



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 05:10 pm GMT

PDB ID : 3C79
Title : Crystal structure of Aplysia californica AChBP in complex with the neonicotinoid imidacloprid
Authors : Talley, T.T.; Harel, M.; Hibbs, R.E.; Tomizawa, M.; Casida, J.E.; Taylor, P.W.
Deposited on : 2008-02-06
Resolution : 2.48 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

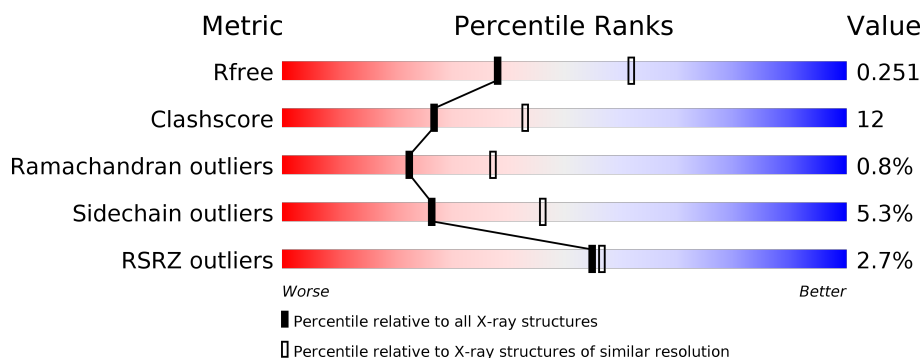
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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}	100719	4719 (2.50-2.46)
Clashscore	112137	5483 (2.50-2.46)
Ramachandran outliers	110173	5388 (2.50-2.46)
Sidechain outliers	110143	5390 (2.50-2.46)
RSRZ outliers	101464	4754 (2.50-2.46)

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. 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	227	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>16%</div> <div>• 7%</div> </div> </div>
1	B	227	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>15%</div> <div>• • 7%</div> </div> </div>
1	C	227	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>19%</div> <div>• 8%</div> </div> </div>
1	D	227	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>19%</div> <div>• 7%</div> </div> </div>
1	E	227	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>23%</div> <div>• • 7%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IM4	A	301	-	-	-	X
2	IM4	B	302	-	-	-	X
2	IM4	D	304	-	-	-	X
3	IPA	A	404	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8648 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 Soluble acetylcholine receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	1	0
			1695	1069	282	335	9			
1	B	212	Total	C	N	O	S	0	1	0
			1703	1073	283	338	9			
1	C	208	Total	C	N	O	S	0	0	0
			1661	1049	275	329	8			
1	D	212	Total	C	N	O	S	0	0	0
			1692	1067	279	337	9			
1	E	211	Total	C	N	O	S	0	1	0
			1693	1067	281	336	9			

There are 40 discrepancies between the modelled and reference sequences:

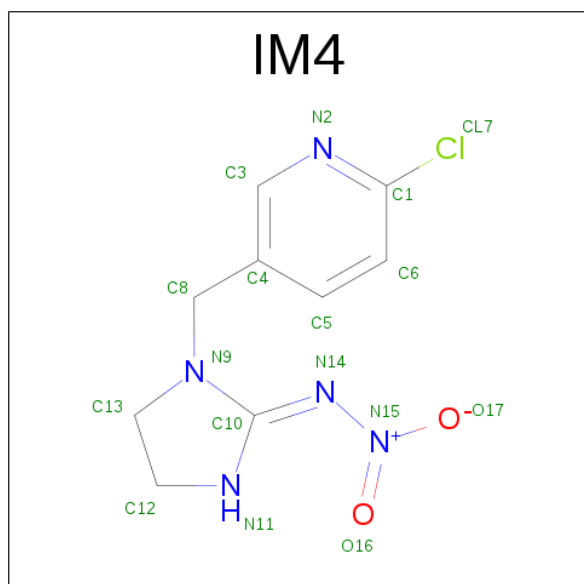
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	TYR	-	expression tag	UNP Q8WSF8
A	-6	LYS	-	expression tag	UNP Q8WSF8
A	-5	ASP	-	expression tag	UNP Q8WSF8
A	-4	ASP	-	expression tag	UNP Q8WSF8
A	-3	ASP	-	expression tag	UNP Q8WSF8
A	-2	ASP	-	expression tag	UNP Q8WSF8
A	-1	LYS	-	expression tag	UNP Q8WSF8
A	0	LEU	-	expression tag	UNP Q8WSF8
B	-7	TYR	-	expression tag	UNP Q8WSF8
B	-6	LYS	-	expression tag	UNP Q8WSF8
B	-5	ASP	-	expression tag	UNP Q8WSF8
B	-4	ASP	-	expression tag	UNP Q8WSF8
B	-3	ASP	-	expression tag	UNP Q8WSF8
B	-2	ASP	-	expression tag	UNP Q8WSF8
B	-1	LYS	-	expression tag	UNP Q8WSF8
B	0	LEU	-	expression tag	UNP Q8WSF8
C	-7	TYR	-	expression tag	UNP Q8WSF8
C	-6	LYS	-	expression tag	UNP Q8WSF8
C	-5	ASP	-	expression tag	UNP Q8WSF8

