



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:46 PM GMT

PDB ID : 4AID
Title : Crystal structure of C. crescentus PNPase bound to RNase E recognition peptide
Authors : Hardwick, S.W.; Gubbey, T.; Hug, I.; Jenal, U.; Luisi, B.F.
Deposited on : 2012-02-09
Resolution : 2.60 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>

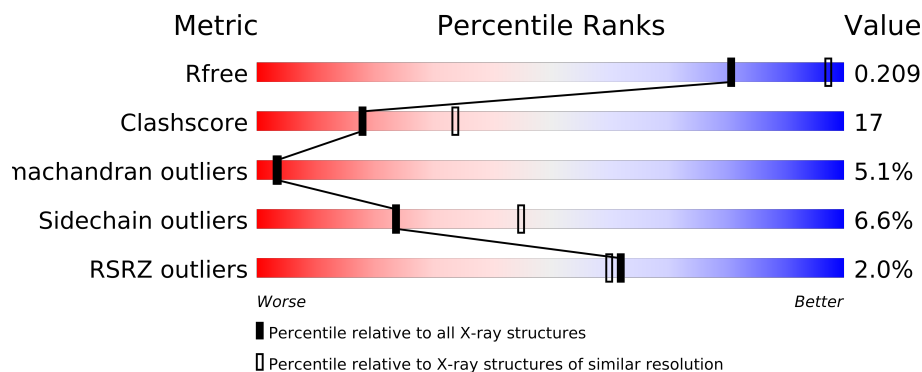
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.60 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	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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	726	
1	B	726	
1	C	726	
2	F	14	
2	G	14	
2	H	14	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12655 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 POLYRIBONUCLEOTIDE NUCLEOTIDYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	573	Total	C	N	O	S	0	1	0
			4248	2686	720	819	23			
1	B	558	Total	C	N	O	S	0	0	0
			4170	2639	706	802	23			
1	C	539	Total	C	N	O	S	0	0	0
			3836	2425	654	735	22			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP Q9AC32
A	-12	GLY	-	EXPRESSION TAG	UNP Q9AC32
A	-11	SER	-	EXPRESSION TAG	UNP Q9AC32
A	-10	SER	-	EXPRESSION TAG	UNP Q9AC32
A	-9	HIS	-	EXPRESSION TAG	UNP Q9AC32
A	-8	HIS	-	EXPRESSION TAG	UNP Q9AC32
A	-7	HIS	-	EXPRESSION TAG	UNP Q9AC32
A	-6	HIS	-	EXPRESSION TAG	UNP Q9AC32
A	-5	HIS	-	EXPRESSION TAG	UNP Q9AC32
A	-4	HIS	-	EXPRESSION TAG	UNP Q9AC32
A	-3	SER	-	EXPRESSION TAG	UNP Q9AC32
A	-2	GLN	-	EXPRESSION TAG	UNP Q9AC32
A	-1	ASP	-	EXPRESSION TAG	UNP Q9AC32
A	0	PRO	-	EXPRESSION TAG	UNP Q9AC32
B	-13	MET	-	EXPRESSION TAG	UNP Q9AC32
B	-12	GLY	-	EXPRESSION TAG	UNP Q9AC32
B	-11	SER	-	EXPRESSION TAG	UNP Q9AC32
B	-10	SER	-	EXPRESSION TAG	UNP Q9AC32
B	-9	HIS	-	EXPRESSION TAG	UNP Q9AC32
B	-8	HIS	-	EXPRESSION TAG	UNP Q9AC32
B	-7	HIS	-	EXPRESSION TAG	UNP Q9AC32
B	-6	HIS	-	EXPRESSION TAG	UNP Q9AC32

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	EXPRESSION TAG	UNP Q9AC32
B	-4	HIS	-	EXPRESSION TAG	UNP Q9AC32
B	-3	SER	-	EXPRESSION TAG	UNP Q9AC32
B	-2	GLN	-	EXPRESSION TAG	UNP Q9AC32
B	-1	ASP	-	EXPRESSION TAG	UNP Q9AC32
B	0	PRO	-	EXPRESSION TAG	UNP Q9AC32
C	-13	MET	-	EXPRESSION TAG	UNP Q9AC32
C	-12	GLY	-	EXPRESSION TAG	UNP Q9AC32
C	-11	SER	-	EXPRESSION TAG	UNP Q9AC32
C	-10	SER	-	EXPRESSION TAG	UNP Q9AC32
C	-9	HIS	-	EXPRESSION TAG	UNP Q9AC32
C	-8	HIS	-	EXPRESSION TAG	UNP Q9AC32
C	-7	HIS	-	EXPRESSION TAG	UNP Q9AC32
C	-6	HIS	-	EXPRESSION TAG	UNP Q9AC32
C	-5	HIS	-	EXPRESSION TAG	UNP Q9AC32
C	-4	HIS	-	EXPRESSION TAG	UNP Q9AC32
C	-3	SER	-	EXPRESSION TAG	UNP Q9AC32
C	-2	GLN	-	EXPRESSION TAG	UNP Q9AC32
C	-1	ASP	-	EXPRESSION TAG	UNP Q9AC32
C	0	PRO	-	EXPRESSION TAG	UNP Q9AC32

- Molecule 2 is a protein called RIBONUCLEASE, RNE/RNG FAMILY PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	7	Total	C	N	O	0	0	0
			66	44	15	7			
2	G	8	Total	C	N	O	0	0	0
			77	50	19	8			
2	H	5	Total	C	N	O	0	0	0
			42	30	7	5			

