



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:34 PM GMT

PDB ID : 4HNT
Title : crystal structure of F403A mutant of *S. aureus* Pyruvate carboxylase
Authors : Yu, L.P.C.; Tong, L.
Deposited on : 2012-10-21
Resolution : 2.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

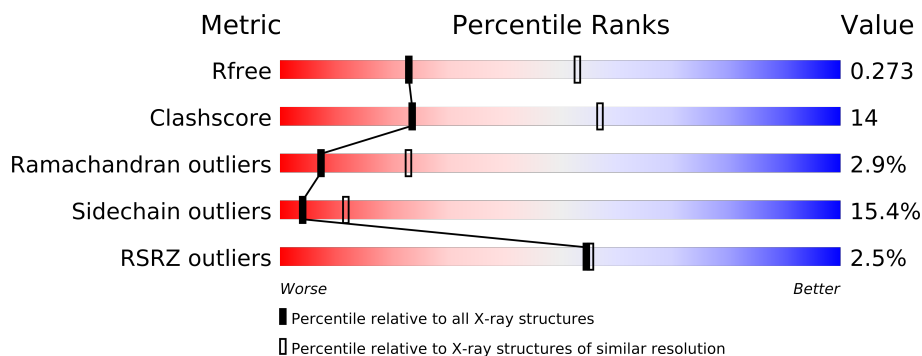
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1173	
1	B	1173	
1	C	1173	
1	D	1173	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32480 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Pyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1052	Total	C	N	O	S	0	0	0
			8336	5286	1404	1619	27			
1	B	989	Total	C	N	O	S	0	0	0
			7832	4969	1321	1516	26			
1	C	1059	Total	C	N	O	S	0	0	0
			8373	5307	1412	1626	28			
1	D	989	Total	C	N	O	S	0	0	0
			7832	4969	1321	1516	26			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	EXPRESSION TAG	UNP Q99UY8
A	12	GLY	-	EXPRESSION TAG	UNP Q99UY8
A	13	SER	-	EXPRESSION TAG	UNP Q99UY8
A	14	SER	-	EXPRESSION TAG	UNP Q99UY8
A	15	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	16	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	17	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	18	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	19	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	20	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	21	SER	-	EXPRESSION TAG	UNP Q99UY8
A	22	SER	-	EXPRESSION TAG	UNP Q99UY8
A	23	GLY	-	EXPRESSION TAG	UNP Q99UY8
A	24	LEU	-	EXPRESSION TAG	UNP Q99UY8
A	25	VAL	-	EXPRESSION TAG	UNP Q99UY8
A	26	PRO	-	EXPRESSION TAG	UNP Q99UY8
A	27	ARG	-	EXPRESSION TAG	UNP Q99UY8
A	28	GLY	-	EXPRESSION TAG	UNP Q99UY8
A	29	SER	-	EXPRESSION TAG	UNP Q99UY8
A	30	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	31	MET	-	EXPRESSION TAG	UNP Q99UY8

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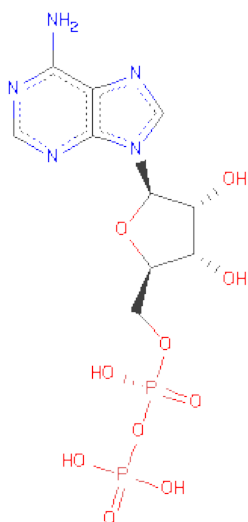
Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ALA	-	EXPRESSION TAG	UNP Q99UY8
A	33	SER	-	EXPRESSION TAG	UNP Q99UY8
B	11	MET	-	EXPRESSION TAG	UNP Q99UY8
B	12	GLY	-	EXPRESSION TAG	UNP Q99UY8
B	13	SER	-	EXPRESSION TAG	UNP Q99UY8
B	14	SER	-	EXPRESSION TAG	UNP Q99UY8
B	15	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	16	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	17	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	18	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	19	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	20	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	21	SER	-	EXPRESSION TAG	UNP Q99UY8
B	22	SER	-	EXPRESSION TAG	UNP Q99UY8
B	23	GLY	-	EXPRESSION TAG	UNP Q99UY8
B	24	LEU	-	EXPRESSION TAG	UNP Q99UY8
B	25	VAL	-	EXPRESSION TAG	UNP Q99UY8
B	26	PRO	-	EXPRESSION TAG	UNP Q99UY8
B	27	ARG	-	EXPRESSION TAG	UNP Q99UY8
B	28	GLY	-	EXPRESSION TAG	UNP Q99UY8
B	29	SER	-	EXPRESSION TAG	UNP Q99UY8
B	30	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	31	MET	-	EXPRESSION TAG	UNP Q99UY8
B	32	ALA	-	EXPRESSION TAG	UNP Q99UY8
B	33	SER	-	EXPRESSION TAG	UNP Q99UY8
C	11	MET	-	EXPRESSION TAG	UNP Q99UY8
C	12	GLY	-	EXPRESSION TAG	UNP Q99UY8
C	13	SER	-	EXPRESSION TAG	UNP Q99UY8
C	14	SER	-	EXPRESSION TAG	UNP Q99UY8
C	15	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	16	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	17	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	18	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	19	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	20	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	21	SER	-	EXPRESSION TAG	UNP Q99UY8
C	22	SER	-	EXPRESSION TAG	UNP Q99UY8
C	23	GLY	-	EXPRESSION TAG	UNP Q99UY8
C	24	LEU	-	EXPRESSION TAG	UNP Q99UY8
C	25	VAL	-	EXPRESSION TAG	UNP Q99UY8
C	26	PRO	-	EXPRESSION TAG	UNP Q99UY8
C	27	ARG	-	EXPRESSION TAG	UNP Q99UY8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	28	GLY	-	EXPRESSION TAG	UNP Q99UY8
C	29	SER	-	EXPRESSION TAG	UNP Q99UY8
C	30	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	31	MET	-	EXPRESSION TAG	UNP Q99UY8
C	32	ALA	-	EXPRESSION TAG	UNP Q99UY8
C	33	SER	-	EXPRESSION TAG	UNP Q99UY8
D	11	MET	-	EXPRESSION TAG	UNP Q99UY8
D	12	GLY	-	EXPRESSION TAG	UNP Q99UY8
D	13	SER	-	EXPRESSION TAG	UNP Q99UY8
D	14	SER	-	EXPRESSION TAG	UNP Q99UY8
D	15	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	16	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	17	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	18	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	19	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	20	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	21	SER	-	EXPRESSION TAG	UNP Q99UY8
D	22	SER	-	EXPRESSION TAG	UNP Q99UY8
D	23	GLY	-	EXPRESSION TAG	UNP Q99UY8
D	24	LEU	-	EXPRESSION TAG	UNP Q99UY8
D	25	VAL	-	EXPRESSION TAG	UNP Q99UY8
D	26	PRO	-	EXPRESSION TAG	UNP Q99UY8
D	27	ARG	-	EXPRESSION TAG	UNP Q99UY8
D	28	GLY	-	EXPRESSION TAG	UNP Q99UY8
D	29	SER	-	EXPRESSION TAG	UNP Q99UY8
D	30	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	31	MET	-	EXPRESSION TAG	UNP Q99UY8
D	32	ALA	-	EXPRESSION TAG	UNP Q99UY8
D	33	SER	-	EXPRESSION TAG	UNP Q99UY8

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

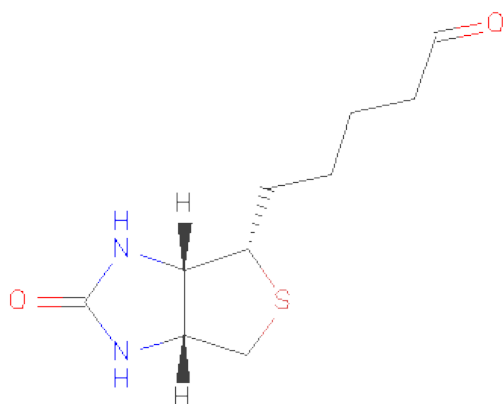


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

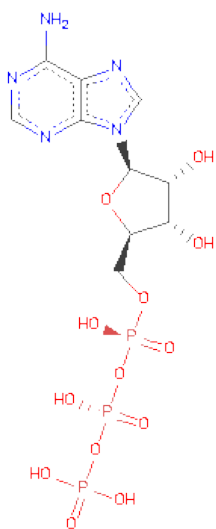
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

- Molecule 4 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (three-letter code: BTI) (formula: C₁₀H₁₆N₂O₂S).



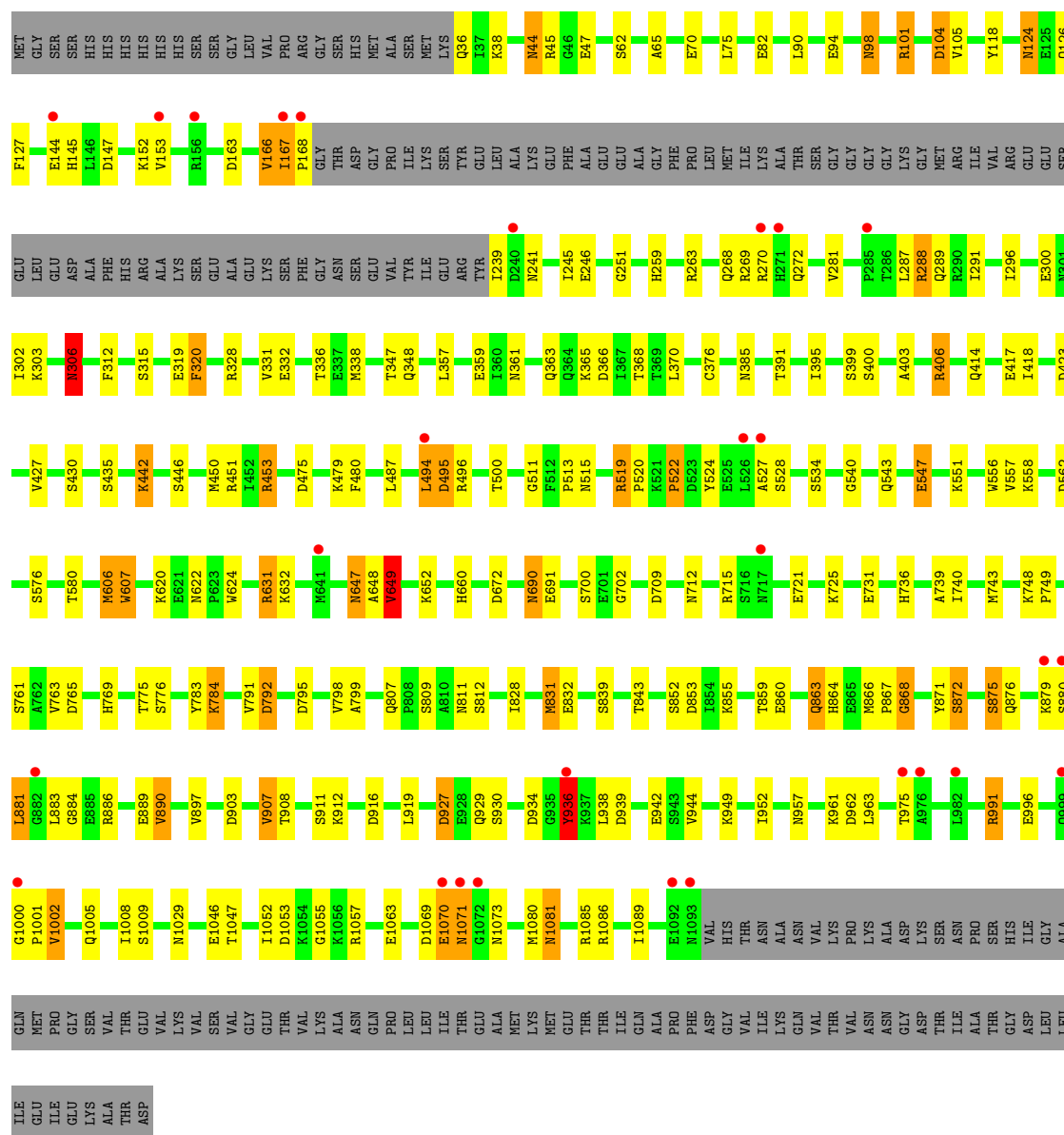
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
4	B	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
4	D	1	Total	C	N	O	S	0	0
			15	10	2	2	1		

