Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:23 PM GMT

PDB ID	:	4XK9
Title	:	Crystal structure of A-AChBP in complex with pinnatoxin G
Authors	:	Bourne, Y.; Sulzenbacher, G.; Marchot, P.
Deposited on	:	2015-01-10
Resolution	:	2.20 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:

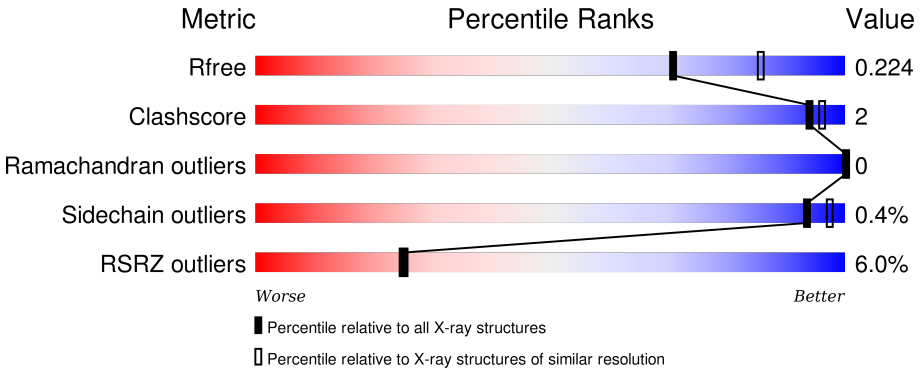
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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 <=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	228	4% 88% • 8%
1	B	228	6% 88% 6% 7%
1	C	228	5% 86% 5% 8%
1	D	228	8% 84% 6% • 9%
1	E	228	4% 89% • 7%

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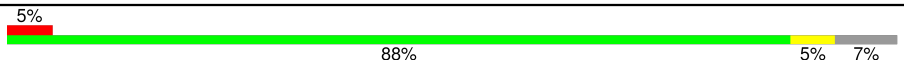
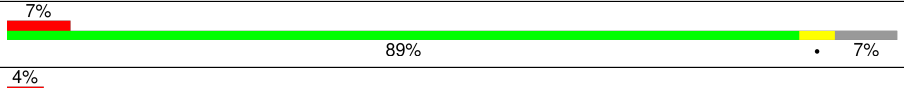
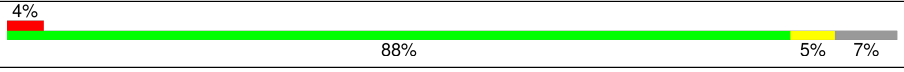
Mol	Chain	Length	Quality of chain
1	F	228	
1	G	228	
1	H	228	
1	I	228	
1	J	228	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18268 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	210	Total	C	N	O	S	0	1	0
			1680	1061	279	331	9			
1	B	213	Total	C	N	O	S	0	2	0
			1702	1075	282	336	9			
1	C	209	Total	C	N	O	S	0	1	0
			1672	1055	278	330	9			
1	D	207	Total	C	N	O	S	0	1	0
			1657	1046	274	328	9			
1	E	212	Total	C	N	O	S	0	1	0
			1691	1068	279	335	9			
1	F	211	Total	C	N	O	S	0	1	0
			1692	1068	281	334	9			
1	G	208	Total	C	N	O	S	0	1	0
			1661	1049	274	329	9			
1	H	212	Total	C	N	O	S	0	1	0
			1693	1070	279	335	9			
1	I	211	Total	C	N	O	S	0	1	0
			1686	1065	278	334	9			
1	J	212	Total	C	N	O	S	0	2	0
			1699	1073	282	335	9			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ASP	-	expression tag	UNP Q8WSF8
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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	ASP	-	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	-8	ASP	-	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
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	-8	ASP	-	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	-8	ASP	-	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
F	-8	ASP	-	expression tag	UNP Q8WSF8
F	-7	TYR	-	expression tag	UNP Q8WSF8
F	-6	LYS	-	expression tag	UNP Q8WSF8
F	-5	ASP	-	expression tag	UNP Q8WSF8
F	-4	ASP	-	expression tag	UNP Q8WSF8
F	-3	ASP	-	expression tag	UNP Q8WSF8