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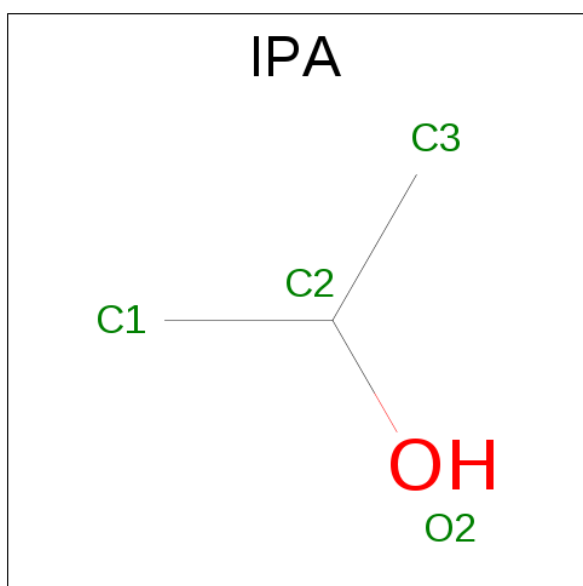
Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	ASP	-	expression tag	UNP Q8WSF8
C	-3	ASP	-	expression tag	UNP Q8WSF8
C	-2	ASP	-	expression tag	UNP Q8WSF8
C	-1	LYS	-	expression tag	UNP Q8WSF8
C	0	LEU	-	expression tag	UNP Q8WSF8
D	-7	TYR	-	expression tag	UNP Q8WSF8
D	-6	LYS	-	expression tag	UNP Q8WSF8
D	-5	ASP	-	expression tag	UNP Q8WSF8
D	-4	ASP	-	expression tag	UNP Q8WSF8
D	-3	ASP	-	expression tag	UNP Q8WSF8
D	-2	ASP	-	expression tag	UNP Q8WSF8
D	-1	LYS	-	expression tag	UNP Q8WSF8
D	0	LEU	-	expression tag	UNP Q8WSF8
E	-7	TYR	-	expression tag	UNP Q8WSF8
E	-6	LYS	-	expression tag	UNP Q8WSF8
E	-5	ASP	-	expression tag	UNP Q8WSF8
E	-4	ASP	-	expression tag	UNP Q8WSF8
E	-3	ASP	-	expression tag	UNP Q8WSF8
E	-2	ASP	-	expression tag	UNP Q8WSF8
E	-1	LYS	-	expression tag	UNP Q8WSF8
E	0	LEU	-	expression tag	UNP Q8WSF8

- Molecule 2 is (2E)-1-[(6-CHLOROPYRIDIN-3-YL)METHYL]-N-NITROIMIDAZOLIDIN-2-IMINE (three-letter code: IM4) (formula: C₉H₁₀ClN₅O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			17	9	1	5	2		
2	B	1	Total	C	Cl	N	O	0	0
			17	9	1	5	2		
2	C	1	Total	C	Cl	N	O	0	0
			17	9	1	5	2		
2	D	1	Total	C	Cl	N	O	0	0
			17	9	1	5	2		

- Molecule 3 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	3	1		
3	C	1	Total	C	O	0	0
			4	3	1		
3	D	1	Total	C	O	0	0
			4	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total	O	0	0
			23	23		
4	B	24	Total	O	0	0
			24	24		
4	C	29	Total	O	0	0
			29	29		

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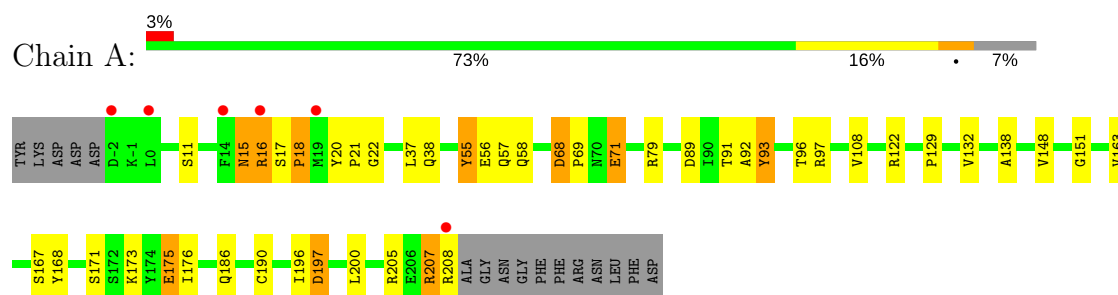
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	19	Total	O	0	0
			19	19		
4	E	29	Total	O	0	0
			29	29		

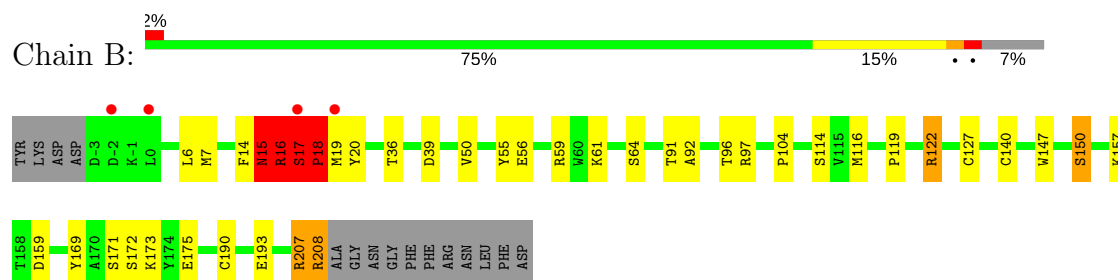
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

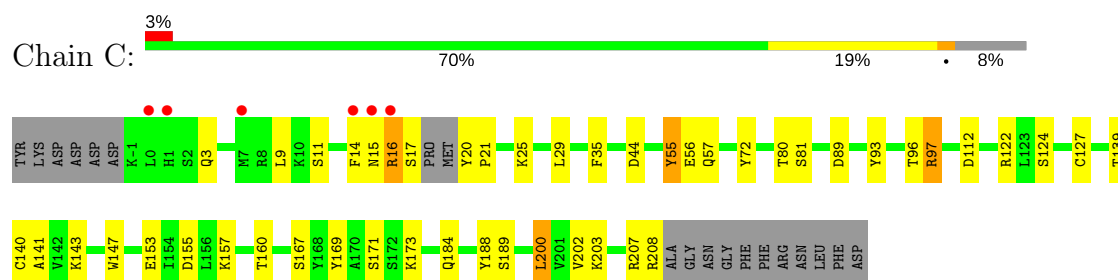
• Molecule 1: Soluble acetylcholine receptor