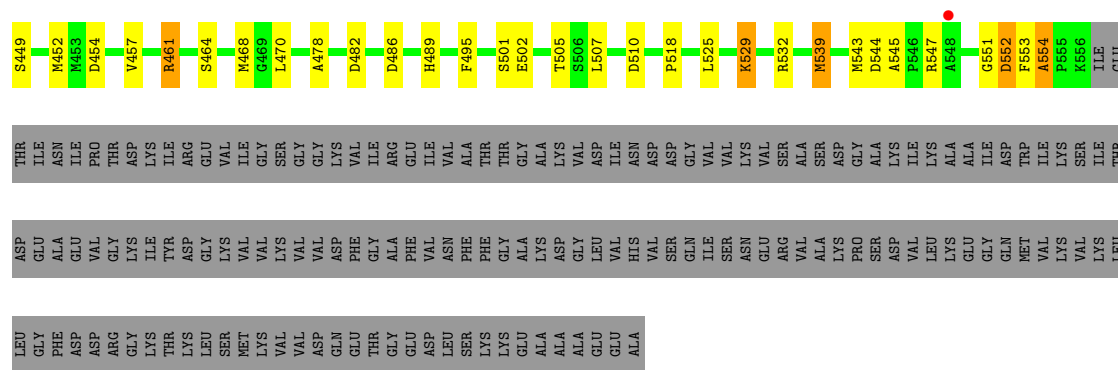
- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		

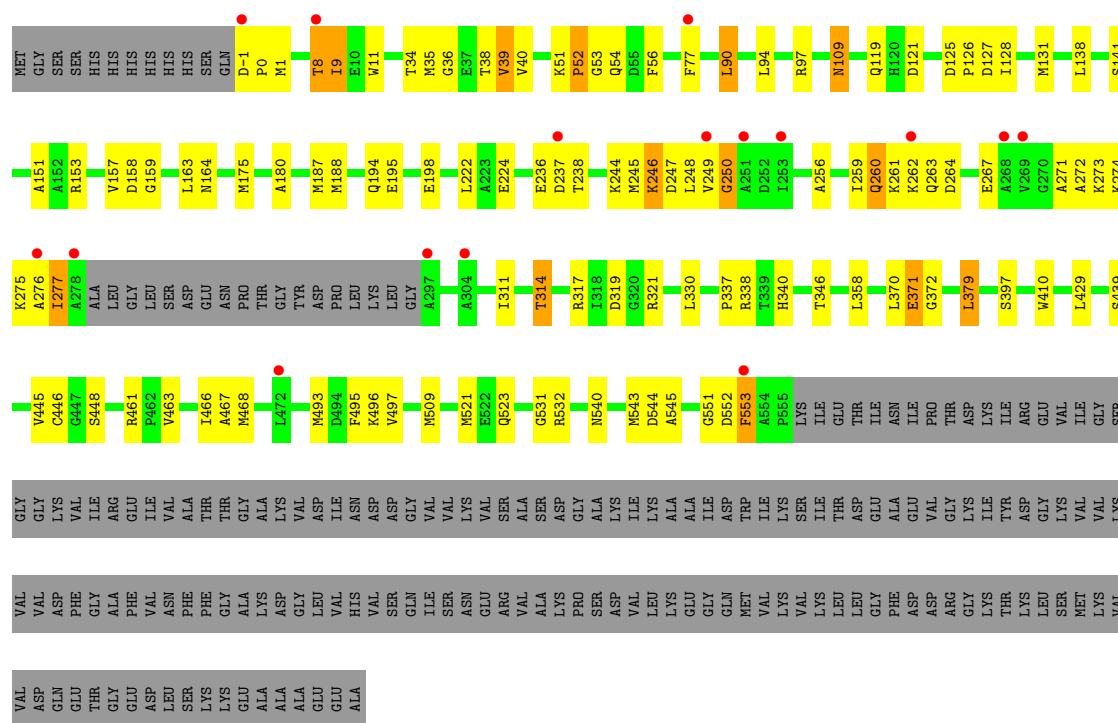
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	96	Total	O	0	0
			96	96		
4	B	80	Total	O	0	0
			80	80		
4	C	24	Total	O	0	0
			24	24		
4	G	1	Total	O	0	0
			1	1		



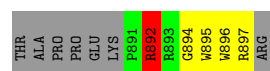
• Molecule 1: POLYRIBONUCLEOTIDE NUCLEOTIDYLTRANSFERASE

Chain C:



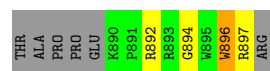
• Molecule 2: RIBONUCLEASE, RNE/RNG FAMILY PROTEIN

Chain F:



• Molecule 2: RIBONUCLEASE, RNE/RNG FAMILY PROTEIN

Chain G:



• Molecule 2: RIBONUCLEASE, RNE/RNG FAMILY PROTEIN

Chain H: 

THR	ALA	PRO	PRO	GLU	LYS	PRO	ARG	F8993	W8996	F8997	ARG
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4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	157.44Å 157.44Å 302.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.60 29.75 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.0 (30.00-2.60) 90.0 (29.75-2.60)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.209 , 0.254 0.190 , 0.209	Depositor DCC
R_{free} test set	2319 reflections (3.09%)	DCC
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 19.5	EDS
Estimated twinning fraction	0.357 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 77316 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12655	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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: PO4