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



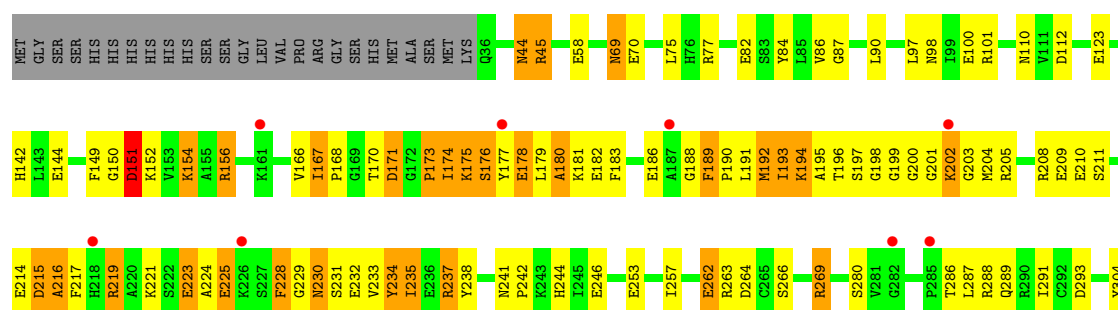
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

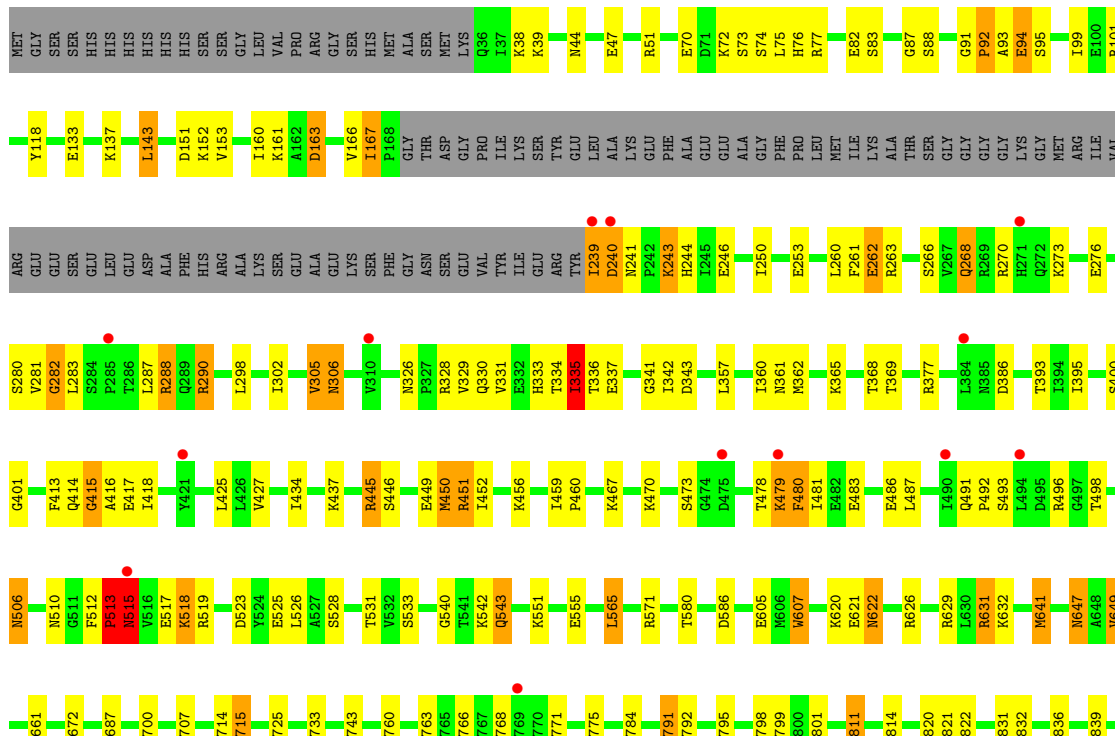
Chain B:



- Molecule 1: Pyruvate carboxylase

Chain C:





THR	SER	Y845
GLY	HIS	
ASP	ILE	S852
LEU	GLY	D853
LEU	ALA	I854
ILE	GLN	K855
GLU	MET	S856
ILE	PRO	
ILE	GLY	D986
LYS	SER	Q863
ALA	VAL	H864
THR	THR	E865
ASP	GLU	M866
	VAL	
	LYS	G869
	VAL	Q870
	VAL	Y871
	VAL	L874
	GLY	S875
	GLU	
	THR	A879
	VAL	
	LYS	G884
	ALA	F885
	ASN	R886
	GLN	F887
	PRO	D888
	LEU	
	LEU	M893
	ILE	
	THR	R896
	GLU	
	ALA	Y907
	MET	T908
	LYS	P909
	MET	S910
	GLU	S911
	THR	
	THR	M917
	ILE	A918
	GLN	L919
	ALA	Y920
	PRO	M921
	PHE	
	ASP	N1093
	GLY	VAL
	VAL	HIS
	ILE	THR
	LYS	ASN
	GLN	ALA
	VAL	ASN
	THR	VAL
	THR	LYS
	VAL	PRO
	ASN	LYS
	GLY	ALA
	ASP	ASP
	THR	LYS
	ILE	SER
	ALA	ASN
		PRO
		L963

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.23Å 256.28Å 126.69Å 90.00° 109.86° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 29.79 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.0 (30.00-2.80) 91.0 (29.79-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.209 , 0.279 0.209 , 0.273	Depositor DCC
R_{free} test set	6458 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	72.2	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.0	EDS
Estimated twinning fraction	0.030 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 128487 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	32480	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, BTI, ATP, ADP

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	0.68	1/8497 (0.0%)	0.73	1/11490 (0.0%)
1	B	0.63	4/7983 (0.1%)	0.66	3/10801 (0.0%)
1	C	0.65	4/8535 (0.0%)	0.68	4/11539 (0.0%)
1	D	0.66	5/7983 (0.1%)	0.70	2/10801 (0.0%)
All	All	0.65	14/32998 (0.0%)	0.69	10/44631 (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	6
1	B	0	3
1	C	0	7
1	D	0	2
All	All	0	18

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	513	PRO	CA-C	14.00	1.80	1.52
1	B	936	TYR	C-N	11.65	1.60	1.34
1	C	513	PRO	C-N	10.85	1.58	1.34
1	C	515	ASN	N-CA	10.62	1.67	1.46
1	B	961	LYS	C-O	10.00	1.42	1.23
1	C	513	PRO	N-CA	8.86	1.62	1.47
1	D	290	ARG	CZ-NH1	8.75	1.44	1.33
1	A	513	PRO	CA-C	8.56	1.70	1.52
1	D	513	PRO	CA-C	7.66	1.68	1.52
1	D	515	ASN	N-CA	7.36	1.61	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	513	PRO	CA-C	7.18	1.67	1.52
1	D	513	PRO	C-N	6.20	1.48	1.34
1	D	513	PRO	N-CA	5.96	1.57	1.47
1	B	763	VAL	N-CA	5.78	1.57	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	513	PRO	C-N-CA	8.07	141.87	121.70
1	D	513	PRO	CA-C-N	7.87	134.51	117.20
1	C	513	PRO	CA-C-N	7.83	134.42	117.20
1	B	763	VAL	CA-C-N	7.35	133.38	117.20
1	C	513	PRO	N-CA-CB	-6.11	95.88	102.60
1	A	513	PRO	CA-C-N	6.09	130.60	117.20
1	B	763	VAL	O-C-N	-5.91	113.25	122.70
1	B	513	PRO	CA-C-N	5.68	129.69	117.20
1	C	513	PRO	O-C-N	-5.66	113.64	122.70
1	D	513	PRO	O-C-N	-5.57	113.78	122.70

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1078	TYR	Peptide
1	A	150	GLY	Peptide
1	A	196	THR	Peptide
1	A	271	HIS	Peptide
1	A	415	GLY	Peptide
1	A	490	ILE	Peptide
1	B	522	PRO	Peptide
1	B	524	TYR	Peptide
1	B	936	TYR	Sidechain
1	C	150	GLY	Peptide
1	C	211	SER	Peptide
1	C	228	PHE	Peptide
1	C	262	GLU	Peptide
1	C	420	PRO	Peptide
1	C	493	SER	Peptide
1	C	494	LEU	Peptide
1	D	415	GLY	Peptide
1	D	416	ALA	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8336	0	488	158	0
1	B	7832	0	7	80	0
1	C	8373	0	526	161	0
1	D	7832	0	7	90	0
2	A	27	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	15	0	16	3	0
4	B	15	0	16	3	0
4	D	15	0	16	2	0
5	C	31	0	12	10	0
All	All	32480	0	1100	482	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (482) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:515:ASN:N	1:C:515:ASN:CA	1.67	1.56
1:C:513:PRO:CA	1:C:513:PRO:C	1.80	1.47
1:A:213:LEU:O	1:A:215:ASP:N	1.87	1.07
1:D:607:TRP:CE3	1:D:641:MET:CE	2.40	1.05
1:A:189:PHE:HB3	1:A:190:PRO:HD3	1.41	1.03
1:B:991:ARG:NH1	1:B:1002:VAL:O	1.92	1.03
1:C:192:MET:HE1	5:C:1202:ATP:C5	1.95	1.02
1:C:977:ARG:NH1	1:C:980:GLU:OE1	1.94	0.99
1:C:170:THR:HG22	1:C:171:ASP:H	1.27	0.98
1:A:334:THR:CG2	1:A:406:ARG:NH1	2.26	0.98
1:C:175:LYS:O	1:C:176:SER:O	1.83	0.97
1:A:179:LEU:H	1:A:179:LEU:HD23	1.26	0.96
1:C:334:THR:CB	1:C:406:ARG:NH1	2.32	0.92
1:C:175:LYS:H	1:C:175:LYS:CD	1.82	0.92

