B	562	HIS	-	expression tag	UNP P07941
B	563	HIS	-	expression tag	UNP P07941
B	564	HIS	-	expression tag	UNP P07941
B	565	HIS	-	expression tag	UNP P07941
D	1	CYS	SER	engineered mutation	UNP P07941
D	123	HIS	ASP	conflict	UNP P07941
D	132	ALA	ARG	conflict	UNP P07941
D	144	ASP	ALA	conflict	UNP P07941
D	211	GLY	-	insertion	UNP P07941
D	212	THR	ASP	conflict	UNP P07941
D	270	THR	ILE	conflict	UNP P07941
D	291	ARG	LEU	conflict	UNP P07941
D	295	ASN	-	insertion	UNP P07941
D	419	GLN	GLU	conflict	UNP P07941
D	526	ILE	LYS	conflict	UNP P07941

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Chain	Residue	Modelled	Actual	Comment	Reference
D	558	LEU	-	expression tag	UNP P07941
D	559	GLU	-	expression tag	UNP P07941
D	560	HIS	-	expression tag	UNP P07941
D	561	HIS	-	expression tag	UNP P07941
D	562	HIS	-	expression tag	UNP P07941
D	563	HIS	-	expression tag	UNP P07941
D	564	HIS	-	expression tag	UNP P07941
D	565	HIS	-	expression tag	UNP P07941
F	1	CYS	SER	engineered mutation	UNP P07941
F	123	HIS	ASP	conflict	UNP P07941
F	132	ALA	ARG	conflict	UNP P07941
F	144	ASP	ALA	conflict	UNP P07941
F	211	GLY	-	insertion	UNP P07941
F	212	THR	ASP	conflict	UNP P07941
F	270	THR	ILE	conflict	UNP P07941
F	291	ARG	LEU	conflict	UNP P07941
F	295	ASN	-	insertion	UNP P07941
F	419	GLN	GLU	conflict	UNP P07941
F	526	ILE	LYS	conflict	UNP P07941
F	558	LEU	-	expression tag	UNP P07941
F	559	GLU	-	expression tag	UNP P07941
F	560	HIS	-	expression tag	UNP P07941
F	561	HIS	-	expression tag	UNP P07941
F	562	HIS	-	expression tag	UNP P07941
F	563	HIS	-	expression tag	UNP P07941
F	564	HIS	-	expression tag	UNP P07941
F	565	HIS	-	expression tag	UNP P07941
H	1	CYS	SER	engineered mutation	UNP P07941
H	123	HIS	ASP	conflict	UNP P07941
H	132	ALA	ARG	conflict	UNP P07941
H	144	ASP	ALA	conflict	UNP P07941
H	211	GLY	-	insertion	UNP P07941
H	212	THR	ASP	conflict	UNP P07941
H	270	THR	ILE	conflict	UNP P07941
H	291	ARG	LEU	conflict	UNP P07941
H	295	ASN	-	insertion	UNP P07941
H	419	GLN	GLU	conflict	UNP P07941
H	526	ILE	LYS	conflict	UNP P07941
H	558	LEU	-	expression tag	UNP P07941
H	559	GLU	-	expression tag	UNP P07941
H	560	HIS	-	expression tag	UNP P07941
H	561	HIS	-	expression tag	UNP P07941

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Chain	Residue	Modelled	Actual	Comment	Reference
H	562	HIS	-	expression tag	UNP P07941
H	563	HIS	-	expression tag	UNP P07941
H	564	HIS	-	expression tag	UNP P07941
H	565	HIS	-	expression tag	UNP P07941

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Ca 1 1	0	0
3	A	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	E	1	Total Ca 1 1	0	0

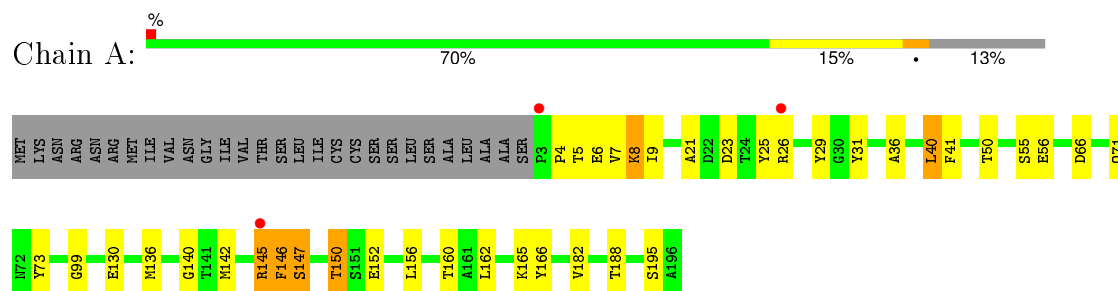
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total O 2 2	0	0
4	B	9	Total O 9 9	0	0
4	C	1	Total O 1 1	0	0
4	D	3	Total O 3 3	0	0
4	F	7	Total O 7 7	0	0
4	G	1	Total O 1 1	0	0
4	H	11	Total O 11 11	0	0

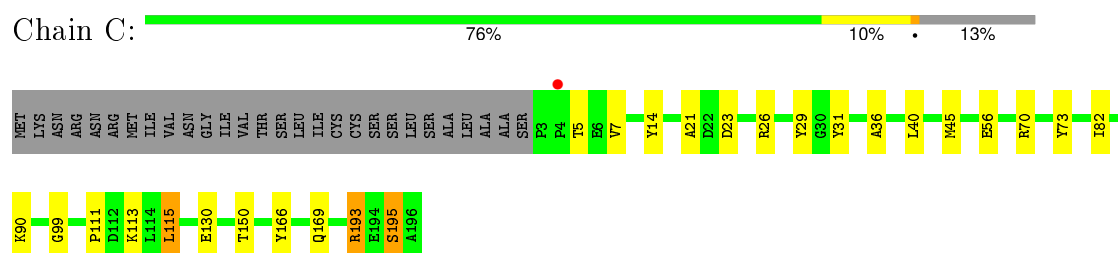
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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.

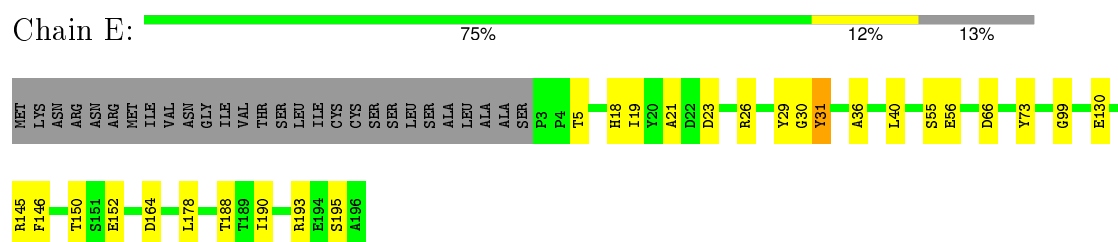
- Molecule 1: Penicillin G acylase subunit alpha



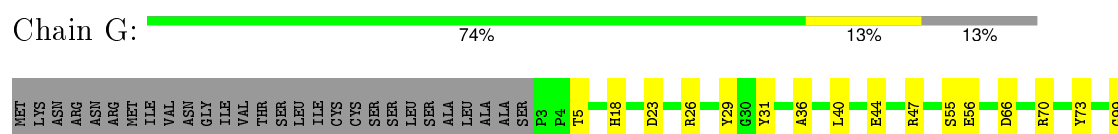
- Molecule 1: Penicillin G acylase subunit alpha