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	1.01	8/4324 (0.2%)	1.15	27/5859 (0.5%)
1	B	1.03	9/4242 (0.2%)	1.21	33/5744 (0.6%)
1	C	0.66	2/3900 (0.1%)	0.87	3/5305 (0.1%)
2	F	1.59	2/70 (2.9%)	1.32	1/94 (1.1%)
2	G	1.30	1/81 (1.2%)	1.14	0/109
2	H	1.49	1/45 (2.2%)	1.03	0/62
All	All	0.94	23/12662 (0.2%)	1.10	64/17173 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	1
2	F	0	1
All	All	0	7

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	896	TRP	CD2-CE2	7.50	1.50	1.41
1	B	81	GLU	CD-OE1	6.69	1.33	1.25
2	G	896	TRP	CD2-CE2	6.34	1.49	1.41
1	A	432	GLU	CD-OE1	6.33	1.32	1.25
1	A	332	GLU	CD-OE1	6.26	1.32	1.25
1	A	11	TRP	CD2-CE2	6.05	1.48	1.41
1	B	432	GLU	CD-OE1	5.86	1.32	1.25
1	B	332	GLU	CD-OE1	5.74	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	147	GLY	N-CA	5.73	1.54	1.46
1	A	376	GLU	CD-OE1	5.72	1.31	1.25
2	F	895	TRP	CD2-CE2	5.68	1.48	1.41
1	A	147	GLY	C-O	-5.62	1.14	1.23
1	B	81	GLU	CD-OE2	5.58	1.31	1.25
1	A	435	GLU	CD-OE1	5.57	1.31	1.25
1	B	11	TRP	CD2-CE2	5.49	1.48	1.41
1	B	199	GLU	CG-CD	5.45	1.60	1.51
1	B	190	GLU	CD-OE1	5.44	1.31	1.25
1	A	190	GLU	CD-OE1	5.40	1.31	1.25
1	A	613	TRP	CD2-CE2	5.37	1.47	1.41
1	C	11	TRP	CD2-CE2	5.34	1.47	1.41
1	B	3	ASP	CB-CG	-5.24	1.40	1.51
1	C	410	TRP	CD2-CE2	5.19	1.47	1.41
2	H	896	TRP	CD2-CE2	5.11	1.47	1.41

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	177	LEU	CB-CG-CD1	-10.79	92.66	111.00
1	B	28	ASP	CB-CG-OD2	10.72	127.95	118.30
1	B	3	ASP	CB-CG-OD1	-10.37	108.97	118.30
1	B	153	ARG	NE-CZ-NH1	9.91	125.26	120.30
1	B	486	ASP	CB-CG-OD1	-9.45	109.80	118.30
1	A	9	ILE	N-CA-C	-9.45	85.50	111.00
1	B	28	ASP	CB-CG-OD1	-9.40	109.84	118.30
1	A	80	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	A	80	ARG	NE-CZ-NH2	-8.95	115.83	120.30
1	A	486	ASP	CB-CG-OD1	-8.28	110.85	118.30
1	B	539	MET	CG-SD-CE	-8.26	86.98	100.20
1	A	97	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	B	55	ASP	CB-CG-OD2	7.99	125.49	118.30
1	A	94	LEU	CB-CG-CD1	-7.84	97.67	111.00
1	B	486	ASP	CB-CG-OD2	7.76	125.28	118.30
1	A	539	MET	CG-SD-CE	-7.54	88.14	100.20
1	B	532	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	A	452	MET	CG-SD-CE	-7.31	88.50	100.20
1	A	553	PHE	N-CA-C	-6.56	93.29	111.00
1	B	525	LEU	CA-CB-CG	-6.45	100.46	115.30
1	B	291	ASP	C-N-CD	-6.45	106.42	120.60
1	A	439	SER	N-CA-C	6.40	128.28	111.00
1	B	83	ARG	NE-CZ-NH1	6.26	123.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	222	LEU	CA-CB-CG	6.24	129.65	115.30
1	B	8	THR	N-CA-C	-6.20	94.26	111.00
1	B	153	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	B	3	ASP	CB-CG-OD2	6.14	123.83	118.30
1	B	452	MET	CG-SD-CE	-6.05	90.52	100.20
1	A	-1	ASP	C-N-CD	6.05	141.10	128.40
1	A	28	ASP	CB-CG-OD1	-6.04	112.87	118.30
1	B	55	ASP	CB-CG-OD1	-5.99	112.91	118.30
1	B	96	ASP	CB-CG-OD1	5.99	123.69	118.30
1	B	401	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	B	461	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	153	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	B	96	ASP	CB-CG-OD2	-5.77	113.10	118.30
1	A	544	ASP	N-CA-CB	-5.67	100.39	110.60
1	A	468	MET	CG-SD-CE	5.63	109.21	100.20
1	B	321	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	B	7	LYS	N-CA-C	-5.57	95.97	111.00
1	B	510	ASP	CB-CG-OD1	5.53	123.28	118.30
1	B	439	SER	N-CA-C	5.50	125.84	111.00
1	A	294	LYS	N-CA-C	-5.49	96.19	111.00
1	A	411	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	B	125	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	428	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	B	3	ASP	N-CA-CB	-5.35	100.97	110.60
2	F	894	GLY	N-CA-C	5.34	126.45	113.10
1	C	90	LEU	CA-CB-CG	5.31	127.51	115.30
1	A	504	LEU	CB-CG-CD2	-5.30	101.99	111.00
1	A	7	LYS	N-CA-C	-5.29	96.71	111.00
1	B	529	LYS	CD-CE-NZ	-5.27	99.59	111.70
1	A	55	ASP	CB-CA-C	-5.25	99.90	110.40
1	B	1	MET	CB-CG-SD	5.23	128.10	112.40
1	A	317	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	B	194	GLN	CA-CB-CG	5.21	124.87	113.40
1	A	28	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	192	GLU	N-CA-C	-5.20	96.97	111.00
1	A	19	GLU	OE1-CD-OE2	-5.12	117.15	123.30
1	A	8	THR	N-CA-C	-5.12	97.18	111.00
1	A	184	ASP	CB-CA-C	-5.10	100.19	110.40
1	B	6	ARG	N-CA-C	-5.10	97.23	111.00
1	A	486	ASP	CB-CG-OD2	5.01	122.81	118.30
1	C	463	VAL	CB-CA-C	-5.01	101.88	111.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	554	ALA	Peptide
1	A	8	THR	Peptide
1	B	554	ALA	Peptide
1	B	6	ARG	Peptide
1	B	9	ILE	Peptide
1	C	35	MET	Peptide
2	F	892	ARG	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	4248	0	2	85	1
1	B	4170	0	0	84	1
1	C	3836	0	0	47	2
2	F	66	0	58	1	0
2	G	77	0	70	1	0
2	H	42	0	26	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
4	A	96	0	0	3	0
4	B	80	0	0	3	0
4	C	24	0	0	2	0
4	G	1	0	0	0	0
All	All	12655	0	156	215	2