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:192:MET:HE1	5:C:1202:ATP:C6	2.08	0.89
1:A:334:THR:CB	1:A:406:ARG:NH1	2.38	0.87
1:C:940:PHE:CB	1:C:944:VAL:CG1	2.56	0.82
1:C:198:GLY:HA3	1:C:228:PHE:HE2	1.43	0.82
1:C:979:GLY:O	1:C:981:TYR:N	2.12	0.82
1:C:918:ALA:O	1:C:922:VAL:CG2	2.29	0.81
1:C:377:ARG:CG	1:C:377:ARG:NH1	2.43	0.80
1:C:198:GLY:HA3	1:C:228:PHE:CE2	2.17	0.80
1:A:213:LEU:C	1:A:215:ASP:H	1.83	0.80
1:A:290:ARG:NH2	1:A:318:ASP:O	2.13	0.80
1:C:1085:ARG:NH1	1:C:1085:ARG:CG	2.44	0.78
1:C:238:TYR:HD1	5:C:1202:ATP:C2	2.01	0.78
1:A:519:ARG:NH2	1:A:847:ASP:OD2	2.17	0.78
1:A:176:SER:O	1:A:179:LEU:HB3	1.84	0.78
1:C:183:PHE:CD2	1:C:183:PHE:O	2.38	0.76
1:A:413:PHE:CZ	1:A:416:ALA:CB	2.69	0.76
1:A:51:ARG:NH2	1:A:337:GLU:OE1	2.19	0.76
1:C:912:LYS:O	1:C:916:ASP:N	2.19	0.76
1:C:188:GLY:HA3	1:C:237:ARG:HH22	1.51	0.76
1:A:189:PHE:HB3	1:A:190:PRO:CD	2.16	0.75
1:B:403:ALA:O	1:B:442:LYS:CE	2.35	0.75
1:C:895:ARG:CG	1:C:895:ARG:NH1	2.49	0.75
1:A:175:LYS:NZ	1:A:232:GLU:HG3	2.02	0.75
1:C:644:ARG:NH1	1:C:650:GLY:O	2.20	0.75
1:C:911:SER:O	1:C:915:GLY:N	2.18	0.75
1:A:1051:GLU:OE1	1:A:1057:ARG:NH2	2.20	0.75
1:C:334:THR:CG2	1:C:406:ARG:NH1	2.49	0.74
1:C:326:ASN:ND2	1:C:330:GLN:OE1	2.20	0.74
1:C:178:GLU:O	1:C:182:GLU:HG3	1.88	0.74
1:C:238:TYR:CD1	5:C:1202:ATP:C2	2.76	0.73
1:A:152:LYS:NZ	1:A:324:GLU:OE2	2.21	0.73
1:D:143:LEU:CD1	1:D:143:LEU:N	2.52	0.72
1:C:893:MET:O	1:C:897:VAL:N	2.22	0.72
1:A:206:ILE:HD11	1:A:238:TYR:CE1	2.24	0.71
1:C:1024:ARG:CG	1:C:1024:ARG:NH1	2.53	0.71
1:C:359:GLU:N	1:C:359:GLU:OE2	2.23	0.71
1:D:917:MET:SD	1:D:921:MET:CE	2.79	0.71
1:C:200:GLY:C	1:C:202:LYS:H	1.92	0.71
1:A:217:PHE:CE2	1:A:221:LYS:HE3	2.26	0.71
1:C:170:THR:HG22	1:C:171:ASP:N	2.04	0.70
1:C:175:LYS:H	1:C:175:LYS:HD3	1.53	0.70
1:C:936:TYR:O	1:C:937:LYS:CG	2.39	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:661:LYS:NZ	1:D:1004:GLU:OE2	2.25	0.69
1:C:230:ASN:HD22	1:C:231:SER:N	1.90	0.69
1:C:893:MET:CA	1:C:896:ARG:CD	2.70	0.69
1:B:927:ASP:N	1:B:927:ASP:OD2	2.25	0.69
1:B:259:HIS:CD2	1:B:296:ILE:CD1	2.76	0.69
1:C:943:SER:OG	1:C:944:VAL:N	2.26	0.69
1:B:631:ARG:NH2	1:B:672:ASP:OD1	2.27	0.68
1:C:156:ARG:NH2	1:C:170:THR:O	2.26	0.68
1:B:288:ARG:NH1	1:B:288:ARG:CG	2.56	0.68
1:A:935:GLY:CA	1:A:966:VAL:CG1	2.72	0.67
1:C:200:GLY:O	1:C:202:LYS:N	2.26	0.67
1:A:194:LYS:NZ	1:A:236:GLU:OE1	2.24	0.67
1:D:263:ARG:NH1	1:D:336:THR:OG1	2.28	0.67
1:A:952:ILE:CG2	1:A:952:ILE:O	2.43	0.66
1:A:398:ARG:CG	1:A:398:ARG:NH1	2.59	0.66
1:C:385:ASN:O	1:C:387:PHE:N	2.28	0.66
1:C:192:MET:CE	5:C:1202:ATP:C6	2.79	0.65
1:B:44:ASN:ND2	1:B:45:ARG:N	2.44	0.65
1:D:330:GLN:O	1:D:333:HIS:ND1	2.30	0.65
1:B:269:ARG:O	1:B:272:GLN:N	2.30	0.65
1:A:206:ILE:CG2	1:A:207:VAL:N	2.60	0.65
1:B:124:ASN:OD1	1:B:127:PHE:N	2.30	0.65
1:A:192:MET:HE1	1:A:238:TYR:CE1	2.32	0.65
1:A:207:VAL:HA	1:A:212:GLU:OE2	1.96	0.65
1:C:175:LYS:CD	1:C:175:LYS:N	2.57	0.64
1:B:268:GLN:CB	1:B:272:GLN:O	2.45	0.64
1:B:101:ARG:CG	1:B:101:ARG:NH1	2.60	0.64
1:C:173:PRO:O	1:C:174:ILE:HD12	1.97	0.64
1:B:338:MET:CE	1:B:430:SER:CB	2.75	0.64
1:D:715:ARG:NH1	1:D:865:GLU:OE2	2.31	0.64
1:C:183:PHE:HD2	1:C:183:PHE:O	1.76	0.64
1:B:647:ASN:O	1:B:649:VAL:N	2.30	0.64
1:C:170:THR:CG2	1:C:171:ASP:H	2.08	0.64
1:D:771:HIS:ND1	1:D:795:ASP:OD2	2.31	0.64
1:A:179:LEU:HA	1:A:182:GLU:OE2	1.96	0.63
1:A:216:ALA:C	1:A:218:HIS:H	2.01	0.63
1:D:492:PRO:O	1:D:493:SER:OG	2.16	0.63
1:A:1018:GLU:OE1	1:A:1018:GLU:CA	2.46	0.63
1:A:216:ALA:O	1:A:218:HIS:N	2.31	0.63
1:A:176:SER:O	1:A:179:LEU:HD22	1.98	0.63
1:C:991:ARG:NH1	1:C:1002:VAL:O	2.31	0.63
1:C:304:TYR:OH	1:C:307:ALA:O	2.16	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:490:ILE:CD1	1:A:490:ILE:O	2.47	0.62
1:A:775:THR:OG1	1:A:861:ILE:CD1	2.47	0.62
1:D:875:SER:OG	1:D:887:PHE:CE1	2.53	0.62
1:D:262:GLU:OE2	1:D:262:GLU:N	2.33	0.62
1:A:77:ARG:NH1	1:A:77:ARG:CG	2.60	0.62
1:B:320:PHE:N	1:B:320:PHE:CD1	2.67	0.61
1:D:93:ALA:O	1:D:95:SER:N	2.33	0.61
1:D:151:ASP:O	1:D:153:VAL:N	2.33	0.61
1:C:221:LYS:O	1:C:224:ALA:HB3	2.01	0.61
1:D:281:VAL:O	1:D:283:LEU:N	2.33	0.61
1:C:949:LYS:CD	1:C:951:GLU:OE1	2.48	0.61
1:B:395:ILE:N	1:B:453:ARG:O	2.34	0.61
1:A:210:GLU:O	1:A:212:GLU:N	2.28	0.61
1:A:860:GLU:OE2	1:A:891:LYS:NZ	2.34	0.61
1:D:335:ILE:CG2	1:D:336:THR:N	2.63	0.60
1:D:498:THR:OG1	1:D:1085:ARG:NH2	2.34	0.60
1:D:166:VAL:CG1	1:D:167:ILE:N	2.64	0.60
1:C:69:ASN:OD1	1:C:69:ASN:N	2.34	0.60
1:A:192:MET:HE2	1:A:238:TYR:CD1	2.37	0.60
1:C:238:TYR:CD1	5:C:1202:ATP:H2	2.20	0.60
1:C:186:GLU:OE2	1:C:186:GLU:N	2.35	0.59
1:A:791:VAL:O	1:A:822:ARG:NH2	2.35	0.59
1:A:192:MET:CE	1:A:238:TYR:CD1	2.85	0.59
1:B:731:GLU:OE1	1:B:765:ASP:N	2.35	0.59
1:A:503:TYR:OH	1:A:1038:PHE:O	2.20	0.59
1:D:512:PHE:CZ	4:D:1201:BTI:H5	2.37	0.59
1:B:167:ILE:CG1	1:B:168:PRO:HD3	2.31	0.59
1:B:1052:ILE:O	1:B:1052:ILE:CG2	2.49	0.59
1:C:193:ILE:HB	1:C:235:ILE:HB	1.84	0.59
1:A:179:LEU:CD2	1:A:179:LEU:H	2.02	0.59
1:A:98:ASN:C	1:A:98:ASN:ND2	2.56	0.59
1:D:920:TYR:OH	1:D:938:LEU:O	2.21	0.58
1:C:811:ASN:ND2	1:C:811:ASN:N	2.51	0.58
1:A:506:ASN:OD1	4:A:1203:BTI:H92	2.03	0.58
1:C:175:LYS:H	1:C:175:LYS:HD2	1.65	0.58
1:C:517:GLU:O	1:C:519:ARG:N	2.36	0.58
1:A:181:LYS:HG2	1:A:185:GLU:OE2	2.03	0.58
1:D:268:GLN:O	1:D:481:ILE:CD1	2.52	0.58
1:C:649:VAL:O	1:C:649:VAL:CG1	2.51	0.58
1:A:194:LYS:HE2	2:A:1201:ADP:N7	2.19	0.58
1:D:513:PRO:CD	4:D:1201:BTI:H4	2.34	0.58
1:B:124:ASN:OD1	1:B:124:ASN:C	2.42	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:180:ALA:O	1:A:183:PHE:N	2.31	0.57
1:C:959:PHE:CD1	1:C:959:PHE:N	2.71	0.57
1:D:986:ASP:C	1:D:986:ASP:OD2	2.42	0.57
1:A:192:MET:HE1	1:A:238:TYR:HE1	1.68	0.57
1:A:206:ILE:HD11	1:A:238:TYR:CZ	2.39	0.57
1:A:174:ILE:HD11	1:A:235:ILE:CG2	2.35	0.57
1:A:445:ARG:NE	1:C:58:GLU:OE2	2.37	0.57
1:C:940:PHE:CB	1:C:941:PRO:CD	2.82	0.57
1:C:192:MET:HE1	5:C:1202:ATP:C4	2.40	0.57
1:B:712:ASN:C	1:B:712:ASN:OD1	2.43	0.57
1:D:622:ASN:ND2	1:D:622:ASN:C	2.58	0.57
1:A:180:ALA:O	1:A:184:ALA:N	2.33	0.56
1:C:961:LYS:O	1:C:964:GLN:N	2.38	0.56
1:A:504:ILE:O	1:A:508:THR:OG1	2.23	0.56
1:A:206:ILE:HG22	1:A:207:VAL:N	2.19	0.56
1:A:175:LYS:HZ2	1:A:232:GLU:HG3	1.68	0.56
1:B:332:GLU:OE1	1:B:332:GLU:N	2.37	0.56
1:D:875:SER:OG	1:D:887:PHE:CZ	2.58	0.56
1:A:631:ARG:NH2	1:A:672:ASP:OD1	2.39	0.56
1:A:382:ASP:O	1:A:387:PHE:N	2.38	0.55
1:C:200:GLY:C	1:C:202:LYS:N	2.59	0.55
1:D:401:GLY:O	1:D:445:ARG:NH2	2.39	0.55
1:C:44:ASN:ND2	1:C:45:ARG:N	2.55	0.55
1:D:513:PRO:O	1:D:515:ASN:CB	2.55	0.55
1:D:768:ILE:N	1:D:792:ASP:OD2	2.40	0.55
1:C:230:ASN:HD22	1:C:230:ASN:C	2.10	0.55
1:B:620:LYS:CG	4:B:1201:BTI:H63	2.37	0.55
1:C:167:ILE:N	1:C:167:ILE:CD1	2.68	0.55
1:B:1080:MET:O	1:B:1081:ASN:C	2.45	0.54
1:A:194:LYS:HD2	1:A:234:TYR:OH	2.07	0.54
1:D:811:ASN:N	1:D:811:ASN:ND2	2.56	0.54
1:A:216:ALA:C	1:A:218:HIS:N	2.59	0.54
1:D:91:GLY:O	1:D:92:PRO:O	2.25	0.54
1:A:334:THR:CG2	1:A:428:LYS:NZ	2.71	0.54
1:C:174:ILE:HG22	1:C:217:PHE:HE1	1.72	0.54
1:B:1070:GLU:OE1	1:B:1071:ASN:N	2.41	0.54
1:A:186:GLU:O	1:A:187:ALA:HB2	2.08	0.54
1:A:512:PHE:CZ	4:A:1203:BTI:H5	2.42	0.53
1:B:1069:ASP:OD2	1:B:1073:ASN:N	2.41	0.53
1:B:624:TRP:CZ2	1:B:1008:ILE:CD1	2.91	0.53
1:B:494:LEU:O	1:B:496:ARG:N	2.42	0.53
1:C:513:PRO:CB	1:C:513:PRO:C	2.74	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:224:ALA:HB3	1:C:231:SER:HB2	1.91	0.53
1:B:798:VAL:CG1	1:B:831:MET:CE	2.86	0.53
1:D:949:LYS:NZ	1:D:971:GLN:OE1	2.40	0.53
1:A:217:PHE:HE2	1:A:221:LYS:HE3	1.71	0.53
1:A:192:MET:HE2	1:A:238:TYR:HD1	1.73	0.53
1:C:192:MET:HB2	1:C:238:TYR:HB2	1.91	0.53
1:B:495:ASP:O	1:B:496:ARG:C	2.47	0.53
1:A:194:LYS:HB3	1:A:234:TYR:CE2	2.44	0.53
1:A:768:ILE:N	1:A:792:ASP:OD2	2.42	0.52
1:B:167:ILE:CG1	1:B:168:PRO:CD	2.87	0.52
1:C:149:PHE:O	1:C:151:ASP:N	2.42	0.52
1:C:1062:LEU:CD1	1:C:1078:TYR:CE2	2.92	0.52
1:D:451:ARG:NH1	1:D:451:ARG:CG	2.73	0.52
1:C:519:ARG:CG	1:C:520:PRO:O	2.57	0.52
1:A:849:GLU:O	1:A:852:SER:C	2.44	0.52
1:A:879:LYS:O	1:A:881:LEU:N	2.42	0.52
1:A:241:ASN:N	1:A:242:PRO:CD	2.72	0.52
1:C:641:MET:CE	1:C:674:PHE:CE1	2.93	0.52
1:C:590:ILE:CG1	1:C:837:TYR:CE2	2.93	0.52
1:C:289:GLN:O	1:C:293:ASP:N	2.43	0.51
1:A:192:MET:CE	1:A:238:TYR:HD1	2.22	0.51
1:C:662:PHE:O	1:C:666:SER:OG	2.29	0.51
1:A:521:LYS:NZ	1:A:1046:GLU:OE1	2.43	0.51
1:A:311:GLU:OE1	1:A:326:ASN:ND2	2.43	0.51
1:D:832:GLU:O	1:D:836:HIS:CD2	2.64	0.51
1:C:948:PHE:CD2	1:C:959:PHE:CD2	2.98	0.51
1:D:540:GLY:N	1:D:543:GLN:NE2	2.59	0.51
1:C:199:GLY:HA2	5:C:1202:ATP:O3B	2.10	0.51
1:D:263:ARG:CD	1:D:335:ILE:CG2	2.89	0.51
1:C:151:ASP:OD1	1:C:154:LYS:N	2.44	0.51
1:D:246:GLU:OE2	1:D:273:LYS:NZ	2.44	0.51
1:A:222:SER:O	1:A:226:LYS:HB2	2.10	0.51
1:C:920:TYR:CE1	1:C:940:PHE:CD2	2.99	0.51
1:D:449:GLU:O	1:D:450:MET:C	2.49	0.51
1:A:794:ILE:CD1	1:A:813:LEU:CD2	2.89	0.51
1:D:160:ILE:O	1:D:161:LYS:C	2.48	0.51
1:B:145:HIS:CE1	1:B:302:ILE:O	2.64	0.51
1:C:173:PRO:C	1:C:174:ILE:HD12	2.32	0.50
1:C:774:ASP:OD2	1:C:779:GLY:N	2.43	0.50
1:C:193:ILE:HG12	1:C:194:LYS:N	2.25	0.50
1:C:647:ASN:N	1:C:647:ASN:OD1	2.44	0.50
1:D:47:GLU:OE2	1:D:118:TYR:OH	2.29	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:337:GLU:OE2	1:C:406:ARG:NH2	2.45	0.50
1:C:798:VAL:O	1:C:799:ALA:C	2.50	0.50
1:B:832:GLU:OE2	1:C:859:THR:OG1	2.28	0.50
1:C:644:ARG:O	1:C:645:ALA:C	2.50	0.50
1:D:337:GLU:CG	1:D:342:ILE:O	2.60	0.50
1:C:189:PHE:H	1:C:190:PRO:CD	2.24	0.50
1:A:912:LYS:NZ	1:A:916:ASP:OD1	2.45	0.50
1:B:385:ASN:CG	1:B:385:ASN:O	2.50	0.50
1:A:334:THR:OG1	1:A:375:GLN:NE2	2.44	0.49
1:C:219:ARG:O	1:C:223:GLU:HB2	2.13	0.49
1:D:459:ILE:N	1:D:460:PRO:CD	2.75	0.49
1:A:886:ARG:O	1:A:889:GLU:N	2.45	0.49
1:C:700:SER:N	1:C:736:HIS:CD2	2.79	0.49
1:C:152:LYS:N	1:C:196:THR:CG2	2.76	0.49
1:A:375:GLN:NE2	1:A:428:LYS:NZ	2.61	0.49
1:A:229:GLY:O	1:A:230:ASN:HB2	2.12	0.49
1:A:206:ILE:CD1	1:A:238:TYR:CE1	2.96	0.49
1:C:715:ARG:NH2	1:C:865:GLU:OE2	2.46	0.49
1:B:867:PRO:O	1:B:868:GLY:C	2.51	0.49
1:A:51:ARG:NH2	1:A:343:ASP:OD2	2.46	0.49
1:B:1055:GLY:O	1:D:83:SER:N	2.46	0.49
1:D:357:LEU:O	1:D:362:MET:CB	2.61	0.49
1:A:863:GLN:O	1:A:895:ARG:CD	2.61	0.49
1:A:184:ALA:HA	1:A:191:LEU:HD11	1.94	0.49
1:D:631:ARG:NH2	1:D:672:ASP:OD1	2.46	0.48
1:A:516:VAL:O	1:A:516:VAL:CG1	2.61	0.48
1:C:968:LEU:O	1:C:969:LYS:C	2.51	0.48