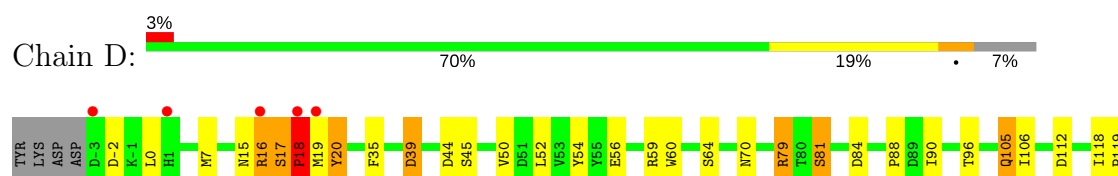
• Molecule 1: Soluble acetylcholine receptor

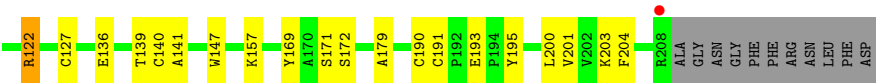


• Molecule 1: Soluble acetylcholine receptor

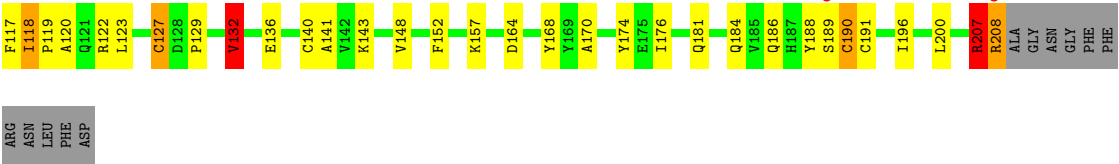
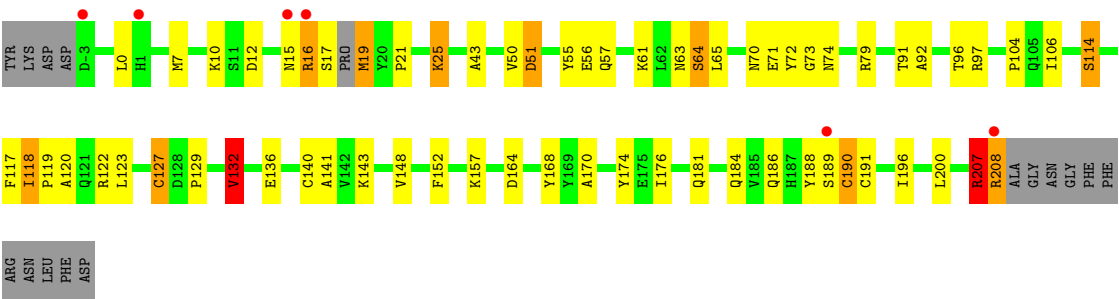


• Molecule 1: Soluble acetylcholine receptor





● Molecule 1: Soluble acetylcholine receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.39Å 116.29Å 132.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.72 – 2.48 47.72 – 2.48	Depositor EDS
% Data completeness (in resolution range)	97.6 (47.72-2.48) 97.7 (47.72-2.48)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.09 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.188 , 0.250 0.192 , 0.251	Depositor DCC
R_{free} test set	2353 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8648	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IPA, IM4

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	1.21	5/1736 (0.3%)	1.11	5/2366 (0.2%)
1	B	1.23	1/1744 (0.1%)	1.06	4/2377 (0.2%)
1	C	1.25	1/1700 (0.1%)	1.10	4/2315 (0.2%)
1	D	1.27	3/1733 (0.2%)	1.09	10/2362 (0.4%)
1	E	1.22	5/1735 (0.3%)	1.03	4/2362 (0.2%)
All	All	1.24	15/8648 (0.2%)	1.08	27/11782 (0.2%)

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
1	B	0	4
1	C	0	2
1	D	0	2
1	E	0	2
All	All	0	11

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	175	GLU	CG-CD	5.96	1.60	1.51
1	E	140	CYS	CB-SG	5.90	1.92	1.82
1	D	105	GLN	CG-CD	5.83	1.64	1.51
1	E	117	PHE	CE1-CZ	5.83	1.48	1.37
1	B	169	TYR	CD2-CE2	-5.81	1.30	1.39
1	E	132	VAL	CB-CG1	-5.80	1.40	1.52
1	A	93	TYR	CG-CD2	5.58	1.46	1.39
1	A	93	TYR	CD2-CE2	5.46	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	ALA	CA-CB	-5.31	1.41	1.52
1	C	55	TYR	CE2-CZ	5.30	1.45	1.38
1	D	136	GLU	CG-CD	5.23	1.59	1.51
1	E	174	TYR	CD2-CE2	5.23	1.47	1.39
1	A	55	TYR	CE1-CZ	5.11	1.45	1.38
1	D	105	GLN	CB-CG	5.01	1.66	1.52
1	E	114	SER	CB-OG	-5.00	1.35	1.42