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 17.

All (215) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:287:PRO:CB	1:A:288:THR:CG2	1.84	1.53
1:A:281:GLY:CA	1:A:289:GLY:O	1.68	1.37
1:B:291:ASP:O	1:B:293:LEU:N	1.61	1.29

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:279:ALA:O	1:B:282:LEU:CD2	1.97	1.13
1:A:287:PRO:CA	1:A:288:THR:CG2	2.28	1.10
1:A:493:MET:CE	1:A:509:MET:CE	2.36	1.03
1:B:279:ALA:O	1:B:282:LEU:CG	2.07	1.02
1:C:52:PRO:O	1:C:54:GLN:N	1.92	1.02
1:A:282:LEU:CA	1:A:292:PRO:CG	2.38	1.00
1:B:97:ARG:NH2	1:B:190:GLU:OE1	1.96	0.97
1:B:275:LYS:O	1:B:277:ILE:N	1.97	0.97
1:A:281:GLY:O	1:A:290:TYR:O	1.82	0.97
1:A:543:MET:O	1:A:544:ASP:CB	2.11	0.94
1:B:263:GLN:O	1:B:266:TYR:N	2.01	0.93
1:B:274:LYS:CA	1:B:277:ILE:CG2	2.47	0.92
1:A:276:ALA:O	1:A:280:LEU:CB	2.19	0.91
1:B:97:ARG:CZ	1:B:188:MET:CE	2.57	0.82
1:A:277:ILE:C	1:A:282:LEU:CD1	2.49	0.81
1:B:278:ALA:O	1:B:282:LEU:CD2	2.28	0.81
1:B:277:ILE:O	1:B:278:ALA:C	2.20	0.80
1:B:291:ASP:C	1:B:293:LEU:N	2.32	0.80
1:A:274:LYS:O	1:A:277:ILE:CG2	2.30	0.79
1:C:319:ASP:OD2	1:C:321:ARG:NH1	2.16	0.78
1:A:284:ASP:OD1	1:A:285:GLU:N	2.18	0.77
1:A:277:ILE:O	1:A:282:LEU:CD1	2.34	0.76
1:A:464:SER:CB	1:A:539:MET:CE	2.64	0.76
1:A:381:HIS:CD2	1:A:428:ARG:NH1	2.54	0.75
1:C:236:GLU:O	1:C:238:THR:N	2.20	0.74
1:A:281:GLY:O	1:A:292:PRO:CD	2.35	0.74
1:B:286:ASN:N	1:B:287:PRO:O	2.20	0.74
1:A:7:LYS:O	1:A:8:THR:C	2.26	0.74
1:B:290:TYR:O	1:B:292:PRO:N	2.21	0.74
1:A:454:ASP:OD1	1:A:547:ARG:NH1	2.20	0.73
1:B:416:MET:CE	1:B:461:ARG:CB	2.67	0.73
1:A:8:THR:O	1:A:9:ILE:CG1	2.37	0.72
1:B:454:ASP:OD1	1:B:547:ARG:NH1	2.22	0.72
1:B:260:GLN:O	1:B:261:LYS:CB	2.35	0.71
1:B:291:ASP:O	1:B:292:PRO:C	2.27	0.71
1:A:54:GLN:O	1:A:55:ASP:CB	2.36	0.70
1:C:446:CYS:SG	4:C:2015:HOH:O	2.50	0.69
1:A:453:MET:CB	1:A:543:MET:CE	2.70	0.69
1:C:157:VAL:O	1:C:159:GLY:N	2.25	0.69
1:B:274:LYS:CD	1:B:277:ILE:CG2	2.70	0.69
1:B:277:ILE:O	1:B:279:ALA:N	2.26	0.69
1:B:263:GLN:O	1:B:267:GLU:N	2.26	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:261:LYS:O	1:B:262:LYS:O	2.11	0.69
1:B:100:ARG:NH1	4:B:2014:HOH:O	2.26	0.69
1:B:275:LYS:CG	1:B:276:ALA:N	2.55	0.68
1:A:181:GLY:CA	1:A:212:MET:CE	2.72	0.68
1:B:364:GLU:OE1	1:B:375:LYS:CE	2.42	0.68
1:B:274:LYS:CD	1:B:277:ILE:CD1	2.72	0.67
1:A:401:ARG:NE	1:A:405:HIS:CE1	2.63	0.66
1:B:313:ASP:O	1:B:314:THR:OG1	2.13	0.65
1:B:97:ARG:NH1	1:B:188:MET:CE	2.59	0.65
1:C:337:PRO:O	1:C:338:ARG:CB	2.41	0.65
1:C:338:ARG:CA	1:C:553:PHE:CE1	2.80	0.65
1:B:303:GLU:O	1:B:306:VAL:CG1	2.44	0.64
1:C:39:VAL:CG1	1:C:119:GLN:CB	2.76	0.64
1:A:266:TYR:O	1:A:267:GLU:C	2.36	0.64
1:A:311:ILE:O	1:A:314:THR:O	2.16	0.63
1:A:502:GLU:O	4:A:2091:HOH:O	2.15	0.63
1:B:337:PRO:O	1:B:338:ARG:CB	2.42	0.63
1:B:287:PRO:CB	1:B:288:THR:CA	2.77	0.63
1:A:281:GLY:C	1:A:289:GLY:O	2.36	0.62
1:C:38:THR:OG1	1:C:121:ASP:N	2.34	0.61
1:C:256:ALA:O	1:C:259:ILE:CB	2.49	0.60
1:A:287:PRO:C	1:A:288:THR:CG2	2.69	0.60
1:B:259:ILE:O	1:B:265:ARG:NH1	2.34	0.60
1:B:282:LEU:CB	1:B:287:PRO:O	2.50	0.59