- Molecule 1: Penicillin G acylase subunit alpha



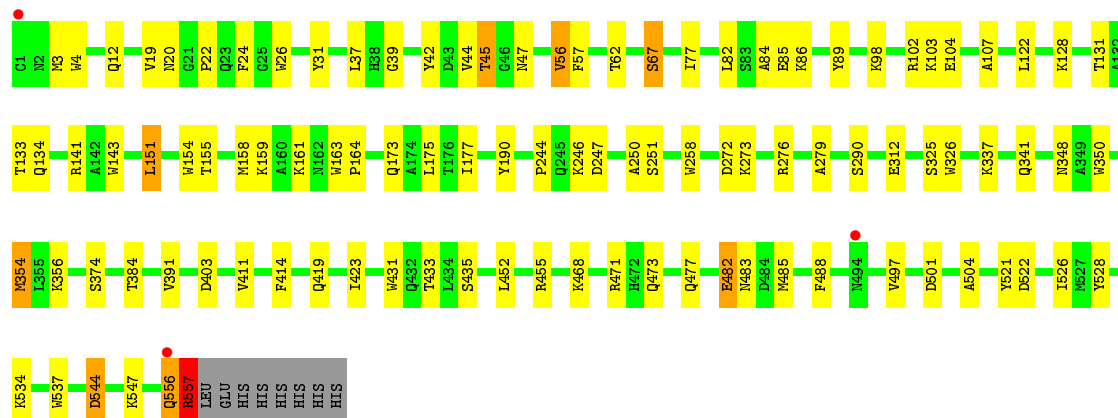
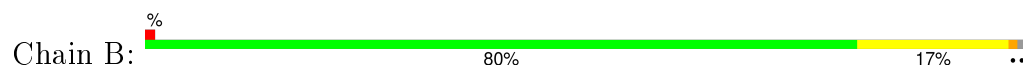
- Molecule 1: Penicillin G acylase subunit alpha



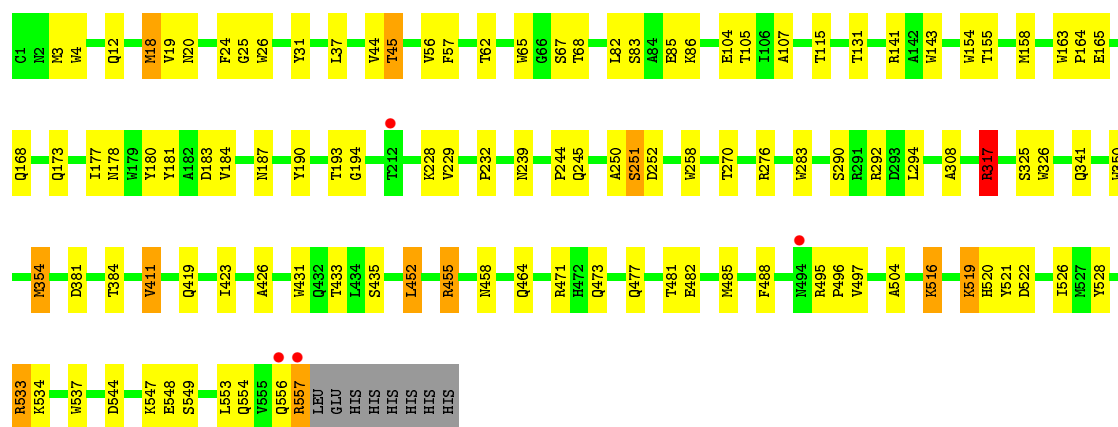
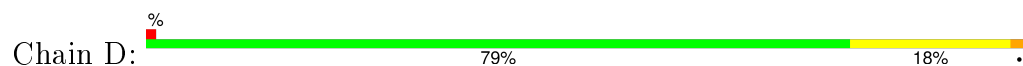




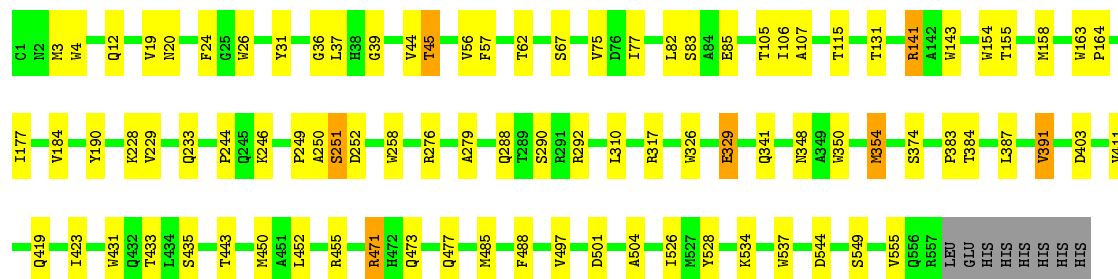
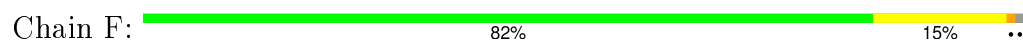
• Molecule 2: Penicillin G acylase subunit beta



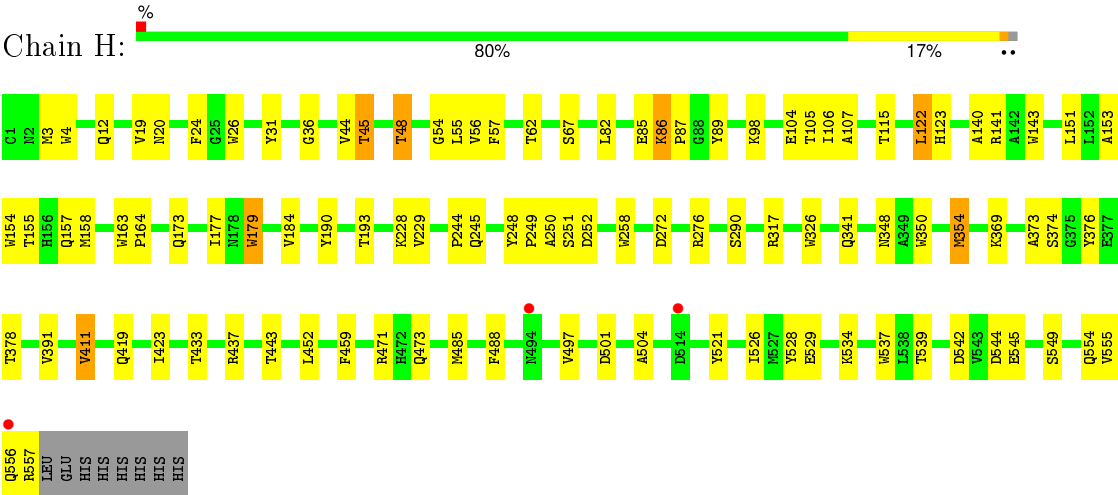
• Molecule 2: Penicillin G acylase subunit beta