1:C:174:ILE:HG22	1:C:217:PHE:CE1	2.48	0.48
1:D:91:GLY:N	1:D:94:GLU:OE2	2.47	0.48
1:C:890:VAL:O	1:C:891:LYS:CG	2.60	0.48
1:D:874:LEU:O	1:D:887:PHE:CE1	2.65	0.48
1:D:413:PHE:O	1:D:415:GLY:N	2.46	0.48
1:A:370:LEU:O	1:A:432:HIS:CE1	2.67	0.48
1:C:921:MET:O	1:C:926:LEU:N	2.46	0.48
1:A:170:THR:HG22	1:A:172:GLY:O	2.13	0.48
1:B:690:ASN:ND2	1:B:700:SER:OG	2.47	0.48
1:A:196:THR:HG22	1:A:232:GLU:O	2.14	0.48
1:A:879:LYS:C	1:A:881:LEU:N	2.68	0.48
1:A:771:HIS:ND1	1:A:795:ASP:OD2	2.47	0.48
1:D:814:TYR:C	1:D:814:TYR:CD2	2.87	0.48
1:D:244:HIS:N	1:D:266:SER:OG	2.46	0.48
1:A:678:ASP:OD2	1:A:685:GLN:NE2	2.47	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:42:VAL:CG2	1:A:53:PHE:CE2	2.97	0.47
1:A:175:LYS:HZ1	1:A:232:GLU:HG3	1.78	0.47
1:D:498:THR:CG2	1:D:1085:ARG:NH2	2.77	0.47
1:A:178:GLU:HG2	1:A:181:LYS:HB2	1.96	0.47
1:C:224:ALA:O	1:C:228:PHE:HD1	1.98	0.47
1:B:395:ILE:CD1	1:B:1086:ARG:O	2.63	0.47
1:A:590:ILE:CG1	1:A:837:TYR:CE2	2.98	0.47
1:A:178:GLU:O	1:A:178:GLU:HG2	2.14	0.47
1:C:264:ASP:OD2	1:C:266:SER:OG	2.33	0.47
1:A:516:VAL:O	1:A:517:GLU:C	2.51	0.47
1:C:892:ASP:O	1:C:896:ARG:CD	2.62	0.47
1:B:769:HIS:NE2	1:B:795:ASP:OD1	2.48	0.47
1:C:82:GLU:OE1	1:C:84:TYR:OH	2.33	0.47
1:B:104:ASP:O	1:B:105:VAL:C	2.53	0.47
1:C:357:LEU:O	1:C:362:MET:CB	2.62	0.47
1:D:51:ARG:NH2	1:D:343:ASP:OD2	2.48	0.47
1:C:811:ASN:OD1	1:C:832:GLU:OE1	2.33	0.47
1:B:859:THR:OG1	1:C:832:GLU:OE2	2.33	0.47
1:B:620:LYS:NZ	4:B:1201:BTI:HN3	2.13	0.47
1:C:177:TYR:OH	1:C:181:LYS:HE3	2.15	0.46
1:C:1035:THR:N	1:C:1036:PRO:CD	2.77	0.46
1:A:598:PHE:O	1:A:601:GLY:N	2.48	0.46
1:A:674:PHE:CD2	1:A:674:PHE:N	2.83	0.46
1:C:690:ASN:OD1	1:C:700:SER:OG	2.32	0.46
1:A:572:ASP:OD1	1:A:771:HIS:CE1	2.68	0.46
1:A:167:ILE:CD1	1:A:323:ILE:CD1	2.94	0.46
1:C:241:ASN:N	1:C:242:PRO:CD	2.77	0.46
1:A:778:ASN:O	1:A:779:GLY:C	2.52	0.46
1:B:860:GLU:O	1:B:863:GLN:N	2.49	0.46
1:A:263:ARG:NH1	1:A:336:THR:OG1	2.49	0.46
1:B:912:LYS:NZ	1:B:916:ASP:OD1	2.48	0.46
1:B:1005:GLN:O	1:B:1009:SER:OG	2.33	0.46
1:A:458:ASN:OD1	1:A:458:ASN:N	2.48	0.46
1:A:214:GLU:O	1:A:218:HIS:CD2	2.68	0.46
1:D:798:VAL:O	1:D:801:MET:N	2.49	0.46
1:C:385:ASN:C	1:C:387:PHE:N	2.69	0.46
1:D:878:ALA:O	1:D:884:GLY:N	2.49	0.46
1:D:70:GLU:CD	1:D:70:GLU:N	2.69	0.46
1:B:263:ARG:NH1	1:B:336:THR:OG1	2.49	0.46
1:D:74:SER:OG	1:D:76:HIS:ND1	2.49	0.46
1:C:813:LEU:O	1:C:814:TYR:C	2.53	0.45
1:D:243:LYS:CB	1:D:243:LYS:NZ	2.74	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:234:TYR:CE1	1:A:236:GLU:HG3	2.51	0.45
1:C:831:MET:O	1:C:835:SER:N	2.49	0.45
1:D:337:GLU:O	1:D:341:GLY:N	2.49	0.45
1:D:512:PHE:CD2	1:D:512:PHE:C	2.90	0.45
1:C:234:TYR:C	1:C:235:ILE:HG22	2.37	0.45
1:D:991:ARG:O	1:D:995:GLU:CG	2.65	0.45
1:C:743:MET:N	1:C:743:MET:SD	2.89	0.45
1:A:207:VAL:HG11	1:A:213:LEU:HD23	1.97	0.45
1:C:192:MET:HB3	1:C:192:MET:HE3	1.87	0.45
1:A:193:ILE:HG13	1:A:194:LYS:N	2.32	0.45
1:D:938:LEU:O	1:D:939:ASP:CB	2.63	0.45
1:B:540:GLY:N	1:B:543:GLN:NE2	2.63	0.45
1:A:864:HIS:CD2	1:A:866:MET:CG	3.00	0.45
1:B:776:SER:O	1:C:812:SER:OG	2.35	0.45
1:A:869:GLY:O	1:A:871:TYR:N	2.49	0.45
1:C:860:GLU:O	1:C:863:GLN:N	2.50	0.45
1:D:305:VAL:O	1:D:306:ASN:CB	2.65	0.45
1:A:179:LEU:HD11	1:A:217:PHE:CE1	2.51	0.45
1:C:979:GLY:C	1:C:981:TYR:N	2.70	0.45
1:D:262:GLU:OE1	1:D:288:ARG:NH1	2.50	0.45
1:B:347:THR:O	1:B:348:GLN:C	2.52	0.45
1:A:44:ASN:ND2	1:A:45:ARG:N	2.65	0.45
1:C:263:ARG:NH1	1:C:336:THR:OG1	2.50	0.45
1:A:873:ASN:O	1:A:875:SER:N	2.49	0.45
1:A:192:MET:CE	1:A:238:TYR:CE1	3.00	0.45
1:A:174:ILE:HD11	1:A:235:ILE:HG22	1.99	0.45
1:B:251:GLY:O	1:B:306:ASN:N	2.50	0.45
1:A:459:ILE:O	1:A:460:PRO:C	2.54	0.45
1:C:513:PRO:CA	1:C:513:PRO:O	2.53	0.45
1:A:606:MET:CE	1:A:639:PHE:CD2	3.00	0.45
1:C:173:PRO:O	1:C:174:ILE:CD1	2.64	0.45
1:A:177:TYR:O	1:A:179:LEU:N	2.50	0.45
1:C:221:LYS:HG3	1:C:233:VAL:HG13	1.99	0.45
1:C:897:VAL:O	1:C:898:ASN:C	2.55	0.45
1:A:512:PHE:C	1:A:512:PHE:CD2	2.90	0.45
1:B:511:GLY:O	4:B:1201:BTI:H102	2.17	0.45
1:B:748:LYS:O	1:B:749:PRO:C	2.55	0.45
1:D:907:VAL:O	1:D:910:SER:N	2.49	0.45
1:D:479:LYS:O	1:D:480:PHE:C	2.55	0.45
1:A:179:LEU:HA	1:A:182:GLU:CD	2.37	0.44
1:D:944:VAL:O	1:D:945:VAL:C	2.54	0.44
1:B:709:ASP:OD1	1:B:748:LYS:NZ	2.50	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:606:MET:CE	1:B:607:TRP:CB	2.95	0.44
1:A:955:PRO:O	1:A:956:VAL:C	2.56	0.44
1:A:470:LYS:CB	1:A:480:PHE:CE1	3.00	0.44
1:A:174:ILE:HD11	1:A:235:ILE:HG21	1.97	0.44
1:B:98:ASN:C	1:B:98:ASN:ND2	2.70	0.44
1:C:1029:ASN:C	1:C:1029:ASN:ND2	2.70	0.44
1:C:191:LEU:HD13	1:C:235:ILE:HD11	2.00	0.44
1:D:276:GLU:OE2	1:D:377:ARG:NH1	2.50	0.44
1:D:571:ARG:NH2	1:D:605:GLU:OE2	2.50	0.44
1:A:413:PHE:O	1:A:414:GLN:C	2.56	0.44
1:C:960:ASN:O	1:C:961:LYS:C	2.56	0.44
1:A:622:ASN:C	1:A:622:ASN:ND2	2.70	0.44
1:B:792:ASP:N	1:B:792:ASP:OD2	2.51	0.44
1:A:893:MET:O	1:A:897:VAL:N	2.51	0.44
1:C:188:GLY:HA3	1:C:237:ARG:NH2	2.28	0.44
1:B:702:GLY:O	1:B:739:ALA:N	2.50	0.44
1:C:926:LEU:CD1	1:C:938:LEU:CD1	2.96	0.44
1:C:907:VAL:O	1:C:911:SER:OG	2.35	0.44
1:B:556:TRP:O	1:B:557:VAL:C	2.56	0.44
1:C:332:GLU:OE2	1:C:332:GLU:N	2.51	0.44
1:A:513:PRO:O	1:A:515:ASN:CB	2.66	0.43
1:A:177:TYR:C	1:A:179:LEU:N	2.69	0.43
1:B:864:HIS:CD2	1:B:866:MET:N	2.86	0.43
1:C:225:GLU:HB3	1:C:231:SER:HB3	1.99	0.43
1:A:622:ASN:ND2	1:A:624:TRP:N	2.66	0.43
1:A:547:GLU:CA	1:A:547:GLU:OE2	2.66	0.43
1:A:225:GLU:OE1	1:A:225:GLU:HA	2.17	0.43
1:C:567:ASP:OD2	1:C:569:THR:OG1	2.35	0.43
1:A:251:GLY:N	1:A:306:ASN:O	2.51	0.43
1:B:1063:GLU:OE1	1:D:1086:ARG:NH1	2.51	0.43
1:C:631:ARG:NH2	1:C:672:ASP:OD1	2.51	0.43
1:B:883:LEU:O	1:B:884:GLY:C	2.56	0.43
1:A:394:ILE:O	1:A:414:GLN:O	2.36	0.43
1:A:1029:ASN:C	1:A:1029:ASN:ND2	2.71	0.43
1:C:216:ALA:O	1:C:217:PHE:C	2.56	0.43
1:A:177:TYR:O	1:A:178:GLU:C	2.56	0.43
1:B:700:SER:N	1:B:736:HIS:CD2	2.86	0.43
1:A:380:THR:O	1:A:390:ASP:N	2.52	0.43
1:D:621:GLU:OE1	1:D:626:ARG:NH2	2.52	0.43
1:C:347:THR:O	1:C:348:GLN:C	2.56	0.42
1:A:118:TYR:C	1:A:118:TYR:CD1	2.91	0.42
1:A:571:ARG:NH2	1:A:605:GLU:OE1	2.52	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:238:TYR:CE1	5:C:1202:ATP:H2	2.37	0.42
1:A:1017:TYR:O	1:A:1018:GLU:C	2.57	0.42
1:B:363:GLN:O	1:B:366:ASP:N	2.52	0.42
1:C:175:LYS:O	1:C:176:SER:C	2.49	0.42
1:A:207:VAL:CG1	1:A:209:GLU:H	2.33	0.42
1:D:93:ALA:C	1:D:95:SER:N	2.73	0.42
1:B:889:GLU:O	1:B:890:VAL:C	2.58	0.42
1:D:586:ASP:OD1	1:D:845:TYR:OH	2.36	0.42
1:A:213:LEU:O	1:A:214:GLU:C	2.55	0.42
1:C:246:GLU:OE1	1:C:330:GLN:NE2	2.52	0.42
1:D:298:LEU:O	1:D:302:ILE:CG1	2.67	0.42
1:B:952:ILE:O	1:B:952:ILE:CG2	2.68	0.42
1:D:518:LYS:CG	1:D:518:LYS:O	2.67	0.42
1:B:47:GLU:OE2	1:B:118:TYR:OH	2.37	0.42
1:C:1080:MET:CE	1:C:1085:ARG:NH2	2.83	0.42
1:A:382:ASP:OD1	1:A:384:LEU:CD1	2.67	0.42
1:C:1029:ASN:ND2	1:C:1031:SER:CB	2.83	0.42
1:B:996:GLU:C	1:B:996:GLU:OE1	2.58	0.42
1:C:979:GLY:O	1:C:982:LEU:N	2.52	0.42
1:B:124:ASN:OD1	1:B:126:GLN:N	2.53	0.42
1:C:831:MET:O	1:C:832:GLU:C	2.58	0.42
1:A:1066:SER:OG	1:A:1075:THR:N	2.52	0.42
1:D:870:GLN:O	1:D:871:TYR:C	2.57	0.42
1:C:803:GLY:O	1:C:804:LEU:C	2.56	0.42
1:C:760:LYS:CE	1:C:790:GLY:O	2.67	0.42
1:C:794:ILE:CD1	1:C:796:THR:CG2	2.97	0.42
1:D:506:ASN:ND2	1:D:510:ASN:ND2	2.67	0.42
1:B:783:TYR:O	1:B:784:LYS:C	2.56	0.42
1:D:647:ASN:ND2	1:D:647:ASN:C	2.74	0.42
1:C:152:LYS:NZ	5:C:1202:ATP:O1A	2.53	0.42
1:C:896:ARG:NE	1:C:928:GLU:OE1	2.53	0.42
1:D:239:ILE:O	1:D:241:ASN:N	2.52	0.42
1:D:791:VAL:O	1:D:822:ARG:NH2	2.53	0.42
1:C:1077:TYR:N	1:C:1077:TYR:CD1	2.88	0.42
1:B:690:ASN:O	1:B:691:GLU:C	2.59	0.41
1:A:219:ARG:HG2	1:A:219:ARG:O	2.19	0.41
1:C:396:ALA:CA	1:C:414:GLN:NE2	2.83	0.41
1:B:406:ARG:N	1:B:430:SER:O	2.53	0.41
1:B:246:GLU:OE1	1:B:263:ARG:NE	2.53	0.41
1:D:479:LYS:NZ	1:D:483:GLU:OE2	2.52	0.41
1:A:225:GLU:OE2	1:A:231:SER:HB3	2.20	0.41
1:A:532:VAL:N	1:A:592:SER:OG	2.52	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:211:SER:H	1:A:213:LEU:HD12	1.85	0.41
1:D:1035:THR:N	1:D:1036:PRO:CD	2.84	0.41
1:C:152:LYS:N	1:C:196:THR:HG23	2.35	0.41
1:C:771:HIS:ND1	1:C:795:ASP:OD2	2.53	0.41
1:D:565:LEU:CD1	1:D:565:LEU:C	2.89	0.41
1:C:170:THR:HG21	1:C:174:ILE:HD11	2.01	0.41
1:B:302:ILE:O	1:B:303:LYS:CB	2.68	0.41
1:B:65:ALA:N	1:B:82:GLU:O	2.54	0.41
1:B:543:GLN:O	1:B:547:GLU:CG	2.68	0.41
1:A:265:CYS:O	1:A:268:GLN:NE2	2.54	0.41
1:D:687:LYS:NZ	1:D:733:GLU:OE2	2.53	0.41
1:D:893:MET:SD	1:D:896:ARG:NH2	2.94	0.41
1:B:1046:GLU:CG	1:B:1047:THR:N	2.84	0.41
1:D:413:PHE:C	1:D:415:GLY:N	2.74	0.41
1:B:519:ARG:CB	1:B:520:PRO:CD	2.98	0.41
1:A:145:HIS:CE1	1:A:302:ILE:O	2.73	0.41
1:B:872:SER:O	1:B:875:SER:N	2.54	0.41
1:A:1063:GLU:OE2	1:C:1086:ARG:NH2	2.54	0.41
1:A:512:PHE:CD2	1:A:513:PRO:N	2.89	0.41
1:A:991:ARG:NH1	1:A:1002:VAL:O	2.54	0.41
1:A:647:ASN:O	1:A:649:VAL:N	2.53	0.41
1:A:980:GLU:OE1	1:A:980:GLU:O	2.39	0.41
1:D:281:VAL:CG1	1:D:282:GLY:N	2.83	0.40
1:A:170:THR:HG22	1:A:172:GLY:H	1.85	0.40
1:B:798:VAL:O	1:B:799:ALA:C	2.59	0.40
1:C:189:PHE:N	1:C:190:PRO:CD	2.84	0.40
1:A:1076:ILE:N	1:A:1087:ILE:O	2.54	0.40
1:A:498:THR:O	1:A:499:LYS:C	2.59	0.40
1:D:39:LYS:NZ	1:D:82:GLU:OE1	2.54	0.40
1:C:1013:TYR:O	1:C:1017:TYR:N	2.54	0.40
1:C:189:PHE:H	1:C:190:PRO:HD2	1.86	0.40
1:D:869:GLY:O	1:D:870:GLN:C	2.59	0.40
1:C:783:TYR:OH	1:C:795:ASP:O	2.38	0.40
1:C:244:HIS:NE2	1:C:311:GLU:OE2	2.54	0.40
1:B:907:VAL:O	1:B:911:SER:N	2.55	0.40
1:A:511:GLY:O	4:A:1203:BTI:H103	2.20	0.40
1:D:400:SER:OG	1:D:401:GLY:N	2.54	0.40
1:D:820:PHE:CB	1:D:821:PRO:CD	2.99	0.40
1:A:170:THR:HG21	1:A:174:ILE:HG23	2.03	0.40
1:C:180:ALA:O	1:C:181:LYS:C	2.60	0.40
1:A:622:ASN:O	1:A:623:PRO:C	2.60	0.40
1:C:995:GLU:O	1:C:998:GLN:O	2.39	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:480:PHE:C	1:C:480:PHE:CD1	2.94	0.40
1:A:606:MET:C	1:A:606:MET:SD	3.00	0.40
1:D:869:GLY:O	1:D:871:TYR:N	2.55	0.40
1:B:245:ILE:O	1:B:312:PHE:N	2.55	0.40
1:D:935:GLY:CA	1:D:966:VAL:CG1	3.00	0.40
1:A:496:ARG:O	1:A:497:GLY:C	2.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1048/1173 (89%)	916 (87%)	102 (10%)	30 (3%)	7	23
1	B	985/1173 (84%)	876 (89%)	85 (9%)	24 (2%)	9	29
1	C	1057/1173 (90%)	923 (87%)	96 (9%)	38 (4%)	5	17
1	D	985/1173 (84%)	864 (88%)	94 (10%)	27 (3%)	8	25
All	All	4075/4692 (87%)	3579 (88%)	377 (9%)	119 (3%)	7	23