1:A:401:ARG:CZ	1:A:405:HIS:CE1	2.85	0.59
1:C:264:ASP:O	1:C:267:GLU:N	2.36	0.59
1:A:275:LYS:O	1:A:278:ALA:N	2.36	0.58
1:C:509:MET:CE	1:C:521:MET:SD	2.91	0.58
1:B:277:ILE:O	1:B:280:LEU:N	2.37	0.58
1:C:249:VAL:CG1	1:C:272:ALA:CB	2.81	0.58
1:A:83:ARG:NH1	1:A:83:ARG:CG	2.68	0.57
1:A:368:ASP:N	1:A:368:ASP:OD1	2.37	0.57
2:G:896:TRP:N	2:G:897:ARG:HA	2.19	0.57
1:A:260:GLN:O	1:A:261:LYS:C	2.42	0.57
1:A:262:LYS:O	1:A:263:GLN:C	2.42	0.57
1:B:97:ARG:NH2	1:B:188:MET:CE	2.68	0.56
1:B:414:ARG:N	1:B:415:PRO:CD	2.67	0.56
1:A:266:TYR:O	1:A:269:VAL:N	2.39	0.56
1:A:285:GLU:O	1:A:286:ASN:ND2	2.40	0.55
1:B:291:ASP:O	1:B:293:LEU:CA	2.52	0.55
1:A:310:GLY:O	1:A:313:ASP:O	2.24	0.55
1:C:246:LYS:O	1:C:247:ASP:C	2.43	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:263:GLN:CG	1:B:264:ASP:N	2.70	0.55
1:A:261:LYS:O	1:A:262:LYS:C	2.45	0.55
1:A:277:ILE:CG2	1:A:278:ALA:N	2.70	0.54
1:B:464:SER:CB	1:B:539:MET:CE	2.85	0.54
1:B:263:GLN:O	1:B:265:ARG:N	2.41	0.54
1:A:502:GLU:OE2	1:B:529:LYS:CE	2.55	0.54
1:A:275:LYS:O	1:A:277:ILE:N	2.40	0.54
1:B:275:LYS:C	1:B:277:ILE:N	2.53	0.54
1:A:261:LYS:O	1:A:262:LYS:O	2.25	0.54
1:A:281:GLY:N	1:A:289:GLY:O	2.39	0.54
1:A:431:SER:OG	1:A:444:THR:CG2	2.56	0.54
1:A:127:ASP:OD1	1:A:128:ILE:N	2.41	0.54
1:A:401:ARG:CD	4:A:2078:HOH:O	2.55	0.53
1:B:246:LYS:O	1:B:250:GLY:N	2.41	0.53
1:B:181:GLY:CA	1:B:212:MET:CE	2.87	0.53
1:C:180:ALA:O	1:C:187:MET:N	2.42	0.53
1:C:340:HIS:CD2	1:C:358:LEU:N	2.77	0.53
1:C:259:ILE:O	1:C:260:GLN:O	2.27	0.52
1:A:97:ARG:NH1	1:A:190:GLU:OE1	2.42	0.52
1:A:412:ALA:O	1:A:505:THR:CG2	2.58	0.52
1:C:94:LEU:CD1	1:C:97:ARG:NH2	2.73	0.52
1:C:249:VAL:CG2	1:C:276:ALA:CB	2.88	0.51
1:B:263:GLN:O	1:B:266:TYR:CA	2.58	0.51
1:A:479:VAL:CG2	1:A:527:GLN:OE1	2.58	0.51
1:A:260:GLN:O	1:A:261:LYS:O	2.28	0.51
1:C:531:GLY:CA	4:C:2020:HOH:O	2.58	0.50
1:A:265:ARG:O	1:A:266:TYR:O	2.29	0.50
1:A:523:GLN:O	1:A:526:ALA:N	2.44	0.50
1:A:543:MET:O	1:A:545:ALA:N	2.44	0.50
1:B:311:ILE:O	1:B:314:THR:O	2.29	0.50
1:B:543:MET:O	1:B:545:ALA:N	2.45	0.50
1:A:313:ASP:O	1:A:314:THR:OG1	2.29	0.50
1:C:-1:ASP:O	1:C:0:PRO:C	2.49	0.49
1:A:263:GLN:O	1:A:264:ASP:C	2.52	0.48
1:C:330:LEU:O	1:C:346:THR:CG2	2.61	0.48
1:C:109:ASN:ND2	1:C:109:ASN:N	2.61	0.48
1:B:281:GLY:O	1:B:289:GLY:O	2.32	0.48
1:B:551:GLY:O	1:B:552:ASP:C	2.51	0.48
1:B:8:THR:O	1:B:9:ILE:C	2.48	0.48
1:C:370:LEU:O	1:C:372:GLY:N	2.47	0.48
1:A:274:LYS:CA	1:A:274:LYS:CE	2.92	0.48
1:C:195:GLU:OE2	1:C:461:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:198:GLU:OE2	1:C:532:ARG:NH2	2.47	0.48
1:A:181:GLY:C	1:A:212:MET:CE	2.82	0.47
1:A:263:GLN:O	1:A:265:ARG:N	2.47	0.47
1:A:249:VAL:CG2	1:A:276:ALA:CB	2.92	0.47
1:A:416:MET:CE	1:A:500:THR:CG2	2.92	0.47
1:A:299:PHE:O	1:A:302:LEU:N	2.48	0.47
1:C:54:GLN:NE2	1:C:56:PHE:CE1	2.82	0.47
1:C:127:ASP:OD1	1:C:128:ILE:N	2.47	0.47
1:C:543:MET:O	1:C:545:ALA:N	2.47	0.47
1:B:283:SER:CB	1:B:287:PRO:CB	2.93	0.47
1:C:8:THR:O	1:C:9:ILE:CB	2.63	0.47
1:C:125:ASP:OD1	1:C:126:PRO:CD	2.64	0.46
1:B:279:ALA:C	1:B:282:LEU:CD2	2.79	0.46