• Molecule 2: Penicillin G acylase subunit beta



• Molecule 2: Penicillin G acylase subunit beta



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.26 Å 96.26 Å 100.21 Å 69.27° 69.27° 76.77°	Depositor
Resolution (Å)	38.24 – 2.80 38.21 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.4 (38.24-2.80) 79.0 (38.21-2.80)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 2.81 Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.214 , 0.251 0.216 , 0.252	Depositor DCC
$R_{free}$ test set	3420 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.8	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 20.1	EDS
Estimated twinning fraction	0.037 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 68028 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	23734	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.64	2/1584 (0.1%)	0.76	2/2146 (0.1%)
1	C	0.48	0/1584	0.67	0/2146
1	E	0.51	0/1584	0.72	1/2146 (0.0%)
1	G	0.51	0/1584	0.72	2/2146 (0.1%)
2	B	0.54	1/4507 (0.0%)	0.73	1/6147 (0.0%)
2	D	0.52	0/4507	0.73	5/6147 (0.1%)
2	F	0.52	0/4507	0.70	3/6147 (0.0%)
2	H	0.52	1/4507 (0.0%)	0.72	2/6147 (0.0%)
All	All	0.53	4/24364 (0.0%)	0.72	16/33172 (0.0%)

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	1
2	B	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	8	LYS	C-N	-11.42	1.07	1.34
1	A	9	ILE	C-N	-7.28	1.17	1.34
2	H	179	TRP	CB-CG	-7.16	1.37	1.50
2	B	557	ARG	CA-C	6.31	1.69	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	557	ARG	N-CA-C	9.25	135.97	111.00
1	G	145	ARG	CB-CA-C	-7.47	95.47	110.40
1	A	40	LEU	N-CA-C	-6.83	92.56	111.00
1	E	164	ASP	CB-CA-C	6.69	123.78	110.40
2	D	354	MET	CG-SD-CE	6.52	110.62	100.20
1	A	41	PHE	N-CA-CB	6.14	121.66	110.60
2	H	48	THR	CB-CA-C	-5.84	95.84	111.60
2	F	141	ARG	CB-CG-CD	5.67	126.33	111.60
1	G	145	ARG	CA-CB-CG	5.41	125.30	113.40
2	D	455	ARG	NE-CZ-NH1	5.35	122.98	120.30
2	D	533	ARG	CB-CA-C	-5.35	99.70	110.40
2	D	317	ARG	NE-CZ-NH2	-5.18	117.71	120.30
2	H	272	ASP	CB-CG-OD2	-5.18	113.64	118.30
2	F	391	VAL	CB-CA-C	-5.17	101.57	111.40
2	D	381	ASP	CB-CG-OD1	5.15	122.94	118.30
2	F	471	ARG	NE-CZ-NH1	5.07	122.83	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	LYS	Mainchain
2	B	556	GLN	Mainchain

## 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	1545	0	1505	36	0
1	C	1545	0	1507	30	0
1	E	1545	0	1507	23	0
1	G	1545	0	1507	52	1
2	B	4379	0	4198	77	1
2	D	4379	0	4198	107	0
2	F	4379	0	4198	62	0
2	H	4379	0	4198	95	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	2	0	0	0	0
4	B	9	0	0	1	0
4	C	1	0	0	0	0
4	D	3	0	0	0	0
4	F	7	0	0	0	0
4	G	1	0	0	0	0
4	H	11	0	0	1	0
All	All	23734	0	22818	414	1

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 9.