All (119) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	ALA
1	A	211	SER
1	A	213	LEU
1	A	214	GLU
1	A	217	PHE
1	A	230	ASN
1	A	396	ALA
1	A	709	ASP
1	A	870	GLN
1	A	880	SER
1	B	163	ASP
1	B	270	ARG

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Mol	Chain	Res	Type
1	B	414	GLN
1	B	495	ASP
1	B	522	PRO
1	B	975	THR
1	C	176	SER
1	C	195	ALA
1	C	201	GLY
1	C	204	MET
1	C	214	GLU
1	C	215	ASP
1	C	386	ASP
1	C	518	LYS
1	C	649	VAL
1	C	886	ARG
1	C	890	VAL
1	C	980	GLU
1	D	92	PRO
1	D	152	LYS
1	D	240	ASP
1	D	515	ASN
1	D	870	GLN
1	A	499	LYS
1	A	527	ALA
1	A	648	ALA
1	A	861	ILE
1	B	166	VAL
1	B	528	SER
1	B	868	GLY
1	B	881	LEU
1	B	903	ASP
1	B	1001	PRO
1	C	87	GLY
1	C	203	GLY
1	C	229	GLY
1	C	385	ASN
1	C	645	ALA
1	C	937	LYS
1	C	938	LEU
1	C	942	GLU
1	D	87	GLY
1	D	94	GLU
1	D	163	ASP