1:B:261:LYS:C	1:B:262:LYS:O	2.52	0.46
1:B:280:LEU:N	1:B:280:LEU:CD1	2.79	0.46
1:B:266:TYR:C	1:B:266:TYR:CD1	2.89	0.46
1:A:265:ARG:O	1:A:266:TYR:C	2.52	0.46
1:C:551:GLY:O	1:C:552:ASP:C	2.52	0.46
1:B:206:ASN:ND2	4:B:2042:HOH:O	2.48	0.46
1:A:373:THR:O	1:A:373:THR:CG2	2.63	0.46
1:C:379:LEU:O	1:C:429:LEU:N	2.49	0.46
1:A:60:THR:CG2	4:A:2012:HOH:O	2.64	0.46
1:B:284:ASP:CA	1:B:285:GLU:CB	2.94	0.46
1:B:55:ASP:N	1:B:55:ASP:OD1	2.48	0.46
1:C:311:ILE:O	1:C:314:THR:O	2.33	0.46
1:B:286:ASN:N	1:B:287:PRO:CA	2.79	0.45
1:B:501:SER:N	4:B:2071:HOH:O	2.49	0.45
1:A:224:GLU:O	2:F:892:ARG:HD3	2.16	0.45
1:B:277:ILE:CG2	1:B:278:ALA:N	2.79	0.45
1:A:236:GLU:O	1:A:238:THR:N	2.49	0.45
1:B:-1:ASP:CB	1:B:0:PRO:CD	2.95	0.45
1:A:275:LYS:C	1:A:277:ILE:N	2.70	0.45
1:B:273:LYS:O	1:B:275:LYS:N	2.50	0.45
1:A:275:LYS:CG	1:A:276:ALA:N	2.76	0.45
1:A:414:ARG:N	1:A:415:PRO:CD	2.80	0.45
1:A:7:LYS:C	1:A:8:THR:O	2.50	0.44
1:A:416:MET:CE	1:A:461:ARG:CB	2.95	0.44
1:B:68:PHE:C	1:B:68:PHE:CD1	2.90	0.44
1:C:256:ALA:O	1:C:259:ILE:N	2.50	0.44
1:C:246:LYS:O	1:C:250:GLY:N	2.50	0.44
1:C:128:ILE:CD1	1:C:153:ARG:CB	2.95	0.44
1:A:266:TYR:O	1:A:268:ALA:N	2.51	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:368:ASP:OD1	1:B:368:ASP:N	2.50	0.44
1:A:3:ASP:N	1:A:3:ASP:OD1	2.50	0.44
1:B:347:ARG:NH2	1:B:439:SER:O	2.51	0.44
1:B:283:SER:N	1:B:284:ASP:C	2.71	0.44
1:A:7:LYS:O	1:A:9:ILE:N	2.50	0.44
1:C:553:PHE:O	1:C:553:PHE:CD1	2.71	0.43
1:A:249:VAL:CG1	1:A:272:ALA:CB	2.96	0.43
1:A:340:HIS:CD2	1:A:358:LEU:N	2.86	0.43
1:B:327:ARG:NH2	1:B:482:ASP:OD1	2.52	0.43
1:B:551:GLY:O	1:B:552:ASP:O	2.37	0.43
1:C:131:MET:CE	1:C:151:ALA:CB	2.97	0.43
1:B:283:SER:N	1:B:285:GLU:N	2.67	0.43
1:A:401:ARG:NH2	1:A:405:HIS:CE1	2.87	0.42
1:C:466:ILE:CG1	1:C:467:ALA:N	2.83	0.42
1:B:304:ALA:O	1:B:308:ARG:CG	2.67	0.42
1:A:11:TRP:N	1:A:14:LYS:O	2.53	0.42
1:A:274:LYS:C	1:A:277:ILE:CG2	2.87	0.42
1:B:83:ARG:NH1	1:B:83:ARG:CB	2.82	0.42
1:B:286:ASN:CA	1:B:287:PRO:O	2.68	0.42
1:B:286:ASN:CB	1:B:287:PRO:O	2.68	0.42
1:B:99:ILE:O	1:B:100:ARG:C	2.58	0.42
1:B:309:ARG:CG	1:B:309:ARG:NH1	2.83	0.42
1:B:93:ARG:NH1	1:B:404:GLY:CA	2.83	0.42
1:B:468:MET:CB	1:B:495:PHE:CZ	3.03	0.41
1:C:317:ARG:NH2	1:C:321:ARG:NH2	2.67	0.41
1:B:470:LEU:CD1	1:B:478:ALA:O	2.68	0.41
1:A:8:THR:C	1:A:9:ILE:CG1	2.89	0.41
1:C:39:VAL:O	1:C:40:VAL:CG2	2.68	0.41
1:B:544:ASP:C	1:B:544:ASP:OD1	2.59	0.41
1:C:163:LEU:O	1:C:164:ASN:C	2.59	0.41
1:A:281:GLY:O	1:A:292:PRO:CG	2.69	0.41
1:B:336:LEU:C	1:B:337:PRO:O	2.59	0.41
1:A:181:GLY:N	1:A:212:MET:CE	2.84	0.41
1:A:245:MET:CE	1:A:299:PHE:CA	2.98	0.41
1:C:493:MET:CE	1:C:495:PHE:CD1	3.04	0.41
1:B:269:VAL:CG1	1:B:270:GLY:N	2.83	0.41
1:C:468:MET:CB	1:C:495:PHE:CE2	3.04	0.40
1:C:138:LEU:O	1:C:141:SER:OG	2.39	0.40
1:A:236:GLU:C	1:A:238:THR:N	2.75	0.40
1:B:191:SER:OG	1:B:507:LEU:O	2.40	0.40
1:A:308:ARG:NH2	1:A:473:GLU:OE2	2.55	0.40
1:B:349:GLU:OE1	1:B:437:ASN:ND2	2.54	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:529:LYS:NZ	1:B:502:GLU:OE1	2.55	0.40
1:C:274:LYS:O	1:C:277:ILE:CB	2.70	0.40