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	7	MET	CG-SD-CE	5.98	109.77	100.20
1	C	112	ASP	CB-CG-OD1	5.96	123.67	118.30
1	E	164	ASP	CB-CG-OD2	5.91	123.62	118.30
1	D	112	ASP	CB-CG-OD1	5.91	123.62	118.30
1	B	140	CYS	CA-CB-SG	-5.89	103.40	114.00
1	E	79	ARG	NE-CZ-NH2	5.89	123.24	120.30
1	D	140	CYS	CA-CB-SG	-5.88	103.42	114.00
1	D	39	ASP	CB-CG-OD1	5.70	123.43	118.30
1	D	122	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	A	68	ASP	CB-CG-OD1	5.61	123.35	118.30
1	A	55	TYR	CB-CG-CD2	-5.59	117.65	121.00
1	C	29	LEU	CB-CG-CD2	-5.57	101.54	111.00
1	C	202	VAL	CB-CA-C	-5.53	100.89	111.40
1	B	122	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	B	207	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	197	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	208	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	E	51	ASP	CB-CG-OD1	5.32	123.09	118.30
1	D	39	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	E	207	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	D	122	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	167	SER	CB-CA-C	-5.27	100.09	110.10
1	A	55	TYR	CA-CB-CG	5.22	123.31	113.40
1	D	52	LEU	CB-CA-C	-5.19	100.34	110.20
1	D	44	ASP	CB-CG-OD1	5.15	122.93	118.30
1	C	44	ASP	CB-CG-OD1	5.10	122.89	118.30
1	D	79	ARG	NE-CZ-NH2	-5.07	117.76	120.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	ASN	Peptide
1	B	15	ASN	Peptide
1	B	16	ARG	Peptide
1	B	17	SER	Peptide
1	B	18	PRO	Peptide
1	C	14	PHE	Peptide
1	C	16	ARG	Peptide
1	D	16	ARG	Peptide
1	D	18	PRO	Peptide
1	E	16	ARG	Peptide
1	E	189	SER	Peptide