All (414) 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:G:107:VAL:HG13	1:G:114:LEU:O	1.12	1.28
1:A:145:ARG:HG2	1:A:146:PHE:N	1.55	1.18
1:G:107:VAL:HA	1:G:114:LEU:HB3	1.18	1.17
1:G:107:VAL:CG1	1:G:114:LEU:O	1.93	1.16
1:G:106:LYS:O	1:G:114:LEU:HD12	1.44	1.16
2:D:354:MET:CE	2:D:423:ILE:HA	1.84	1.07
1:G:106:LYS:O	1:G:114:LEU:CD1	2.01	1.06
2:D:25:GLY:O	2:D:481:THR:CG2	2.02	1.06
2:D:25:GLY:O	2:D:481:THR:HG22	1.58	1.03
1:C:14:TYR:CG	2:D:534:LYS:HE3	1.94	1.03
2:B:47:ASN:OD1	2:B:482:GLU:OE1	1.80	0.99
1:A:162:LEU:O	1:A:165:LYS:O	1.78	0.98
2:D:308:ALA:O	2:D:317:ARG:NH2	1.97	0.96
2:D:354:MET:HE3	2:D:423:ILE:HA	1.44	0.96
1:E:26:ARG:NH1	2:F:555:VAL:O	1.98	0.96
2:B:556:GLN:HG2	2:B:557:ARG:N	1.80	0.95
1:G:106:LYS:C	1:G:114:LEU:HD13	1.88	0.93
2:B:556:GLN:HG2	2:B:557:ARG:H	1.32	0.92
2:H:48:THR:CG2	2:H:55:LEU:HA	1.98	0.92
2:F:141:ARG:HD2	2:F:143:TRP:CZ2	2.05	0.91
2:D:173:GLN:HB3	2:D:193:THR:HG21	1.51	0.90
2:B:556:GLN:CG	2:B:557:ARG:H	1.84	0.90
1:A:145:ARG:HG2	1:A:146:PHE:H	1.18	0.89
1:A:50:THR:HG23	1:A:140:GLY:HA3	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ARG:CG	1:A:146:PHE:N	2.36	0.88
1:A:23:ASP:OD1	1:A:26:ARG:HD3	1.73	0.86
1:C:14:TYR:CD2	2:D:534:LYS:HE3	2.12	0.84
2:B:151:LEU:HD12	2:B:151:LEU:O	1.80	0.82
2:D:25:GLY:O	2:D:481:THR:HG21	1.80	0.82
2:H:154:TRP:CZ3	2:H:179:TRP:CH2	2.68	0.82
2:D:354:MET:HE1	2:D:423:ILE:HA	1.59	0.82
1:G:110:SER:O	1:G:114:LEU:HB2	1.80	0.81
2:D:18:MET:HE1	2:D:65:TRP:O	1.79	0.81
1:G:107:VAL:HG13	1:G:114:LEU:C	2.00	0.81
2:F:383:PRO:CG	2:F:450:MET:HE2	2.11	0.81
2:F:383:PRO:CG	2:F:450:MET:CE	2.59	0.80
1:G:106:LYS:C	1:G:114:LEU:CD1	2.47	0.80
2:D:556:GLN:HG3	2:D:557:ARG:H	1.43	0.80
1:A:5:THR:C	1:A:26:ARG:HH12	1.84	0.80
2:H:542:ASP:O	2:H:545:GLU:O	2.02	0.78
2:F:383:PRO:HG3	2:F:450:MET:CE	2.14	0.77
1:G:44:GLU:OE2	1:G:47:ARG:NH2	2.18	0.76
2:D:68:THR:HG21	2:D:239:ASN:OD1	1.84	0.76
2:H:154:TRP:CE3	2:H:179:TRP:CH2	2.73	0.76
1:A:23:ASP:CG	1:A:26:ARG:HD3	2.05	0.76
1:A:50:THR:HG21	1:A:136:MET:O	1.84	0.76
2:D:68:THR:HG23	2:D:178:ASN:HD22	1.52	0.75
2:H:179:TRP:CD1	2:H:193:THR:HG21	2.22	0.75
2:D:228:LYS:O	2:D:229:VAL:HG23	1.88	0.74
2:H:154:TRP:CZ3	2:H:179:TRP:CZ2	2.76	0.74
1:G:110:SER:HB2	1:G:114:LEU:HG	1.70	0.73
1:A:23:ASP:OD1	1:A:26:ARG:CD	2.37	0.72
2:D:68:THR:CG2	2:D:178:ASN:HB2	2.21	0.71
2:F:383:PRO:HG3	2:F:450:MET:HE2	1.70	0.71
1:A:150:THR:HG22	1:A:152:GLU:HG3	1.72	0.71
2:D:68:THR:HG22	2:D:178:ASN:HB2	1.73	0.70
2:D:3:MET:HE1	2:D:18:MET:HG3	1.72	0.70
1:G:5:THR:HG23	2:H:556:GLN:HE21	1.57	0.70
2:D:556:GLN:CG	2:D:557:ARG:H	2.05	0.69
1:A:23:ASP:OD2	1:A:26:ARG:HD3	1.92	0.69
1:C:195:SER:HB2	2:D:245:GLN:HE21	1.56	0.69
2:D:183:ASP:OD2	2:D:187:ASN:ND2	2.25	0.69
2:B:482:GLU:HG3	2:B:483:ASN:N	2.05	0.69
2:F:228:LYS:O	2:F:229:VAL:HG23	1.93	0.69
2:H:48:THR:HG22	2:H:56:VAL:H	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:LEU:O	1:A:160:THR:HG23	1.93	0.69
1:G:23:ASP:OD1	1:G:26:ARG:NH1	2.26	0.68
2:H:48:THR:HG23	2:H:55:LEU:HA	1.73	0.68
1:A:7:VAL:HG12	1:A:21:ALA:HB2	1.76	0.68
1:G:110:SER:HB2	1:G:114:LEU:CG	2.24	0.68
2:B:279:ALA:O	2:B:485:MET:HE1	1.94	0.67
2:B:356:LYS:HD3	2:H:369:LYS:HG3	1.75	0.67
2:B:557:ARG:CG	2:B:557:ARG:HH11	2.07	0.67
2:D:250:ALA:HB2	2:D:258:TRP:CE3	2.30	0.67
2:F:19:VAL:HG22	2:F:485:MET:HG3	1.76	0.67
2:H:250:ALA:HB2	2:H:258:TRP:CE3	2.30	0.67
2:H:153:ALA:HB3	2:H:173:GLN:HG3	1.77	0.67
1:G:145:ARG:HD3	2:H:459:PHE:CZ	2.30	0.67
2:F:279:ALA:O	2:F:485:MET:HE3	1.94	0.67
2:H:151:LEU:HD23	2:H:151:LEU:C	2.16	0.67
1:C:7:VAL:HG12	1:C:21:ALA:HB2	1.78	0.66
2:D:354:MET:HE2	2:D:426:ALA:HB3	1.77	0.66
2:B:173:GLN:HE22	2:B:175:LEU:HB2	1.61	0.66
1:G:107:VAL:HA	1:G:114:LEU:CB	2.11	0.66
2:D:18:MET:HE1	2:D:65:TRP:C	2.14	0.65
1:G:23:ASP:OD1	1:G:26:ARG:HD2	1.96	0.65
1:A:50:THR:CG2	1:A:136:MET:O	2.44	0.65
1:C:150:THR:HG22	2:D:252:ASP:OD2	1.97	0.65
1:G:145:ARG:HD3	2:H:459:PHE:CE1	2.31	0.65
1:C:45:MET:HE2	1:C:45:MET:HA	1.79	0.64
2:F:250:ALA:HB2	2:F:258:TRP:CE3	2.32	0.64
1:G:110:SER:O	1:G:114:LEU:N	2.30	0.64
2:B:250:ALA:HB2	2:B:258:TRP:CE3	2.32	0.64
1:A:145:ARG:NH1	2:B:31:TYR:OH	2.31	0.63
1:G:145:ARG:NE	1:G:146:PHE:CE2	2.66	0.63
2:B:455:ARG:HH22	2:H:437:ARG:HG3	1.63	0.63
2:D:292:ARG:O	2:D:294:LEU:HD12	1.97	0.63
2:H:24:PHE:CD2	2:H:31:TYR:CE2	2.87	0.63
2:F:24:PHE:CD2	2:F:31:TYR:CE2	2.86	0.63
2:D:24:PHE:CD2	2:D:31:TYR:CE2	2.87	0.63
1:A:150:THR:CG2	1:A:152:GLU:HG3	2.29	0.62
2:D:354:MET:CE	2:D:426:ALA:HB3	2.29	0.62
1:C:82:ILE:O	1:C:90:LYS:NZ	2.31	0.62