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:8:THR:OG1	1:C:540:ASN:O[2_555]	1.87	0.33
1:B:6:ARG:NH2	1:C:224:GLU:OE2[3_565]	2.10	0.10

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	570/726 (78%)	502 (88%)	37 (6%)	31 (5%)	3	3
1	B	556/726 (77%)	490 (88%)	41 (7%)	25 (4%)	4	4
1	C	535/726 (74%)	476 (89%)	32 (6%)	27 (5%)	3	4
2	F	5/14 (36%)	4 (80%)	0	1 (20%)	0	0
2	G	6/14 (43%)	5 (83%)	0	1 (17%)	0	0
2	H	3/14 (21%)	2 (67%)	1 (33%)	0	100	100
All	All	1675/2220 (76%)	1479 (88%)	111 (7%)	85 (5%)	3	3

All (85) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	55	ASP
1	A	239	ASP
1	A	248	LEU
1	A	262	LYS
1	A	263	GLN
1	A	266	TYR
1	A	275	LYS

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Mol	Chain	Res	Type
1	A	294	LYS
1	A	554	ALA
1	B	248	LEU
1	B	264	ASP
1	B	276	ALA
1	B	278	ALA
1	B	287	PRO
1	B	290	TYR
1	B	291	ASP
1	B	292	PRO
1	B	552	ASP
1	B	554	ALA
1	C	8	THR
1	C	53	GLY
1	C	158	ASP
1	C	237	ASP
1	C	244	LYS
1	C	248	LEU
1	C	262	LYS
1	C	271	ALA
1	C	275	LYS
1	C	277	ILE
1	C	397	SER
1	C	544	ASP
1	A	54	GLN
1	A	246	LYS
1	A	261	LYS
1	A	264	ASP
1	A	267	GLU
1	A	276	ALA
1	A	278	ALA
1	A	284	ASP
1	A	318	ILE
1	A	396	GLY
1	B	261	LYS
1	B	262	LYS
1	B	269	VAL
1	B	273	LYS
1	B	274	LYS
1	B	277	ILE
1	B	396	GLY
1	B	439	SER