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	1695	0	1630	38	0
1	B	1703	0	1634	39	0
1	C	1661	0	1598	37	0
1	D	1692	0	1621	32	0
1	E	1693	0	1626	57	0
2	A	17	0	10	4	0
2	B	17	0	10	3	0
2	C	17	0	10	2	0
2	D	17	0	10	5	0
3	A	4	0	8	3	0
3	C	4	0	8	0	0
3	D	4	0	8	1	0
4	A	23	0	0	0	0
4	B	24	0	0	0	0
4	C	29	0	0	3	0
4	D	19	0	0	0	0
4	E	29	0	0	0	0
All	All	8648	0	8173	190	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (190) 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)
2:A:301:IM4:N15	2:A:301:IM4:O16	1.57	1.38
1:D:15:ASN:O	1:D:16:ARG:HG3	1.37	1.20
1:C:127:CYS:CB	1:C:140:CYS:SG	2.36	1.13
1:A:93:TYR:HB2	3:A:404:IPA:H32	1.19	1.11
1:A:93:TYR:HB2	3:A:404:IPA:C3	1.86	1.04
1:C:97:ARG:HG2	1:C:97:ARG:HH11	0.92	1.04
1:E:17:SER:O	1:E:19:MET:HG3	1.57	1.03
1:E:17:SER:C	1:E:19:MET:HG3	1.78	1.03
1:C:127:CYS:SG	1:C:140:CYS:CB	2.48	1.01
1:C:97:ARG:HG2	1:C:97:ARG:NH1	1.68	1.00
1:E:15:ASN:O	1:E:16:ARG:HD2	1.62	0.99
1:C:97:ARG:HH11	1:C:97:ARG:CG	1.79	0.96
1:B:15:ASN:O	1:B:16:ARG:HG3	1.72	0.90
1:E:15:ASN:ND2	1:E:16:ARG:HH11	1.72	0.87
1:A:68:ASP:HB3	1:A:71:GLU:OE2	1.75	0.86
1:E:208:ARG:NH1	1:E:208:ARG:HA	1.93	0.84
1:B:15:ASN:C	1:B:16:ARG:HD2	2.00	0.81
1:B:15:ASN:O	1:B:16:ARG:HD2	1.80	0.80
1:B:15:ASN:O	1:B:16:ARG:CG	2.30	0.79
1:E:15:ASN:O	1:E:16:ARG:CD	2.30	0.79
1:B:15:ASN:O	1:B:16:ARG:CD	2.30	0.79
1:C:35:PHE:CE1	1:C:56:GLU:HG3	2.19	0.77
2:D:304:IM4:N11	2:D:304:IM4:O16	2.09	0.76
1:E:17:SER:HB3	1:E:19:MET:N	2.02	0.75
1:C:93:TYR:CE2	1:C:188:TYR:OH	2.39	0.74
1:C:93:TYR:HE2	1:C:188:TYR:OH	1.70	0.74
1:C:97:ARG:NH1	1:C:97:ARG:CG	2.41	0.73
1:A:190:CYS:HB3	2:A:301:IM4:O16	1.87	0.73
1:E:57:GLN:HG3	1:E:118:ILE:HD13	1.71	0.72
1:B:172:SER:N	1:B:207:ARG:NH2	2.38	0.72
1:A:168:TYR:CE1	1:A:176:ILE:HD11	2.25	0.72
1:E:15:ASN:HD22	1:E:16:ARG:HH11	1.37	0.72
1:C:173:LYS:HE3	1:D:45:SER:O	1.89	0.72
1:E:17:SER:CB	1:E:19:MET:N	2.54	0.70
1:E:97[B]:ARG:HH11	1:E:97[B]:ARG:CG	2.05	0.69
1:E:15:ASN:ND2	1:E:16:ARG:NH1	2.41	0.69
1:B:175:GLU:HB3	1:B:207:ARG:HH11	1.58	0.68
1:B:6:LEU:HD23	1:C:21:PRO:HG2	1.76	0.68
1:C:207:ARG:HD2	4:C:421:HOH:O	1.95	0.67
1:B:50:VAL:HG21	1:B:127:CYS:SG	2.35	0.67
1:B:172:SER:N	1:B:207:ARG:HH21	1.93	0.67
1:A:93:TYR:CB	3:A:404:IPA:H32	2.11	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:ASN:O	1:D:16:ARG:CG	2.30	0.66
1:A:15:ASN:O	1:A:16:ARG:C	2.34	0.66
1:B:104:PRO:HG3	1:C:89:ASP:HB2	1.77	0.66
1:D:15:ASN:C	1:D:16:ARG:HG3	2.14	0.66
1:E:15:ASN:O	1:E:16:ARG:CG	2.44	0.66
1:B:16:ARG:HD2	1:B:16:ARG:N	2.12	0.65
1:B:15:ASN:O	1:B:16:ARG:NH1	2.30	0.65
1:C:143:LYS:NZ	1:C:184:GLN:HE22	1.96	0.64
1:E:168:TYR:CE1	1:E:176:ILE:HD11	2.32	0.63
1:B:7:MET:CE	1:C:20:TYR:N	2.62	0.63
1:A:168:TYR:CE1	1:A:176:ILE:CD1	2.81	0.63
1:E:61:LYS:HD3	1:E:114:SER:HB3	1.81	0.63
2:A:301:IM4:O17	2:A:301:IM4:N11	2.21	0.63
1:E:17:SER:C	1:E:19:MET:CG	2.63	0.63
1:E:57:GLN:HG3	1:E:118:ILE:CD1	2.29	0.62
1:A:207:ARG:HG3	1:A:207:ARG:HH21	1.65	0.61
1:E:208:ARG:HH11	1:E:208:ARG:HA	1.63	0.61
1:A:79:ARG:HG3	1:A:108:VAL:HG22	1.83	0.60
1:B:6:LEU:HD23	1:C:21:PRO:CG	2.32	0.60
1:A:122:ARG:HD2	1:B:96:THR:O	2.02	0.59
1:B:15:ASN:N	1:B:15:ASN:OD1	2.36	0.59
1:C:155:ASP:OD2	1:C:157:LYS:HE2	2.02	0.59
1:D:118:ILE:HD12	3:D:402:IPA:H13	1.84	0.59
1:A:207:ARG:O	1:A:208:ARG:HG3	2.03	0.58
1:C:139:THR:OG1	1:C:203:LYS:HG2	2.04	0.58
1:A:96:THR:O	1:E:122:ARG:HD2	2.04	0.58
1:C:25:LYS:HE3	1:C:153:GLU:OE2	2.03	0.57
1:B:36:THR:HG21	1:B:55:TYR:CZ	2.40	0.57
1:A:186:GLN:HG2	1:A:197:ASP:OD2	2.05	0.57
1:B:39:ASP:OD1	1:B:172:SER:HB2	2.05	0.57
1:E:71:GLU:HG2	1:E:71:GLU:O	2.06	0.56
1:E:17:SER:HB2	1:E:19:MET:N	2.21	0.56
1:E:168:TYR:CZ	1:E:176:ILE:CD1	2.88	0.56
1:D:139:THR:OG1	1:D:203:LYS:HG2	2.06	0.56
2:A:301:IM4:N2	1:E:118:ILE:HG13	2.21	0.55
1:C:55:TYR:CE1	2:D:304:IM4:O16	2.59	0.55
1:E:15:ASN:HD22	1:E:16:ARG:NH1	2.04	0.55
1:B:7:MET:HE2	1:C:20:TYR:N	2.21	0.55
1:D:141:ALA:HA	1:D:200:LEU:O	2.06	0.54
1:E:63:ASN:C	1:E:65:LEU:H	2.10	0.54
1:D:88:PRO:HB2	1:D:90:ILE:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ASN:HA	1:B:18:PRO:HG3	1.90	0.54
1:E:168:TYR:CZ	1:E:176:ILE:HD11	2.43	0.54
1:D:88:PRO:HB2	1:D:90:ILE:CD1	2.38	0.54
1:D:122:ARG:HD2	1:E:96:THR:O	2.09	0.53
1:D:39:ASP:OD1	1:D:172:SER:HB2	2.07	0.53
2:B:302:IM4:N11	2:B:302:IM4:O16	2.38	0.53
1:A:207:ARG:HG3	1:A:207:ARG:NH2	2.23	0.53
1:B:91:THR:HG22	1:B:92:ALA:O	2.08	0.53
2:C:303:IM4:O17	2:C:303:IM4:N11	2.42	0.53
1:A:151:GLY:HA3	1:A:196:ILE:CD1	2.39	0.52
1:E:15:ASN:O	1:E:16:ARG:HG3	2.08	0.52