1:G:56:GLU:HG3	2:H:107:ALA:HB3	1.81	0.62
1:G:145:ARG:HG2	2:H:459:PHE:CE1	2.35	0.61
2:H:179:TRP:CD1	2:H:193:THR:CG2	2.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:539:THR:HG23	2:H:542:ASP:H	1.65	0.61
1:G:107:VAL:N	1:G:114:LEU:HD13	2.15	0.61
2:H:67:SER:HG	2:H:154:TRP:HH2	1.47	0.61
1:A:146:PHE:O	1:A:147:SER:CB	2.49	0.60
2:H:154:TRP:CE3	2:H:179:TRP:HH2	2.17	0.60
2:D:67:SER:HG	2:D:154:TRP:HH2	1.49	0.60
1:E:150:THR:HG22	2:F:252:ASP:OD2	2.02	0.60
1:G:145:ARG:CZ	1:G:146:PHE:CE2	2.84	0.60
2:F:383:PRO:HG2	2:F:450:MET:CE	2.30	0.60
1:G:145:ARG:NH1	2:H:31:TYR:OH	2.35	0.60
1:C:14:TYR:CG	2:D:534:LYS:CE	2.80	0.59
2:H:154:TRP:CE3	2:H:179:TRP:CZ2	2.90	0.59
1:C:14:TYR:CD2	2:D:534:LYS:CE	2.83	0.59
2:B:556:GLN:CG	2:B:557:ARG:N	2.42	0.59
1:A:23:ASP:OD1	1:A:26:ARG:NE	2.35	0.59
1:C:26:ARG:HE	2:D:556:GLN:HE22	1.50	0.59
2:B:24:PHE:CD2	2:B:31:TYR:CE2	2.90	0.59
1:G:195:SER:HB3	2:H:245:GLN:HE21	1.68	0.59
2:B:557:ARG:HG2	2:B:557:ARG:HH11	1.68	0.58
2:D:173:GLN:HB3	2:D:193:THR:CG2	2.31	0.58
2:B:151:LEU:C	2:B:151:LEU:HD12	2.21	0.58
1:E:56:GLU:HG3	2:F:107:ALA:HB3	1.86	0.58
1:C:111:PRO:HB3	1:C:115:LEU:HD23	1.86	0.58
2:B:19:VAL:HG22	2:B:485:MET:HG3	1.86	0.57
1:A:165:LYS:O	1:A:166:TYR:HB2	2.04	0.57
2:H:48:THR:HG21	2:H:55:LEU:HA	1.84	0.57
1:G:107:VAL:CA	1:G:114:LEU:HB3	2.12	0.57
2:B:56:VAL:HG23	2:B:57:PHE:CE1	2.39	0.57
2:D:3:MET:HG3	2:D:4:TRP:N	2.20	0.57
1:G:110:SER:C	1:G:114:LEU:HB2	2.24	0.56
1:G:107:VAL:HG22	1:G:114:LEU:O	2.05	0.56
2:B:272:ASP:O	2:B:273:LYS:HB3	2.02	0.56
1:A:25:TYR:CE1	2:B:557:ARG:HD2	2.40	0.56
2:D:556:GLN:HA	2:D:556:GLN:OE1	2.05	0.56
2:D:85:GLU:O	2:D:86:LYS:HB2	2.06	0.56
1:E:19:ILE:CD1	1:E:31:TYR:N	2.69	0.56
2:F:141:ARG:HD2	2:F:143:TRP:CH2	2.40	0.56
2:H:376:TYR:O	2:H:378:THR:HG23	2.05	0.56
1:G:145:ARG:NE	1:G:146:PHE:CD2	2.74	0.55
1:G:150:THR:HG22	2:H:252:ASP:OD2	2.06	0.55
2:D:350:TRP:NE1	2:D:354:MET:HE2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:MET:O	1:A:146:PHE:O	2.24	0.55
1:G:145:ARG:CG	2:H:459:PHE:CE1	2.90	0.55
1:G:23:ASP:OD1	1:G:26:ARG:CZ	2.55	0.55
2:H:26:TRP:CD2	2:H:452:LEU:HD11	2.42	0.55
2:B:56:VAL:HB	2:B:154:TRP:CZ3	2.42	0.54
2:D:163:TRP:HB3	2:D:164:PRO:HD3	1.90	0.54
2:H:48:THR:HG21	2:H:54:GLY:O	2.08	0.54
2:H:373:ALA:HB1	4:H:708:HOH:O	2.07	0.54
2:D:190:TYR:OH	2:D:244:PRO:HB3	2.08	0.54
2:D:193:THR:HG22	2:D:194:GLY:N	2.22	0.54
2:H:163:TRP:HB3	2:H:164:PRO:HD3	1.90	0.54
1:C:7:VAL:HG23	2:D:553:LEU:HB2	1.90	0.54
1:C:45:MET:HA	1:C:45:MET:CE	2.37	0.53
2:D:283:TRP:CZ2	2:D:533:ARG:HG2	2.43	0.53
2:F:163:TRP:HB3	2:F:164:PRO:HD3	1.90	0.53
1:A:56:GLU:HG3	2:B:107:ALA:HB3	1.89	0.53
2:H:19:VAL:HG22	2:H:485:MET:HG3	1.91	0.53
2:B:557:ARG:HG2	2:B:557:ARG:NH1	2.22	0.53
2:B:419:GLN:HB2	1:C:193:ARG:HH21	1.73	0.53
2:B:190:TYR:OH	2:B:244:PRO:HB3	2.08	0.53
2:B:163:TRP:HB3	2:B:164:PRO:HD3	1.91	0.53
2:F:26:TRP:CD2	2:F:452:LEU:HD11	2.44	0.53
2:D:547:LYS:O	2:D:548:GLU:HG3	2.09	0.53
2:H:190:TYR:OH	2:H:244:PRO:HB3	2.08	0.53
2:F:190:TYR:OH	2:F:244:PRO:HB3	2.08	0.53
2:H:179:TRP:HD1	2:H:193:THR:CG2	2.21	0.53
2:B:26:TRP:CD2	2:B:452:LEU:HD11	2.44	0.53
2:D:516:LYS:O	2:D:516:LYS:HG2	2.08	0.53
1:G:5:THR:HG23	2:H:555:VAL:O	2.08	0.53
2:F:310:LEU:O	2:F:317:ARG:HD2	2.09	0.53
1:G:107:VAL:CG2	1:G:114:LEU:O	2.57	0.52
1:G:145:ARG:HG2	2:H:459:PHE:HE1	1.74	0.52
1:G:107:VAL:CB	1:G:114:LEU:O	2.56	0.52
2:D:83:SER:HB3	2:D:85:GLU:O	2.09	0.52
1:E:19:ILE:HD12	1:E:31:TYR:N	2.25	0.52
2:D:19:VAL:HG22	2:D:485:MET:HG3	1.90	0.52
2:F:45:THR:HG21	2:F:537:TRP:O	2.10	0.52
2:F:3:MET:HG3	2:F:4:TRP:N	2.24	0.52
2:D:473:GLN:NE2	2:D:477:GLN:OE1	2.43	0.52
1:A:4:PRO:O	1:A:26:ARG:NH1	2.43	0.51
2:D:354:MET:HE2	2:D:426:ALA:CB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:83:SER:HB3	2:F:85:GLU:O	2.10	0.51
1:C:5:THR:HG23	2:D:554:GLN:HG2	1.91	0.51
2:D:556:GLN:CG	2:D:557:ARG:N	2.73	0.51
2:D:56:VAL:HG12	2:D:57:PHE:CE1	2.46	0.51
2:F:431:TRP:O	2:F:435:SER:OG	2.25	0.51
2:D:68:THR:HG23	2:D:178:ASN:HB2	1.93	0.51
2:F:3:MET:CE	2:F:20:ASN:CG	2.80	0.51
2:H:173:GLN:NE2	2:H:179:TRP:CE2	2.79	0.51
2:D:283:TRP:CH2	2:D:533:ARG:HG2	2.46	0.51
2:B:45:THR:HG21	2:B:537:TRP:O	2.11	0.51
2:H:3:MET:HG3	2:H:4:TRP:N	2.26	0.51
2:H:56:VAL:HG12	2:H:57:PHE:CE1	2.46	0.50
2:H:45:THR:HG21	2:H:537:TRP:O	2.11	0.50
2:H:452:LEU:HB3	2:H:473:GLN:HB2	1.92	0.50
2:B:473:GLN:NE2	2:B:477:GLN:OE1	2.44	0.50
2:B:3:MET:HG3	2:B:4:TRP:N	2.26	0.50
2:D:431:TRP:O	2:D:435:SER:OG	2.23	0.50
1:E:21:ALA:O	2:F:39:GLY:HA3	2.12	0.50
2:B:471:ARG:NH2	2:B:521:TYR:CE2	2.79	0.50