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Mol	Chain	Res	Type
1	C	1	MET
1	C	9	ILE
1	C	36	GLY
1	C	52	PRO
1	C	260	GLN
1	C	261	LYS
1	C	263	GLN
1	C	371	GLU
1	C	439	SER
1	A	244	LYS
1	A	280	LEU
1	A	283	SER
1	A	290	TYR
1	B	279	ALA
1	B	285	GLU
1	B	371	GLU
1	C	246	LYS
1	B	294	LYS
1	C	245	MET
1	C	273	LYS
1	C	314	THR
2	G	894	GLY
1	A	237	ASP
1	A	292	PRO
1	A	439	SER
1	A	552	ASP
1	B	267	GLU
1	B	397	SER
2	F	892	ARG
1	A	1	MET
1	A	281	GLY
1	B	52	PRO
1	C	51	LYS
1	C	250	GLY
1	A	555	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	432/578 (75%)	401 (93%)	31 (7%)	21	39
1	B	428/578 (74%)	397 (93%)	31 (7%)	21	39
1	C	364/578 (63%)	348 (96%)	16 (4%)	39	68
2	F	5/12 (42%)	3 (60%)	2 (40%)	0	0
2	G	6/12 (50%)	5 (83%)	1 (17%)	3	5
2	H	2/12 (17%)	2 (100%)	0	100	100
All	All	1237/1770 (70%)	1156 (94%)	81 (6%)	24	46

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	ASP
1	A	1	MET
1	A	3	ASP
1	A	7	LYS
1	A	35	MET
1	A	54	GLN
1	A	55	ASP
1	A	60	THR
1	A	80	ARG
1	A	83	ARG
1	A	140	LEU
1	A	153	ARG
1	A	157	VAL
1	A	186	VAL
1	A	200	ILE
1	A	221	ASP
1	A	239	ASP
1	A	280	LEU
1	A	282	LEU
1	A	283	SER
1	A	290	TYR
1	A	312	LEU
1	A	355	VAL
1	A	401	ARG
1	A	430	VAL
1	A	457	VAL
1	A	463	VAL
1	A	481	SER
1	A	505	THR
1	A	553	PHE

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Mol	Chain	Res	Type
1	A	613	TRP
1	B	-1	ASP
1	B	1	MET
1	B	8	THR
1	B	10	GLU
1	B	31	VAL
1	B	64	GLN
1	B	83	ARG
1	B	120	HIS
1	B	177	LEU
1	B	178	VAL
1	B	188	MET
1	B	194	GLN
1	B	200	ILE
1	B	202	LEU
1	B	242	LYS
1	B	290	TYR
1	B	293	LEU
1	B	308	ARG
1	B	309	ARG
1	B	333	VAL
1	B	335	ILE
1	B	336	LEU
1	B	368	ASP
1	B	431	SER
1	B	445	VAL
1	B	449	SER
1	B	457	VAL
1	B	489	HIS
1	B	505	THR
1	B	518	PRO
1	B	553	PHE
1	C	34	THR
1	C	39	VAL
1	C	77	PHE
1	C	90	LEU
1	C	109	ASN
1	C	175	MET
1	C	188	MET
1	C	194	GLN
1	C	371	GLU
1	C	379	LEU

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Mol	Chain	Res	Type
1	C	445	VAL
1	C	448	SER
1	C	496	LYS
1	C	497	VAL
1	C	523	GLN
1	C	553	PHE
2	F	892	ARG
2	F	897	ARG
2	G	892	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PO4	A	1614	-	4,4,4	0.14	0	6,6,6	0.35	0
3	PO4	B	1557	-	4,4,4	0.08	0	6,6,6	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	C	1556	-	4,4,4	0.18	0	6,6,6	0.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	A	1614	-	-	0/0/0/0	0/0/0/0
3	PO4	B	1557	-	-	0/0/0/0	0/0/0/0
3	PO4	C	1556	-	-	0/0/0/0	0/0/0/0

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.

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	573/726 (78%)	-0.24	15 (2%) 53 50	24, 34, 123, 161	0
1	B	558/726 (76%)	-0.29	3 (0%) 88 90	24, 33, 109, 147	0
1	C	539/726 (74%)	0.04	16 (2%) 48 45	53, 87, 184, 253	0
2	F	7/14 (50%)	-0.13	0 100 100	40, 67, 84, 94	0
2	G	8/14 (57%)	-0.11	0 100 100	37, 68, 86, 93	0
2	H	5/14 (35%)	0.07	0 100 100	82, 97, 103, 107	0
All	All	1690/2220 (76%)	-0.16	34 (2%) 62 60	24, 49, 135, 253	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	251	ALA	5.3
1	A	278	ALA	4.6
1	C	268	ALA	4.2
1	C	269	VAL	3.9
1	C	278	ALA	3.6
1	A	247	ASP	3.6
1	A	254	ALA	3.5
1	C	472	LEU	3.4
1	C	297	ALA	3.3
1	C	276	ALA	3.3
1	A	251	ALA	3.2
1	A	611	ILE	3.1
1	A	279	ALA	2.9
1	C	249	VAL	2.8
1	C	253	ILE	2.7
1	A	293	LEU	2.7
1	C	553	PHE	2.6
1	C	237	ASP	2.5
1	B	288	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	264	ASP	2.4
1	A	610	ALA	2.4
1	C	262	LYS	2.3
1	C	-1	ASP	2.3
1	C	8	THR	2.3
1	A	255	ALA	2.3
1	C	304	ALA	2.3
1	B	548	ALA	2.3
1	A	259	ILE	2.2
1	B	284	ASP	2.1
1	A	605	ALA	2.1
1	A	284	ASP	2.1
1	C	77	PHE	2.1
1	A	271	ALA	2.0
1	A	269	VAL	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	PO4	C	1556	5/5	0.19	1.15	86,89,109,117	0
3	PO4	B	1557	5/5	0.11	-1.61	76,82,92,104	0
3	PO4	A	1614	5/5	0.10	-3.21	58,60,69,75	0

6.5 Other polymers ⓘ

There are no such residues in this entry.