1:A:151:GLY:CA	1:A:196:ILE:HD12	2.40	0.52
1:D:35:PHE:CE1	1:D:56:GLU:HG3	2.45	0.52
1:D:147:TRP:O	2:D:304:IM4:H13	2.09	0.52
1:D:56:GLU:O	1:D:119:PRO:HD2	2.10	0.52
1:B:14:PHE:C	1:B:15:ASN:OD1	2.49	0.51
1:A:175:GLU:OE2	1:A:205:ARG:NH2	2.42	0.51
1:A:56:GLU:OE2	1:A:58:GLN:NE2	2.36	0.51
1:D:191:CYS:HB3	1:D:193:GLU:OE1	2.11	0.51
1:E:97[B]:ARG:HG3	1:E:97[B]:ARG:HH11	1.76	0.50
1:E:91:THR:HG22	1:E:92:ALA:O	2.12	0.50
1:A:17:SER:O	1:A:18:PRO:O	2.30	0.50
1:E:176:ILE:N	1:E:176:ILE:HD12	2.27	0.50
1:E:181:GLN:HG3	1:E:181:GLN:O	2.11	0.50
1:B:7:MET:HE3	1:C:20:TYR:N	2.26	0.50
1:C:122:ARG:HD2	1:D:96:THR:O	2.12	0.50
1:B:16:ARG:N	1:B:16:ARG:CD	2.74	0.49
1:B:59:ARG:NH1	1:B:159:ASP:OD1	2.46	0.49
1:E:168:TYR:CE1	1:E:176:ILE:CD1	2.95	0.49
1:E:129:PRO:O	1:E:132:VAL:HG22	2.13	0.49
1:B:17:SER:O	1:B:18:PRO:O	2.30	0.48
1:A:129:PRO:O	1:A:132:VAL:HB	2.13	0.48
1:A:175:GLU:HB3	1:A:207:ARG:NH2	2.29	0.48
1:B:56:GLU:O	1:B:119:PRO:HD2	2.14	0.48
1:D:50:VAL:HG21	1:D:127:CYS:SG	2.54	0.48
1:E:56:GLU:O	1:E:119:PRO:HD2	2.14	0.47
1:A:21:PRO:HD3	1:E:7:MET:HE2	1.96	0.47
1:C:97:ARG:NH1	4:C:402:HOH:O	2.23	0.47
1:E:170:ALA:O	1:E:207:ARG:NH1	2.46	0.47
1:D:60:TRP:CH2	1:D:88:PRO:HD2	2.50	0.47
1:C:93:TYR:HE2	1:C:188:TYR:CZ	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:THR:HG22	1:A:92:ALA:O	2.15	0.47
1:D:17:SER:HA	1:D:18:PRO:HD3	1.29	0.47
1:A:37:LEU:HD23	1:A:176:ILE:HD13	1.97	0.47
1:E:50:VAL:HG21	1:E:127:CYS:SG	2.55	0.47
1:C:147:TRP:CH2	2:C:303:IM4:H12	2.50	0.46
1:A:89:ASP:HB2	1:E:104:PRO:HG2	1.96	0.46
1:E:141:ALA:HA	1:E:200:LEU:O	2.16	0.46
1:B:190:CYS:HB3	2:B:302:IM4:O17	2.14	0.46
1:E:188:TYR:O	1:E:191:CYS:N	2.40	0.46
1:C:93:TYR:HE2	1:C:188:TYR:HH	1.40	0.46
1:E:73:GLY:O	1:E:74:ASN:HB2	2.16	0.46
1:A:151:GLY:CA	1:A:196:ILE:CD1	2.93	0.46
1:B:59:ARG:HD3	1:B:116:MET:HE2	1.97	0.46
1:C:9:LEU:HB2	1:C:72:TYR:CD1	2.51	0.46
1:D:204:PHE:N	1:D:204:PHE:CD2	2.84	0.46
1:B:122:ARG:HD2	1:C:96:THR:O	2.16	0.46
1:D:179:ALA:HA	1:D:201:VAL:O	2.16	0.46
1:D:16:ARG:O	1:D:17:SER:O	2.34	0.46
1:C:143:LYS:HZ3	1:C:184:GLN:HE22	1.62	0.45
1:D:81:SER:O	1:D:84:ASP:HB2	2.16	0.45
1:D:106:ILE:HB	1:E:148:VAL:HG11	1.98	0.45
1:A:207:ARG:CG	1:A:207:ARG:HH21	2.28	0.45
1:D:195:TYR:CE1	2:D:304:IM4:H8	2.52	0.45
1:A:20:TYR:CE1	1:A:22:GLY:HA2	2.52	0.45
1:D:54:TYR:C	1:D:54:TYR:CD1	2.89	0.44
1:E:63:ASN:C	1:E:65:LEU:N	2.71	0.44
1:A:173:LYS:HA	1:A:173:LYS:HD2	1.70	0.44
1:B:173:LYS:HA	1:B:173:LYS:HD2	1.83	0.44
1:D:190:CYS:C	1:D:191:CYS:SG	2.95	0.44
1:B:50:VAL:CG2	1:B:127:CYS:SG	3.03	0.44
1:E:143:LYS:NZ	1:E:184:GLN:HE22	2.16	0.44
1:E:188:TYR:O	1:E:190:CYS:N	2.51	0.43
1:B:17:SER:HA	1:B:18:PRO:HD3	1.80	0.43
1:B:61:LYS:HA	1:B:114:SER:HA	2.01	0.43
1:E:97[B]:ARG:HH11	1:E:97[B]:ARG:HG2	1.82	0.43
1:A:16:ARG:O	1:A:17:SER:HB2	2.18	0.43
1:A:163:VAL:HG21	1:A:200:LEU:CD1	2.48	0.43
1:C:3:GLN:HE21	1:D:20:TYR:HD2	1.65	0.43
1:E:25:LYS:HE3	1:E:152:PHE:CD1	2.54	0.43
1:C:169:TYR:CZ	1:C:171:SER:HB2	2.53	0.43
1:E:208:ARG:HA	1:E:208:ARG:CZ	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ASN:O	1:A:17:SER:C	2.57	0.43
1:A:151:GLY:HA3	1:A:196:ILE:HD12	1.99	0.42
1:D:147:TRP:CZ3	2:D:304:IM4:H12	2.54	0.42
1:B:150:SER:HB2	1:B:193:GLU:HG2	2.01	0.42
1:B:171:SER:C	1:B:207:ARG:HH21	2.22	0.42
1:E:51:ASP:HA	1:E:123:LEU:O	2.19	0.42
1:E:70:ASN:ND2	1:E:74:ASN:OD1	2.52	0.42
1:C:143:LYS:HZ2	1:C:184:GLN:HE22	1.68	0.42
1:A:68:ASP:HA	1:A:69:PRO:HD2	1.68	0.41
1:B:147:TRP:CH2	2:B:302:IM4:H12	2.55	0.41
1:C:141:ALA:HA	1:C:200:LEU:O	2.20	0.41
1:C:3:GLN:NE2	1:D:20:TYR:HD2	2.17	0.41
1:A:148:VAL:HG21	1:E:106:ILE:HG21	2.02	0.41
1:B:97[B]:ARG:HH11	1:B:97[B]:ARG:HG3	1.85	0.41
1:E:65:LEU:HA	1:E:65:LEU:HD23	1.89	0.41
1:A:68:ASP:CB	1:A:71:GLU:OE2	2.57	0.41
1:C:11:SER:HA	1:C:15:ASN:HD22	1.85	0.41
1:D:79:ARG:HD2	1:D:79:ARG:N	2.36	0.41
1:E:61:LYS:HD3	1:E:114:SER:CB	2.50	0.41
1:E:55:TYR:HB3	1:E:120:ALA:HA	2.03	0.40
1:A:97[B]:ARG:HH21	1:A:97[B]:ARG:HG2	1.86	0.40
1:C:57:GLN:HB2	4:C:427:HOH:O	2.20	0.40
1:E:12:ASP:OD2	1:E:72:TYR:OH	2.32	0.40
1:E:43:ALA:HA	1:E:50:VAL:HG22	2.03	0.40
1:D:169:TYR:CZ	1:D:171:SER:HB2	2.57	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	210/227 (92%)	202 (96%)	6 (3%)	2 (1%)	18 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	211/227 (93%)	203 (96%)	6 (3%)	2 (1%)	20	34
1	C	204/227 (90%)	199 (98%)	5 (2%)	0	100	100
1	D	210/227 (92%)	203 (97%)	5 (2%)	2 (1%)	18	30
1	E	208/227 (92%)	197 (95%)	9 (4%)	2 (1%)	18	30
All	All	1043/1135 (92%)	1004 (96%)	31 (3%)	8 (1%)	22	37