2:F:387:LEU:HD21	2:F:450:MET:HE3	1.94	0.50
2:F:473:GLN:NE2	2:F:477:GLN:OE1	2.45	0.50
1:A:36:ALA:O	1:A:40:LEU:HB2	2.12	0.50
2:F:56:VAL:HG12	2:F:57:PHE:CE1	2.46	0.50
1:G:166:TYR:CE1	2:H:411:VAL:HG11	2.46	0.49
1:A:4:PRO:O	1:A:26:ARG:CZ	2.60	0.49
2:H:473:GLN:NE2	2:H:529:GLU:HB3	2.28	0.49
1:G:66:ASP:HB3	2:H:106:ILE:HD13	1.93	0.49
2:D:45:THR:HG21	2:D:537:TRP:O	2.12	0.49
1:E:19:ILE:HD13	1:E:30:GLY:C	2.33	0.49
2:H:56:VAL:HG13	2:H:154:TRP:CZ3	2.48	0.49
2:B:47:ASN:CG	2:B:482:GLU:OE1	2.48	0.49
2:F:348:ASN:ND2	2:F:374:SER:OG	2.46	0.49
2:H:173:GLN:NE2	2:H:179:TRP:NE1	2.61	0.48
2:F:383:PRO:CD	2:F:450:MET:HE2	2.43	0.48
2:H:350:TRP:O	2:H:354:MET:HB2	2.13	0.48
2:H:86:LYS:HG2	2:H:89:TYR:CD1	2.48	0.48
1:G:141:THR:HB	1:G:145:ARG:CZ	2.44	0.48
2:B:326:TRP:CD1	2:B:341:GLN:HG3	2.48	0.48
2:B:348:ASN:ND2	2:B:374:SER:OG	2.46	0.48
2:B:102:ARG:NH1	2:B:104:GLU:OE2	2.46	0.48
1:C:195:SER:HB2	2:D:245:GLN:NE2	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:455:ARG:HH22	2:H:437:ARG:CG	2.27	0.48
2:B:452:LEU:HB3	2:B:473:GLN:HB3	1.95	0.48
1:E:36:ALA:O	1:E:40:LEU:HB2	2.13	0.48
2:D:471:ARG:NH2	2:D:521:TYR:CE2	2.82	0.48
2:B:431:TRP:O	2:B:435:SER:OG	2.24	0.48
2:B:89:TYR:CE2	2:B:98:LYS:HG2	2.49	0.48
2:F:62:THR:O	2:F:184:VAL:HG23	2.14	0.48
2:F:292:ARG:NH2	2:F:329:GLU:OE1	2.47	0.48
1:C:14:TYR:CB	2:D:534:LYS:HE3	2.42	0.47
2:H:154:TRP:CH2	2:H:179:TRP:CZ2	3.02	0.47
1:E:193:ARG:NH1	2:F:233:GLN:HE22	2.12	0.47
2:D:350:TRP:O	2:D:354:MET:HB2	2.14	0.47
2:H:85:GLU:O	2:H:87:PRO:HD3	2.14	0.47
2:B:89:TYR:CZ	2:B:98:LYS:HG2	2.49	0.47
2:D:62:THR:O	2:D:184:VAL:HG23	2.13	0.47
2:H:348:ASN:ND2	2:H:374:SER:OG	2.48	0.47
1:C:36:ALA:O	1:C:40:LEU:HB2	2.15	0.47
2:D:458:ASN:OD1	2:D:464:GLN:OE1	2.32	0.47
2:B:350:TRP:O	2:B:354:MET:HB2	2.14	0.47
2:D:56:VAL:HG13	2:D:154:TRP:CZ3	2.50	0.47
2:H:473:GLN:HE22	2:H:528:TYR:HD2	1.62	0.47
2:B:44:VAL:HG11	2:B:158:MET:HB3	1.97	0.47
2:H:326:TRP:CD1	2:H:341:GLN:HG3	2.50	0.47
2:H:157:GLN:OE1	2:H:179:TRP:CZ3	2.68	0.47
1:C:56:GLU:HG3	2:D:107:ALA:HB3	1.97	0.47
2:D:44:VAL:HG11	2:D:158:MET:HB3	1.97	0.47
2:B:67:SER:HG	2:B:154:TRP:HH2	1.60	0.47
2:F:501:ASP:OD1	2:F:534:LYS:HE3	2.15	0.47
1:C:195:SER:CB	2:D:245:GLN:HE21	2.24	0.47
1:G:36:ALA:O	1:G:40:LEU:HB2	2.14	0.47
2:H:62:THR:O	2:H:184:VAL:HG23	2.14	0.47
2:F:350:TRP:O	2:F:354:MET:HB2	2.14	0.46
2:H:44:VAL:HG11	2:H:158:MET:HB3	1.97	0.46
2:D:350:TRP:CZ2	2:D:354:MET:HG2	2.51	0.46
2:F:452:LEU:HB3	2:F:473:GLN:HB3	1.96	0.46
2:H:122:LEU:HD22	2:H:123:HIS:N	2.29	0.46
1:E:19:ILE:CD1	1:E:30:GLY:C	2.83	0.46
2:D:26:TRP:CE2	2:D:452:LEU:HD21	2.50	0.46
1:A:165:LYS:O	1:A:166:TYR:CB	2.63	0.46
2:H:473:GLN:NE2	2:H:528:TYR:HD2	2.14	0.46
2:B:62:THR:HG21	2:B:161:LYS:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:354:MET:HE1	2:D:423:ILE:CA	2.39	0.46
1:C:14:TYR:CB	2:D:534:LYS:CE	2.93	0.46
1:E:66:ASP:HB3	2:F:106:ILE:HD13	1.97	0.46
2:F:44:VAL:HG11	2:F:158:MET:HB3	1.98	0.46
2:F:383:PRO:HG3	2:F:450:MET:HE3	1.95	0.45
1:G:145:ARG:NH1	2:H:459:PHE:CE2	2.83	0.45
2:B:468:LYS:HE2	2:B:468:LYS:HB2	1.53	0.45
2:D:519:LYS:HE3	2:D:520:HIS:CE1	2.51	0.45
2:F:12:GLN:HB2	2:F:276:ARG:HB3	1.98	0.45
2:D:68:THR:CG2	2:D:180:TYR:OH	2.64	0.45
2:H:350:TRP:CZ2	2:H:354:MET:HG2	2.51	0.45
1:E:55:SER:OG	1:E:66:ASP:OD2	2.31	0.45
2:F:326:TRP:CD1	2:F:341:GLN:HG3	2.51	0.45
2:H:122:LEU:C	2:H:122:LEU:HD22	2.37	0.45
1:E:18:HIS:CD2	2:F:36:GLY:HA3	2.52	0.45
1:G:145:ARG:CD	2:H:459:PHE:CE1	2.99	0.45
1:C:166:TYR:CE1	2:D:411:VAL:HG11	2.51	0.45
2:B:84:ALA:HB2	2:B:134:GLN:NE2	2.32	0.45
1:E:190:ILE:HG23	2:F:229:VAL:HG21	1.99	0.45
2:B:384:THR:HG22	2:B:455:ARG:NH2	2.31	0.45
2:B:471:ARG:NH2	2:B:521:TYR:CZ	2.85	0.45
2:D:471:ARG:NH1	2:D:522:ASP:OD1	2.49	0.45
1:A:145:ARG:NH2	2:B:31:TYR:OH	2.50	0.45
2:B:414:PHE:CZ	2:B:419:GLN:HG2	2.52	0.45
2:B:471:ARG:NH1	2:B:522:ASP:OD1	2.50	0.45
2:D:504:ALA:HB2	2:D:528:TYR:HB2	1.99	0.45
1:C:150:THR:HA	2:D:252:ASP:OD1	2.17	0.45
2:B:12:GLN:HB2	2:B:276:ARG:HB3	1.98	0.45
2:B:501:ASP:OD1	2:B:534:LYS:HE3	2.17	0.45
2:D:165:GLU:O	2:D:168:GLN:HG2	2.17	0.45
2:D:354:MET:CE	2:D:426:ALA:CB	2.94	0.44
2:B:356:LYS:HD3	2:H:369:LYS:CG	2.42	0.44
2:H:105:THR:HG23	2:H:115:THR:HG22	1.98	0.44
2:H:228:LYS:O	2:H:229:VAL:HG13	2.16	0.44
2:F:105:THR:HG23	2:F:115:THR:HG22	1.99	0.44
2:F:488:PHE:CD1	2:F:497:VAL:HG22	2.53	0.44
2:D:12:GLN:HB2	2:D:276:ARG:HB3	1.98	0.44
1:C:29:TYR:O	1:C:99:GLY:HA3	2.18	0.44
2:F:350:TRP:CZ2	2:F:354:MET:HG2	2.52	0.44
1:C:150:THR:HG22	2:D:252:ASP:CG	2.37	0.44