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Mol	Chain	Res	Type
1	D	306	ASN
1	D	414	GLN
1	D	450	MET
1	D	649	VAL
1	D	799	ALA
1	D	884	GLY
1	D	888	ASP
1	A	94	GLU
1	A	517	GLU
1	B	475	ASP
1	B	1002	VAL
1	B	1081	ASN
1	C	151	ASP
1	C	197	SER
1	C	981	TYR
1	C	1053	ASP
1	D	334	THR
1	D	517	GLU
1	D	518	LYS
1	D	1069	ASP
1	A	44	ASN
1	A	209	GLU
1	A	882	GLY
1	B	306	ASN
1	B	648	ALA
1	B	649	VAL
1	B	1000	GLY
1	C	173	PRO
1	C	216	ALA
1	C	269	ARG
1	C	355	ALA
1	C	821	PRO
1	D	133	GLU
1	D	261	PHE
1	D	480	PHE
1	D	513	PRO
1	B	527	ALA
1	B	1053	ASP
1	C	898	ASN
1	C	935	GLY
1	D	335	ILE
1	D	854	ILE

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Mol	Chain	Res	Type
1	A	92	PRO
1	A	110	ASN
1	A	189	PHE
1	A	241	ASN
1	A	306	ASN
1	B	480	PHE
1	B	562	ASP
1	C	174	ILE
1	C	180	ALA
1	C	1001	PRO
1	A	1001	PRO
1	D	282	GLY
1	A	282	GLY
1	A	1014	PRO
1	B	890	VAL
1	C	189	PHE
1	A	868	GLY
1	C	291	ILE
1	C	327	PRO
1	A	956	VAL
1	C	168	PRO
1	A	935	GLY
1	D	1014	PRO

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	907/1005 (90%)	778 (86%)	129 (14%)	5	14
1	B	855/1005 (85%)	726 (85%)	129 (15%)	4	12
1	C	909/1005 (90%)	751 (83%)	158 (17%)	3	8
1	D	855/1005 (85%)	727 (85%)	128 (15%)	4	12
All	All	3526/4020 (88%)	2982 (85%)	544 (15%)	4	12

All (544) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LYS
1	A	44	ASN
1	A	62	SER
1	A	66	ILE
1	A	69	ASN
1	A	70	GLU
1	A	73	SER
1	A	75	LEU
1	A	77	ARG
1	A	94	GLU
1	A	95	SER
1	A	97	LEU
1	A	98	ASN
1	A	108	GLN
1	A	110	ASN
1	A	143	LEU
1	A	144	GLU
1	A	156	ARG
1	A	161	LYS
1	A	163	ASP
1	A	175	LYS
1	A	179	LEU
1	A	182	GLU
1	A	186	GLU
1	A	193	ILE
1	A	194	LYS
1	A	210	GLU
1	A	212	GLU
1	A	214	GLU
1	A	215	ASP
1	A	225	GLU
1	A	234	TYR
1	A	237	ARG
1	A	239	ILE
1	A	257	ILE
1	A	271	HIS
1	A	283	LEU
1	A	286	THR
1	A	287	LEU
1	A	306	ASN
1	A	313	LEU
1	A	329	VAL
1	A	331	VAL