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	PRO
1	D	18	PRO
1	A	16	ARG
1	D	17	SER
1	B	19	MET
1	B	18	PRO
1	E	64	SER
1	E	21	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	193/205 (94%)	186 (96%)	7 (4%)	40	65
1	B	194/205 (95%)	186 (96%)	8 (4%)	35	59
1	C	189/205 (92%)	178 (94%)	11 (6%)	23	41
1	D	193/205 (94%)	183 (95%)	10 (5%)	27	47
1	E	193/205 (94%)	178 (92%)	15 (8%)	15	26
All	All	962/1025 (94%)	911 (95%)	51 (5%)	26	46

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	38	GLN
1	A	55	TYR
1	A	57	GLN
1	A	71	GLU
1	A	171	SER
1	A	207	ARG
1	B	15	ASN
1	B	16	ARG
1	B	17	SER
1	B	20	TYR
1	B	64	SER
1	B	150	SER
1	B	157	LYS
1	B	208	ARG
1	C	16	ARG
1	C	17	SER
1	C	80	THR
1	C	81	SER
1	C	97	ARG
1	C	124	SER
1	C	160	THR
1	C	167	SER
1	C	189	SER
1	C	200	LEU
1	C	208	ARG
1	D	-2	ASP
1	D	0	LEU
1	D	19	MET
1	D	20	TYR
1	D	59	ARG
1	D	64	SER
1	D	70	ASN
1	D	81	SER
1	D	105	GLN
1	D	157	LYS
1	E	0	LEU
1	E	10	LYS
1	E	19	MET
1	E	25	LYS
1	E	64	SER
1	E	118	ILE
1	E	127	CYS

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Mol	Chain	Res	Type
1	E	132	VAL
1	E	136	GLU
1	E	157	LYS
1	E	186	GLN
1	E	190	CYS
1	E	196	ILE
1	E	207	ARG
1	E	208	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	184	GLN
1	C	15	ASN
1	C	111	HIS
1	C	184	GLN
1	C	186	GLN
1	C	187	HIS
1	D	70	ASN
1	D	105	GLN
1	D	184	GLN
1	E	15	ASN
1	E	184	GLN
1	E	186	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

7 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
2	IM4	A	301	-	15,18,18	3.47	4 (26%)	17,24,24	3.50	7 (41%)
3	IPA	A	404	-	3,3,3	0.20	0	3,3,3	0.74	0
2	IM4	B	302	-	15,18,18	3.13	3 (20%)	17,24,24	2.70	6 (35%)
2	IM4	C	303	-	15,18,18	3.27	5 (33%)	17,24,24	3.39	6 (35%)
3	IPA	C	401	-	3,3,3	0.53	0	3,3,3	0.38	0
2	IM4	D	304	-	15,18,18	3.65	4 (26%)	17,24,24	3.43	9 (52%)
3	IPA	D	402	-	3,3,3	0.77	0	3,3,3	0.31	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
2	IM4	A	301	-	-	0/6/18/18	0/2/2/2
3	IPA	A	404	-	-	0/0/0/0	0/0/0/0
2	IM4	B	302	-	-	0/6/18/18	0/2/2/2
2	IM4	C	303	-	-	0/6/18/18	0/2/2/2
3	IPA	C	401	-	-	0/0/0/0	0/0/0/0
2	IM4	D	304	-	-	0/6/18/18	0/2/2/2
3	IPA	D	402	-	-	0/0/0/0	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	IM4	C1-CL7	-12.28	1.52	1.74
2	D	304	IM4	C1-CL7	-11.99	1.53	1.74
2	C	303	IM4	C1-CL7	-11.32	1.54	1.74
2	B	302	IM4	C1-CL7	-11.08	1.54	1.74
2	C	303	IM4	C8-C4	2.08	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	303	IM4	C6-C1	2.14	1.42	1.37
2	B	302	IM4	C1-N2	2.28	1.37	1.32
2	D	304	IM4	C1-N2	2.36	1.38	1.32
2	B	302	IM4	C3-C4	2.60	1.43	1.38
2	A	301	IM4	C1-N2	2.61	1.38	1.32
2	C	303	IM4	C8-N9	2.62	1.51	1.46
2	C	303	IM4	C1-N2	2.75	1.38	1.32
2	A	301	IM4	C5-C6	2.81	1.43	1.38
2	A	301	IM4	C8-C4	2.96	1.56	1.51
2	D	304	IM4	C8-C4	3.36	1.57	1.51
2	D	304	IM4	C3-C4	3.96	1.45	1.38