2:D:471:ARG:NH2	2:D:521:TYR:CZ	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:12:GLN:HB2	2:H:276:ARG:HB3	1.98	0.44
2:B:544:ASP:OD1	2:B:547:LYS:HE3	2.17	0.44
2:F:3:MET:CG	2:F:4:TRP:N	2.81	0.44
2:D:326:TRP:CD1	2:D:341:GLN:HG3	2.53	0.44
1:C:70:ARG:NH1	2:D:104:GLU:OE1	2.50	0.44
2:B:3:MET:CE	2:B:20:ASN:CG	2.86	0.44
2:H:471:ARG:NH2	2:H:521:TYR:CE2	2.86	0.44
2:F:504:ALA:HB2	2:F:528:TYR:HB2	2.00	0.44
2:D:317:ARG:NH2	2:H:98:LYS:HE3	2.32	0.44
1:G:114:LEU:HA	1:G:114:LEU:HD23	1.82	0.43
1:E:5:THR:HA	1:E:26:ARG:NH1	2.33	0.43
2:H:539:THR:CG2	2:H:542:ASP:H	2.31	0.43
1:A:182:VAL:HG11	2:B:247:ASP:HA	2.00	0.43
2:D:105:THR:HG23	2:D:115:THR:HG22	2.00	0.43
1:G:5:THR:HG22	2:H:554:GLN:HA	2.00	0.43
1:E:145:ARG:HD3	1:E:146:PHE:CE2	2.53	0.43
1:E:188:THR:HG21	2:F:246:LYS:N	2.34	0.43
2:D:173:GLN:OE1	2:D:193:THR:HG21	2.19	0.43
2:H:504:ALA:HB2	2:H:528:TYR:HB2	2.01	0.43
1:E:145:ARG:CZ	1:E:146:PHE:CZ	3.02	0.43
2:D:141:ARG:HD3	2:D:143:TRP:CH2	2.54	0.43
1:A:6:GLU:O	1:A:26:ARG:NH2	2.51	0.43
2:D:3:MET:HE2	2:D:19:VAL:O	2.19	0.43
2:D:3:MET:HE3	2:D:20:ASN:HB2	1.99	0.43
2:B:488:PHE:CD1	2:B:497:VAL:HG22	2.53	0.43
2:D:384:THR:HG22	2:D:455:ARG:NH2	2.33	0.43
2:D:3:MET:CG	2:D:4:TRP:N	2.82	0.43
2:D:516:LYS:O	2:D:516:LYS:CG	2.67	0.43
2:H:3:MET:CE	2:H:20:ASN:CG	2.86	0.43
2:H:419:GLN:O	2:H:423:ILE:HG13	2.19	0.43
2:D:488:PHE:CD1	2:D:497:VAL:HG22	2.54	0.43
1:A:21:ALA:O	2:B:39:GLY:HA3	2.19	0.43
2:B:141:ARG:HD3	2:B:143:TRP:CH2	2.54	0.43
2:D:419:GLN:O	2:D:423:ILE:HG13	2.19	0.43
2:D:68:THR:CG2	2:D:178:ASN:HD22	2.27	0.43
1:G:145:ARG:CD	2:H:459:PHE:CZ	3.01	0.43
1:E:145:ARG:HG2	1:E:146:PHE:CD2	2.54	0.43
2:B:504:ALA:HB2	2:B:528:TYR:HB2	2.01	0.43
2:H:539:THR:HG22	2:H:542:ASP:HB2	2.01	0.42
2:B:272:ASP:O	2:B:273:LYS:CB	2.67	0.42
1:C:23:ASP:C	1:C:23:ASP:OD2	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:419:GLN:O	2:F:423:ILE:HG13	2.20	0.42
1:E:23:ASP:OD1	1:E:26:ARG:HG3	2.19	0.42
1:C:150:THR:HG22	2:D:252:ASP:OD1	2.20	0.42
2:B:455:ARG:HH12	2:H:437:ARG:HA	1.84	0.42
1:E:152:GLU:HB2	2:F:77:ILE:HG13	2.00	0.42
1:E:29:TYR:O	1:E:99:GLY:HA3	2.20	0.42
2:H:488:PHE:CD1	2:H:497:VAL:HG22	2.54	0.42
2:D:163:TRP:HB3	2:D:164:PRO:CD	2.49	0.42
2:B:419:GLN:O	2:B:423:ILE:HG13	2.19	0.42
1:A:188:THR:HG21	2:B:246:LYS:N	2.34	0.42
1:A:55:SER:OG	1:A:66:ASP:OD2	2.32	0.42
2:F:384:THR:HG22	2:F:455:ARG:NH2	2.35	0.42
2:H:157:GLN:NE2	2:H:179:TRP:CZ3	2.85	0.42
1:A:5:THR:CA	1:A:26:ARG:HH12	2.32	0.42
1:C:195:SER:CB	2:D:245:GLN:NE2	2.82	0.42
1:G:29:TYR:O	1:G:99:GLY:HA3	2.18	0.42
2:B:557:ARG:CG	2:B:557:ARG:NH1	2.73	0.42
2:D:68:THR:HG22	2:D:178:ASN:CB	2.46	0.42
2:F:163:TRP:HB3	2:F:164:PRO:CD	2.49	0.42
2:H:471:ARG:NH2	2:H:521:TYR:CZ	2.88	0.42
2:D:229:VAL:HG11	2:D:232:PRO:HB3	2.01	0.42
1:G:23:ASP:OD1	1:G:26:ARG:CD	2.65	0.42
2:B:356:LYS:HG2	2:H:369:LYS:HE3	2.00	0.42
2:D:37:LEU:HB2	2:D:44:VAL:CG2	2.50	0.42
1:A:152:GLU:HB2	2:B:77:ILE:HG13	2.02	0.41
1:E:150:THR:HG23	2:F:75:VAL:HB	2.01	0.41
2:F:288:GLN:HA	2:F:329:GLU:OE2	2.19	0.41
1:G:110:SER:HB2	1:G:114:LEU:CD1	2.50	0.41
1:A:29:TYR:O	1:A:99:GLY:HA3	2.20	0.41
2:F:56:VAL:HG13	2:F:154:TRP:CZ3	2.55	0.41
2:D:26:TRP:CD2	2:D:452:LEU:HD21	2.55	0.41
1:G:18:HIS:CD2	2:H:36:GLY:HA3	2.56	0.41
2:H:141:ARG:HD3	2:H:143:TRP:CH2	2.55	0.41
2:H:539:THR:HG23	2:H:542:ASP:N	2.34	0.41
2:F:3:MET:HE3	2:F:20:ASN:CG	2.40	0.41
2:H:3:MET:CG	2:H:4:TRP:N	2.83	0.41
2:B:37:LEU:HB2	2:B:44:VAL:CG2	2.51	0.41
2:H:123:HIS:O	2:H:140:ALA:HA	2.21	0.41
2:B:85:GLU:O	2:B:86:LYS:HG3	2.21	0.41
2:H:151:LEU:CD2	2:H:151:LEU:C	2.87	0.41
2:B:163:TRP:HB3	2:B:164:PRO:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:248:TYR:HA	2:H:249:PRO:HD3	1.99	0.41
2:B:42:TYR:CZ	2:B:159:LYS:HE3	2.55	0.41
2:D:181:TYR:HE1	2:D:187:ASN:OD1	2.04	0.41
2:B:3:MET:CG	2:B:4:TRP:N	2.83	0.41
2:D:350:TRP:NE1	2:D:354:MET:CE	2.83	0.40
2:F:383:PRO:HG2	2:F:450:MET:HE1	2.02	0.40
2:F:37:LEU:HB2	2:F:44:VAL:CG2	2.51	0.40
1:G:146:PHE:CZ	2:H:24:PHE:HD1	2.39	0.40
2:H:163:TRP:HB3	2:H:164:PRO:CD	2.51	0.40
2:F:288:GLN:O	2:F:329:GLU:OE2	2.38	0.40
1:G:70:ARG:NH1	2:H:104:GLU:OE1	2.53	0.40
2:H:501:ASP:OD1	2:H:534:LYS:HE3	2.21	0.40
2:F:387:LEU:HD11	2:F:450:MET:CE	2.51	0.40
2:D:283:TRP:CZ2	2:D:533:ARG:CG	3.04	0.40
2:B:312:GLU:O	2:B:312:GLU:HG2	2.21	0.40
2:D:495:ARG:HB3	2:D:496:PRO:HD2	2.04	0.40
2:B:22:PRO:HB2	2:B:24:PHE:CE2	2.57	0.40
1:C:14:TYR:CB	2:D:534:LYS:NZ	2.85	0.40
2:F:383:PRO:HD3	2:F:450:MET:HE2	2.04	0.40
2:D:68:THR:HG21	2:D:180:TYR:OH	2.22	0.40
2:B:455:ARG:NH1	4:B:707:HOH:O	2.37	0.40