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Mol	Chain	Res	Type
1	A	335	ILE
1	A	386	ASP
1	A	391	THR
1	A	398	ARG
1	A	419	SER
1	A	427	VAL
1	A	428	LYS
1	A	434	ILE
1	A	437	LYS
1	A	440	GLU
1	A	442	LYS
1	A	455	VAL
1	A	472	THR
1	A	473	SER
1	A	487	LEU
1	A	491	GLN
1	A	496	ARG
1	A	512	PHE
1	A	518	LYS
1	A	525	GLU
1	A	526	LEU
1	A	528	SER
1	A	535	SER
1	A	536	LYS
1	A	547	GLU
1	A	551	LYS
1	A	565	LEU
1	A	580	THR
1	A	588	ILE
1	A	590	ILE
1	A	592	SER
1	A	606	MET
1	A	607	TRP
1	A	613	ASP
1	A	620	LYS
1	A	622	ASN
1	A	631	ARG
1	A	649	VAL
1	A	672	ASP
1	A	679	SER
1	A	685	GLN
1	A	715	ARG

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Mol	Chain	Res	Type
1	A	719	THR
1	A	725	LYS
1	A	743	MET
1	A	750	LYS
1	A	760	LYS
1	A	766	LEU
1	A	775	THR
1	A	781	LEU
1	A	784	LYS
1	A	811	ASN
1	A	828	ILE
1	A	831	MET
1	A	835	SER
1	A	855	LYS
1	A	861	ILE
1	A	863	GLN
1	A	870	GLN
1	A	876	GLN
1	A	880	SER
1	A	904	ILE
1	A	907	VAL
1	A	908	THR
1	A	919	LEU
1	A	923	GLN
1	A	926	LEU
1	A	931	VAL
1	A	932	ILE
1	A	944	VAL
1	A	961	LYS
1	A	980	GLU
1	A	993	LEU
1	A	999	GLN
1	A	1008	ILE
1	A	1018	GLU
1	A	1019	GLN
1	A	1029	ASN
1	A	1043	ARG
1	A	1044	ASN
1	A	1048	VAL
1	A	1051	GLU
1	A	1064	THR
1	A	1076	ILE

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Mol	Chain	Res	Type
1	A	1080	MET
1	A	1089	ILE
1	B	36	GLN
1	B	38	LYS
1	B	44	ASN
1	B	62	SER
1	B	70	GLU
1	B	75	LEU
1	B	90	LEU
1	B	94	GLU
1	B	98	ASN
1	B	101	ARG
1	B	104	ASP
1	B	124	ASN
1	B	144	GLU
1	B	147	ASP
1	B	152	LYS
1	B	153	VAL
1	B	166	VAL
1	B	167	ILE
1	B	239	ILE
1	B	241	ASN
1	B	281	VAL
1	B	287	LEU
1	B	288	ARG
1	B	289	GLN
1	B	291	ILE
1	B	300	GLU
1	B	306	ASN
1	B	315	SER
1	B	319	GLU
1	B	320	PHE
1	B	328	ARG
1	B	331	VAL
1	B	357	LEU
1	B	359	GLU
1	B	361	ASN
1	B	365	LYS
1	B	368	THR
1	B	370	LEU
1	B	376	CYS
1	B	391	THR

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Mol	Chain	Res	Type
1	B	399	SER
1	B	400	SER
1	B	406	ARG
1	B	417	GLU
1	B	418	ILE
1	B	423	ASP
1	B	427	VAL
1	B	435	SER
1	B	442	LYS
1	B	446	SER
1	B	450	MET
1	B	451	ARG
1	B	453	ARG
1	B	479	LYS
1	B	487	LEU
1	B	494	LEU
1	B	500	THR
1	B	515	ASN
1	B	519	ARG
1	B	534	SER
1	B	547	GLU
1	B	551	LYS
1	B	558	LYS
1	B	576	SER
1	B	580	THR
1	B	606	MET
1	B	607	TRP
1	B	622	ASN
1	B	631	ARG
1	B	632	LYS
1	B	647	ASN
1	B	649	VAL
1	B	652	LYS
1	B	660	HIS
1	B	690	ASN
1	B	715	ARG
1	B	721	GLU
1	B	725	LYS
1	B	740	ILE
1	B	743	MET
1	B	761	SER
1	B	775	THR

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Mol	Chain	Res	Type
1	B	784	LYS
1	B	791	VAL
1	B	792	ASP
1	B	807	GLN
1	B	809	SER
1	B	811	ASN
1	B	812	SER
1	B	828	ILE
1	B	831	MET
1	B	839	SER
1	B	843	THR
1	B	852	SER
1	B	853	ASP
1	B	855	LYS
1	B	863	GLN
1	B	871	TYR
1	B	872	SER
1	B	875	SER
1	B	876	GLN
1	B	879	LYS
1	B	880	SER
1	B	881	LEU
1	B	886	ARG
1	B	897	VAL
1	B	907	VAL
1	B	908	THR
1	B	919	LEU
1	B	927	ASP
1	B	929	GLN
1	B	930	SER
1	B	934	ASP
1	B	936	TYR
1	B	938	LEU
1	B	939	ASP
1	B	942	GLU
1	B	944	VAL
1	B	949	LYS
1	B	957	ASN
1	B	962	ASP
1	B	963	LEU
1	B	991	ARG
1	B	1029	ASN

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Mol	Chain	Res	Type
1	B	1057	ARG
1	B	1070	GLU
1	B	1071	ASN
1	B	1085	ARG
1	B	1089	ILE
1	C	44	ASN
1	C	45	ARG
1	C	69	ASN
1	C	70	GLU
1	C	75	LEU
1	C	77	ARG
1	C	86	VAL
1	C	90	LEU
1	C	97	LEU
1	C	98	ASN
1	C	100	GLU
1	C	101	ARG
1	C	110	ASN
1	C	112	ASP
1	C	123	GLU
1	C	142	HIS
1	C	144	GLU
1	C	151	ASP
1	C	154	LYS
1	C	156	ARG
1	C	166	VAL
1	C	167	ILE
1	C	171	ASP
1	C	175	LYS
1	C	178	GLU
1	C	179	LEU
1	C	192	MET
1	C	193	ILE
1	C	194	LYS
1	C	202	LYS
1	C	205	ARG
1	C	208	ARG
1	C	209	GLU
1	C	210	GLU
1	C	215	ASP
1	C	219	ARG
1	C	223	GLU

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Mol	Chain	Res	Type
1	C	225	GLU
1	C	230	ASN
1	C	232	GLU
1	C	234	TYR
1	C	235	ILE
1	C	237	ARG
1	C	253	GLU
1	C	257	ILE
1	C	262	GLU
1	C	269	ARG
1	C	280	SER
1	C	286	THR
1	C	287	LEU
1	C	288	ARG
1	C	306	ASN
1	C	315	SER
1	C	318	ASP
1	C	324	GLU
1	C	358	GLU
1	C	359	GLU
1	C	365	LYS
1	C	368	THR
1	C	377	ARG
1	C	384	LEU
1	C	386	ASP
1	C	391	THR
1	C	395	ILE
1	C	414	GLN
1	C	437	LYS
1	C	442	LYS
1	C	444	VAL
1	C	446	SER
1	C	451	ARG
1	C	453	ARG
1	C	467	LYS
1	C	469	LYS
1	C	473	SER
1	C	491	GLN
1	C	493	SER
1	C	494	LEU
1	C	531	THR
1	C	533	SER

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Mol	Chain	Res	Type
1	C	537	ILE
1	C	539	SER
1	C	543	GLN
1	C	545	LEU
1	C	547	GLU
1	C	559	LYS
1	C	563	VAL
1	C	589	ASN
1	C	606	MET
1	C	607	TRP
1	C	616	TYR
1	C	622	ASN
1	C	631	ARG
1	C	641	MET
1	C	646	SER
1	C	647	ASN
1	C	649	VAL
1	C	652	LYS
1	C	660	HIS
1	C	661	LYS
1	C	680	LEU
1	C	695	GLU
1	C	707	THR
1	C	717	ASN
1	C	719	THR
1	C	725	LYS
1	C	743	MET
1	C	750	LYS
1	C	760	LYS
1	C	781	LEU
1	C	783	TYR
1	C	784	LYS
1	C	807	GLN
1	C	811	ASN
1	C	833	SER
1	C	835	SER
1	C	839	SER
1	C	843	THR
1	C	852	SER
1	C	855	LYS
1	C	856	SER
1	C	860	GLU

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Mol	Chain	Res	Type
1	C	861	ILE
1	C	863	GLN
1	C	866	MET
1	C	870	GLN
1	C	872	SER
1	C	876	GLN
1	C	881	LEU
1	C	885	GLU
1	C	892	ASP
1	C	893	MET
1	C	895	ARG
1	C	896	ARG
1	C	907	VAL
1	C	908	THR
1	C	923	GLN
1	C	927	ASP
1	C	928	GLU
1	C	938	LEU
1	C	949	LYS
1	C	959	PHE
1	C	960	ASN
1	C	967	ILE
1	C	968	LEU
1	C	971	GLN
1	C	980	GLU
1	C	986	ASP
1	C	997	GLU
1	C	1015	LYS
1	C	1024	ARG
1	C	1029	ASN
1	C	1031	SER
1	C	1048	VAL
1	C	1052	ILE
1	C	1067	GLU
1	C	1076	ILE
1	C	1085	ARG
1	C	1090	LYS
1	D	38	LYS
1	D	44	ASN
1	D	72	LYS
1	D	73	SER
1	D	75	LEU

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Mol	Chain	Res	Type
1	D	77	ARG
1	D	88	SER
1	D	99	ILE
1	D	101	ARG
1	D	137	LYS
1	D	143	LEU
1	D	163	ASP
1	D	167	ILE
1	D	239	ILE
1	D	240	ASP
1	D	243	LYS
1	D	250	ILE
1	D	253	GLU
1	D	260	LEU
1	D	262	GLU
1	D	268	GLN
1	D	270	ARG
1	D	280	SER
1	D	287	LEU
1	D	288	ARG
1	D	290	ARG
1	D	305	VAL
1	D	326	ASN
1	D	328	ARG
1	D	329	VAL
1	D	331	VAL
1	D	335	ILE
1	D	360	ILE
1	D	361	ASN
1	D	365	LYS
1	D	368	THR
1	D	369	THR
1	D	386	ASP
1	D	393	THR
1	D	395	ILE
1	D	417	GLU
1	D	418	ILE
1	D	425	LEU
1	D	427	VAL
1	D	434	ILE
1	D	437	LYS
1	D	445	ARG