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	IM4	C6-C1-N2	-8.04	112.78	124.81
2	C	303	IM4	C6-C1-N2	-5.79	116.14	124.81
2	D	304	IM4	C6-C1-N2	-5.18	117.05	124.81
2	C	303	IM4	C4-C3-N2	-4.90	115.95	123.92
2	B	302	IM4	C6-C1-N2	-4.79	117.64	124.81
2	D	304	IM4	C6-C5-C4	-2.75	117.22	121.02
2	D	304	IM4	C8-C4-C5	-2.56	115.91	120.78
2	B	302	IM4	CL7-C1-N2	2.01	120.27	116.10
2	A	301	IM4	C8-N9-C13	2.04	126.47	120.85
2	B	302	IM4	C8-N9-C13	2.15	126.79	120.85
2	C	303	IM4	C5-C4-C3	2.38	120.42	117.08
2	A	301	IM4	C6-C1-CL7	2.53	124.70	119.20
2	D	304	IM4	C8-C4-C3	2.63	125.75	120.96
2	A	301	IM4	CL7-C1-N2	3.08	122.50	116.10
2	D	304	IM4	C8-N9-C13	3.48	130.45	120.85
2	B	302	IM4	C5-C6-C1	3.53	121.09	117.44
2	A	301	IM4	C5-C6-C1	4.03	121.61	117.44
2	C	303	IM4	CL7-C1-N2	4.07	124.56	116.10
2	D	304	IM4	CL7-C1-N2	4.85	126.18	116.10
2	C	303	IM4	N11-C10-N9	5.07	113.72	109.87
2	B	302	IM4	C3-N2-C1	5.15	123.00	116.37
2	D	304	IM4	C3-N2-C1	5.20	123.06	116.37
2	A	301	IM4	N11-C10-N9	5.22	113.84	109.87
2	D	304	IM4	C5-C6-C1	5.94	123.58	117.44
2	B	302	IM4	N11-C10-N9	6.46	114.77	109.87
2	D	304	IM4	N11-C10-N9	6.73	114.98	109.87
2	A	301	IM4	C3-N2-C1	8.23	126.96	116.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	303	IM4	C3-N2-C1	8.81	127.71	116.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	IM4	4	0
3	A	404	IPA	3	0
2	B	302	IM4	3	0
2	C	303	IM4	2	0
2	D	304	IM4	5	0
3	D	402	IPA	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	211/227 (92%)	-0.21	6 (2%) 53 55	27, 37, 58, 84	0
1	B	212/227 (93%)	-0.21	4 (1%) 67 68	24, 35, 66, 88	0
1	C	208/227 (91%)	-0.24	6 (2%) 52 54	24, 35, 56, 84	0
1	D	212/227 (93%)	-0.22	6 (2%) 53 55	27, 37, 59, 88	0
1	E	211/227 (92%)	-0.16	6 (2%) 53 55	26, 36, 63, 84	0
All	All	1054/1135 (92%)	-0.21	28 (2%) 55 56	24, 36, 63, 88	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	19	MET	5.9
1	B	0	LEU	3.8
1	E	16	ARG	3.7
1	B	19	MET	3.3
1	A	208	ARG	3.3
1	A	0	LEU	3.3
1	C	15	ASN	3.2
1	D	1	HIS	3.2
1	A	14	PHE	3.1
1	D	-3	ASP	3.0
1	E	208	ARG	3.0
1	A	16	ARG	2.9
1	B	17	SER	2.8
1	C	16	ARG	2.8
1	A	19	MET	2.7
1	C	1	HIS	2.6
1	D	208	ARG	2.6
1	E	1	HIS	2.6
1	E	-3	ASP	2.5
1	C	14	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	-2	ASP	2.3
1	C	7	MET	2.3
1	E	189	SER	2.3
1	D	16	ARG	2.3
1	C	0	LEU	2.2
1	B	-2	ASP	2.1
1	D	18	PRO	2.1
1	E	15	ASN	2.1

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	IM4	D	304	17/17	0.86	0.29	3.66	28,45,58,62	0
3	IPA	A	404	4/4	0.94	0.19	3.58	56,56,56,56	0
2	IM4	A	301	17/17	0.82	0.19	2.31	13,35,47,47	0
2	IM4	B	302	17/17	0.83	0.18	2.12	16,34,47,50	0
3	IPA	D	402	4/4	0.93	0.16	1.90	43,44,45,45	0
3	IPA	C	401	4/4	0.97	0.17	1.42	38,38,39,40	0
2	IM4	C	303	17/17	0.83	0.17	1.35	7,32,39,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.