All (1) 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)
2:B:103:LYS:NZ	1:G:108:ASN:O[1_565]	1.90	0.30

## 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	192/222 (86%)	184 (96%)	8 (4%)	0	100	100
1	C	192/222 (86%)	186 (97%)	6 (3%)	0	100	100
1	E	192/222 (86%)	187 (97%)	5 (3%)	0	100	100
1	G	192/222 (86%)	184 (96%)	8 (4%)	0	100	100
2	B	555/565 (98%)	537 (97%)	18 (3%)	0	100	100
2	D	555/565 (98%)	533 (96%)	21 (4%)	1 (0%)	52	84
2	F	555/565 (98%)	538 (97%)	16 (3%)	1 (0%)	52	84
2	H	555/565 (98%)	535 (96%)	19 (3%)	1 (0%)	52	84
All	All	2988/3148 (95%)	2884 (96%)	101 (3%)	3 (0%)	56	87

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	251	SER
2	D	251	SER
2	F	251	SER

### 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	164/188 (87%)	155 (94%)	9 (6%)	27	59
1	C	164/188 (87%)	156 (95%)	8 (5%)	31	65
1	E	164/188 (87%)	159 (97%)	5 (3%)	48	82
1	G	164/188 (87%)	159 (97%)	5 (3%)	48	82
2	B	449/457 (98%)	425 (95%)	24 (5%)	28	61
2	D	449/457 (98%)	428 (95%)	21 (5%)	32	67
2	F	449/457 (98%)	429 (96%)	20 (4%)	34	68
2	H	449/457 (98%)	432 (96%)	17 (4%)	40	74
All	All	2452/2580 (95%)	2343 (96%)	109 (4%)	35	69

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	TYR
1	A	71	GLN
1	A	73	TYR
1	A	130	GLU
1	A	145	ARG
1	A	146	PHE
1	A	147	SER
1	A	150	THR
1	A	195	SER
2	B	45	THR
2	B	56	VAL
2	B	67	SER
2	B	82	LEU
2	B	122	LEU
2	B	128	LYS
2	B	131	THR
2	B	133	THR
2	B	151	LEU
2	B	155	THR
2	B	177	ILE
2	B	251	SER
2	B	290	SER
2	B	325	SER
2	B	337	LYS
2	B	354	MET
2	B	391	VAL
2	B	403	ASP
2	B	411	VAL
2	B	433	THR
2	B	482	GLU
2	B	526	ILE
2	B	544	ASP
2	B	557	ARG
1	C	31	TYR
1	C	73	TYR
1	C	113	LYS
1	C	115	LEU
1	C	130	GLU
1	C	169	GLN
1	C	193	ARG
1	C	195	SER
2	D	18	MET

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Mol	Chain	Res	Type
2	D	45	THR
2	D	82	LEU
2	D	131	THR
2	D	155	THR
2	D	177	ILE
2	D	251	SER
2	D	270	THR
2	D	290	SER
2	D	317	ARG
2	D	325	SER
2	D	411	VAL
2	D	433	THR
2	D	452	LEU
2	D	482	GLU
2	D	516	LYS
2	D	519	LYS
2	D	526	ILE
2	D	544	ASP
2	D	549	SER
2	D	557	ARG
1	E	31	TYR
1	E	73	TYR
1	E	130	GLU
1	E	178	LEU
1	E	195	SER
2	F	45	THR
2	F	67	SER
2	F	82	LEU
2	F	131	THR
2	F	155	THR
2	F	177	ILE
2	F	249	PRO
2	F	251	SER
2	F	290	SER
2	F	329	GLU
2	F	354	MET
2	F	391	VAL
2	F	403	ASP
2	F	411	VAL
2	F	433	THR
2	F	443	THR
2	F	471	ARG

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Mol	Chain	Res	Type
2	F	526	ILE
2	F	544	ASP
2	F	549	SER
1	G	31	TYR
1	G	55	SER
1	G	73	TYR
1	G	113	LYS
1	G	130	GLU
2	H	45	THR
2	H	82	LEU
2	H	86	LYS
2	H	122	LEU
2	H	155	THR
2	H	177	ILE
2	H	290	SER
2	H	317	ARG
2	H	354	MET
2	H	391	VAL
2	H	411	VAL
2	H	433	THR
2	H	443	THR
2	H	526	ILE
2	H	544	ASP
2	H	549	SER
2	H	557	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	47	ASN
2	B	173	GLN
2	B	203	HIS
2	B	348	ASN
2	B	432	GLN
1	C	169	GLN
2	D	203	HIS
2	D	245	GLN
2	D	274	GLN
2	F	233	GLN
2	F	274	GLN
2	F	348	ASN
2	F	432	GLN

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Mol	Chain	Res	Type
2	F	494	ASN
1	G	169	GLN
2	H	203	HIS
2	H	245	GLN
2	H	348	ASN
2	H	556	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are 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 ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	9:ILE	C	10:VAL	N	1.17
1	A	8:LYS	C	9:ILE	N	1.07

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	194/222 (87%)	-0.43	3 (1%) 76 68	26, 47, 78, 114	0
1	C	194/222 (87%)	-0.38	1 (0%) 91 88	24, 54, 82, 98	0
1	E	194/222 (87%)	-0.57	0 100 100	26, 43, 67, 98	0
1	G	194/222 (87%)	-0.44	1 (0%) 91 88	31, 47, 68, 93	0
2	B	557/565 (98%)	-0.39	3 (0%) 91 88	23, 45, 73, 113	0
2	D	557/565 (98%)	-0.33	4 (0%) 89 84	27, 50, 79, 103	0
2	F	557/565 (98%)	-0.45	0 100 100	25, 44, 67, 93	0
2	H	557/565 (98%)	-0.40	3 (0%) 91 88	24, 45, 68, 101	0
All	All	3004/3148 (95%)	-0.41	15 (0%) 91 88	23, 46, 74, 114	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	556	GLN	4.4
1	G	114	LEU	3.6
1	A	3	PRO	3.4
2	H	556	GLN	2.9
2	D	557	ARG	2.4
2	D	494	ASN	2.3
2	B	494	ASN	2.3
2	B	556	GLN	2.3
2	D	212	THR	2.2
2	H	494	ASN	2.2
1	C	4	PRO	2.1
1	A	26	ARG	2.1
2	B	1	CYS	2.1
2	H	514	ASP	2.1
1	A	145	ARG	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CA	A	601	1/1	0.98	0.09	-1.41	30,30,30,30	0
3	CA	E	601	1/1	0.99	0.10	-1.52	31,31,31,31	0
3	CA	C	601	1/1	0.99	0.07	-2.76	34,34,34,34	0
3	CA	G	601	1/1	0.97	0.06	-3.43	44,44,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.