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Mol	Chain	Res	Type
1	D	446	SER
1	D	451	ARG
1	D	452	ILE
1	D	456	LYS
1	D	467	LYS
1	D	470	LYS
1	D	473	SER
1	D	478	THR
1	D	479	LYS
1	D	486	GLU
1	D	487	LEU
1	D	491	GLN
1	D	496	ARG
1	D	506	ASN
1	D	513	PRO
1	D	519	ARG
1	D	523	ASP
1	D	525	GLU
1	D	526	LEU
1	D	528	SER
1	D	531	THR
1	D	533	SER
1	D	542	LYS
1	D	543	GLN
1	D	551	LYS
1	D	555	GLU
1	D	565	LEU
1	D	580	THR
1	D	607	TRP
1	D	620	LYS
1	D	622	ASN
1	D	629	ARG
1	D	631	ARG
1	D	632	LYS
1	D	641	MET
1	D	647	ASN
1	D	649	VAL
1	D	700	SER
1	D	707	THR
1	D	714	GLU
1	D	715	ARG
1	D	725	LYS

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Mol	Chain	Res	Type
1	D	743	MET
1	D	760	LYS
1	D	763	VAL
1	D	766	LEU
1	D	775	THR
1	D	784	LYS
1	D	791	VAL
1	D	811	ASN
1	D	831	MET
1	D	839	SER
1	D	852	SER
1	D	853	ASP
1	D	856	SER
1	D	863	GLN
1	D	866	MET
1	D	870	GLN
1	D	885	GLU
1	D	886	ARG
1	D	907	VAL
1	D	908	THR
1	D	911	SER
1	D	917	MET
1	D	919	LEU
1	D	926	LEU
1	D	927	ASP
1	D	944	VAL
1	D	952	ILE
1	D	963	LEU
1	D	977	ARG
1	D	996	GLU
1	D	1046	GLU
1	D	1052	ILE
1	D	1054	LYS
1	D	1057	ARG
1	D	1061	LYS
1	D	1064	THR
1	D	1080	MET
1	D	1083	GLN
1	D	1085	ARG

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

Mol	Chain	Res	Type
1	C	230	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	$\# Z > 2$
2	ADP	A	1201	-	29,29,29	1.19	3 (10%)	45,45,45	1.93	10 (22%)
4	BTI	A	1203	-	16,16,16	1.60	2 (12%)	21,21,21	1.85	4 (19%)
4	BTI	B	1201	-	16,16,16	1.55	3 (18%)	21,21,21	1.90	5 (23%)
5	ATP	C	1202	-	33,33,33	1.14	5 (15%)	52,52,52	1.74	9 (17%)
4	BTI	D	1201	-	16,16,16	1.56	2 (12%)	21,21,21	1.71	5 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	1201	-	-	0/16/32/32	0/1/3/3
4	BTI	A	1203	-	-	0/6/27/27	0/0/2/2
4	BTI	B	1201	-	-	0/6/27/27	0/0/2/2
5	ATP	C	1202	-	-	0/22/38/38	0/1/3/3
4	BTI	D	1201	-	-	0/6/27/27	0/0/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1203	BTI	O3-C3	4.61	1.34	1.23
4	B	1201	BTI	O3-C3	4.59	1.34	1.23
4	D	1201	BTI	O3-C3	4.41	1.33	1.23
5	C	1202	ATP	C5-C4	3.25	1.47	1.40
4	A	1203	BTI	C2-S1	-3.15	1.76	1.82
2	A	1201	ADP	C5-C4	3.07	1.47	1.40
4	D	1201	BTI	C2-S1	-2.90	1.77	1.82
4	B	1201	BTI	C2-S1	-2.57	1.77	1.82
2	A	1201	ADP	C4-N9	-2.44	1.34	1.37
5	C	1202	ATP	C4-N9	-2.41	1.34	1.37
2	A	1201	ADP	PA-O3A	2.39	1.64	1.59
5	C	1202	ATP	PB-O3B	2.36	1.64	1.59
5	C	1202	ATP	PG-O3B	2.24	1.64	1.60
5	C	1202	ATP	O4'-C1'	2.13	1.44	1.41
4	B	1201	BTI	C3-N2	-2.03	1.32	1.35

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	ADP	N3-C2-N1	-6.39	123.36	128.71
4	A	1203	BTI	C5-C6-S1	5.67	110.56	106.04
4	B	1201	BTI	C2-C4-N2	-5.52	105.42	113.27
5	C	1202	ATP	N3-C2-N1	-5.49	124.12	128.71
2	A	1201	ADP	N3-C4-N9	5.35	135.09	125.43
5	C	1202	ATP	N3-C4-N9	5.14	134.72	125.43
5	C	1202	ATP	PA-O3A-PB	-4.08	119.71	131.68
2	A	1201	ADP	O4'-C1'-N9	4.05	112.21	108.44
4	D	1201	BTI	N2-C3-N3	4.00	111.39	108.99
4	D	1201	BTI	C2-C4-N2	-3.85	107.80	113.27
5	C	1202	ATP	C2'-C1'-N9	-3.59	104.06	113.27
5	C	1202	ATP	C4-C5-N7	-3.37	106.64	109.52
4	B	1201	BTI	N2-C3-N3	3.32	110.98	108.99
2	A	1201	ADP	C5-C4-N3	-3.28	118.55	125.70
2	A	1201	ADP	C3'-C2'-C1'	3.23	105.96	100.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1201	BTI	C6-C5-N3	-3.11	106.80	112.56
4	A	1203	BTI	C6-C5-N3	-3.11	106.80	112.56
5	C	1202	ATP	C5-C4-N3	-3.10	118.95	125.70
2	A	1201	ADP	C4-C5-N7	-3.07	106.89	109.52
4	D	1201	BTI	C6-C5-N3	-2.95	107.10	112.56
4	A	1203	BTI	N2-C3-N3	2.94	110.76	108.99
5	C	1202	ATP	PB-O3B-PG	-2.91	123.16	131.68
4	D	1201	BTI	C5-C6-S1	2.87	108.33	106.04
5	C	1202	ATP	O3A-PB-O3B	-2.68	96.22	101.66
2	A	1201	ADP	PA-O3A-PB	-2.63	123.98	131.68
2	A	1201	ADP	C2-N3-C4	2.45	120.98	114.01
5	C	1202	ATP	C2-N3-C4	2.17	120.20	114.01
2	A	1201	ADP	C2'-C1'-N9	-2.14	107.77	113.27
4	B	1201	BTI	C4-C2-S1	2.12	107.94	105.29
2	A	1201	ADP	O3B-PB-O2B	2.12	115.86	107.61
4	B	1201	BTI	O3-C3-N2	-2.06	122.89	125.84
4	D	1201	BTI	C8-C7-C2	-2.04	108.52	113.40
4	A	1203	BTI	C4-N2-C3	-2.01	110.82	112.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	1052/1173 (89%)	-0.24	24 (2%) 57 58	49, 72, 115, 131	0
1	B	989/1173 (84%)	-0.15	28 (2%) 50 52	55, 87, 129, 178	0
1	C	1059/1173 (90%)	-0.08	35 (3%) 44 45	55, 84, 126, 177	0
1	D	989/1173 (84%)	-0.21	14 (1%) 72 72	47, 78, 130, 167	0
All	All	4089/4692 (87%)	-0.17	101 (2%) 54 55	47, 80, 125, 178	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	229	GLY	5.3
1	D	490	ILE	5.3
1	A	233	VAL	5.0
1	C	877	GLN	4.4
1	A	231	SER	4.4
1	C	933	THR	4.3
1	A	1001	PRO	4.2
1	D	240	ASP	4.2
1	A	177	TYR	4.1
1	C	936	TYR	4.1
1	B	168	PRO	4.0
1	D	285	PRO	3.6
1	D	475	ASP	3.6
1	B	526	LEU	3.6
1	C	932	ILE	3.5
1	A	1000	GLY	3.5
1	A	175	LYS	3.4
1	C	890	VAL	3.3
1	C	1093	ASN	3.2
1	C	282	GLY	3.2
1	D	271	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	515	ASN	3.1
1	C	881	LEU	3.1
1	B	527	ALA	3.1
1	C	1070	GLU	3.1
1	A	230	ASN	3.0
1	B	1093	ASN	3.0
1	C	876	GLN	3.0
1	D	515	ASN	3.0
1	B	167	ILE	3.0
1	A	493	SER	2.9
1	D	310	VAL	2.9
1	A	1072	GLY	2.9
1	A	999	GLN	2.9
1	C	922	VAL	2.9
1	A	193	ILE	2.9
1	B	271	HIS	2.9
1	D	239	ILE	2.8
1	A	197	SER	2.8
1	A	174	ILE	2.8
1	C	516	VAL	2.8
1	B	494	LEU	2.8
1	C	492	PRO	2.7
1	A	227	SER	2.7
1	B	156	ARG	2.7
1	C	177	TYR	2.7
1	C	879	LYS	2.7
1	C	999	GLN	2.6
1	C	937	LYS	2.6
1	C	919	LEU	2.6
1	A	219	ARG	2.6
1	C	226	LYS	2.6
1	C	739	ALA	2.5
1	A	494	LEU	2.5
1	B	1072	GLY	2.5
1	B	975	THR	2.5
1	B	153	VAL	2.4
1	C	202	LYS	2.4
1	C	968	LEU	2.4
1	D	494	LEU	2.4
1	B	717	ASN	2.3
1	C	1072	GLY	2.3
1	A	222	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	285	PRO	2.3
1	D	421	TYR	2.3
1	A	228	PHE	2.3
1	C	285	PRO	2.3
1	B	1000	GLY	2.3
1	C	1001	PRO	2.3
1	C	766	LEU	2.2
1	B	976	ALA	2.2
1	C	741	LYS	2.2
1	B	999	GLN	2.2
1	B	882	GLY	2.2
1	A	223	GLU	2.2
1	B	1092	GLU	2.2
1	C	935	GLY	2.2
1	D	384	LEU	2.2
1	C	187	ALA	2.2
1	B	936	TYR	2.2
1	B	1070	GLU	2.2
1	C	218	HIS	2.2
1	D	479	LYS	2.1
1	A	421	TYR	2.1
1	B	270	ARG	2.1
1	B	880	SER	2.1
1	B	641	MET	2.1
1	A	1070	GLU	2.1
1	C	923	GLN	2.1
1	C	884	GLY	2.1
1	A	189	PHE	2.1
1	B	240	ASP	2.1
1	B	879	LYS	2.1
1	B	1071	ASN	2.0
1	C	713	PRO	2.0
1	A	568	THR	2.0
1	D	1070	GLU	2.0
1	B	144	GLU	2.0
1	B	982	LEU	2.0
1	C	161	LYS	2.0
1	D	769	HIS	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	MN	D	1202	1/1	0.18	-	74,74,74,74	0
3	MN	B	1202	1/1	0.19	-	82,82,82,82	0
3	MN	C	1201	1/1	0.28	-	76,76,76,76	0
2	ADP	A	1201	27/27	0.17	-	86,91,110,110	0
5	ATP	C	1202	31/31	0.16	-	102,108,115,115	0
3	MN	A	1202	1/1	0.20	-	74,74,74,74	0
4	BTI	D	1201	15/15	0.28	-	105,109,113,116	0
4	BTI	B	1201	15/15	0.34	-	105,109,114,115	0
4	BTI	A	1203	15/15	0.33	-	92,99,104,105	0

6.5 Other polymers ⓘ

There are no such residues in this entry.