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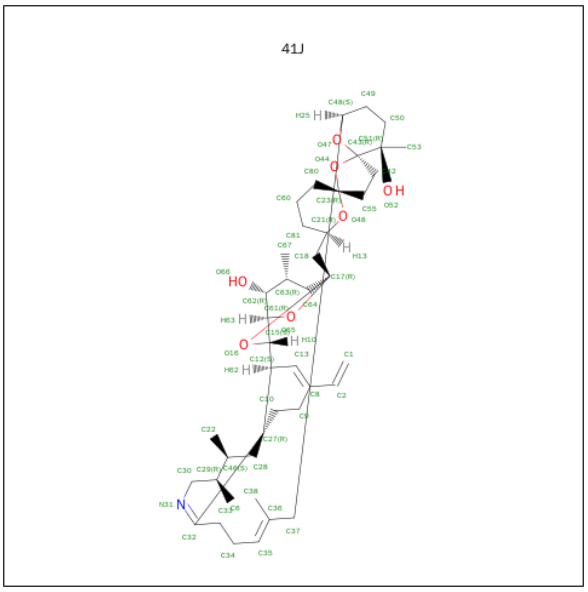
Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	ASP	-	expression tag	UNP Q8WSF8
F	-1	LYS	-	expression tag	UNP Q8WSF8
F	0	LEU	-	expression tag	UNP Q8WSF8
G	-8	ASP	-	expression tag	UNP Q8WSF8
G	-7	TYR	-	expression tag	UNP Q8WSF8
G	-6	LYS	-	expression tag	UNP Q8WSF8
G	-5	ASP	-	expression tag	UNP Q8WSF8
G	-4	ASP	-	expression tag	UNP Q8WSF8
G	-3	ASP	-	expression tag	UNP Q8WSF8
G	-2	ASP	-	expression tag	UNP Q8WSF8
G	-1	LYS	-	expression tag	UNP Q8WSF8
G	0	LEU	-	expression tag	UNP Q8WSF8
H	-8	ASP	-	expression tag	UNP Q8WSF8
H	-7	TYR	-	expression tag	UNP Q8WSF8
H	-6	LYS	-	expression tag	UNP Q8WSF8
H	-5	ASP	-	expression tag	UNP Q8WSF8
H	-4	ASP	-	expression tag	UNP Q8WSF8
H	-3	ASP	-	expression tag	UNP Q8WSF8
H	-2	ASP	-	expression tag	UNP Q8WSF8
H	-1	LYS	-	expression tag	UNP Q8WSF8
H	0	LEU	-	expression tag	UNP Q8WSF8
I	-8	ASP	-	expression tag	UNP Q8WSF8
I	-7	TYR	-	expression tag	UNP Q8WSF8
I	-6	LYS	-	expression tag	UNP Q8WSF8
I	-5	ASP	-	expression tag	UNP Q8WSF8
I	-4	ASP	-	expression tag	UNP Q8WSF8
I	-3	ASP	-	expression tag	UNP Q8WSF8
I	-2	ASP	-	expression tag	UNP Q8WSF8
I	-1	LYS	-	expression tag	UNP Q8WSF8
I	0	LEU	-	expression tag	UNP Q8WSF8
J	-8	ASP	-	expression tag	UNP Q8WSF8
J	-7	TYR	-	expression tag	UNP Q8WSF8
J	-6	LYS	-	expression tag	UNP Q8WSF8
J	-5	ASP	-	expression tag	UNP Q8WSF8
J	-4	ASP	-	expression tag	UNP Q8WSF8
J	-3	ASP	-	expression tag	UNP Q8WSF8
J	-2	ASP	-	expression tag	UNP Q8WSF8
J	-1	LYS	-	expression tag	UNP Q8WSF8
J	0	LEU	-	expression tag	UNP Q8WSF8

- Molecule 2 is Pinnatoxin G (three-letter code: 41J) (formula: $C_{42}H_{63}NO_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			50	42	1	7		
2	B	1	Total	C	N	O	0	0
			50	42	1	7		
2	C	1	Total	C	N	O	0	0
			50	42	1	7		
2	D	1	Total	C	N	O	0	0
			50	42	1	7		
2	E	1	Total	C	N	O	0	0
			50	42	1	7		
2	F	1	Total	C	N	O	0	0
			50	42	1	7		
2	G	1	Total	C	N	O	0	0
			50	42	1	7		
2	H	1	Total	C	N	O	0	0
			50	42	1	7		
2	I	1	Total	C	N	O	0	0
			50	42	1	7		
2	J	1	Total	C	N	O	0	0
			50	42	1	7		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Cl	0	0
			1	1		
3	J	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total Cl 1 1	0	0
3	H	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	A	1	Total Cl 1 1	0	0

- Molecule 4 is water.

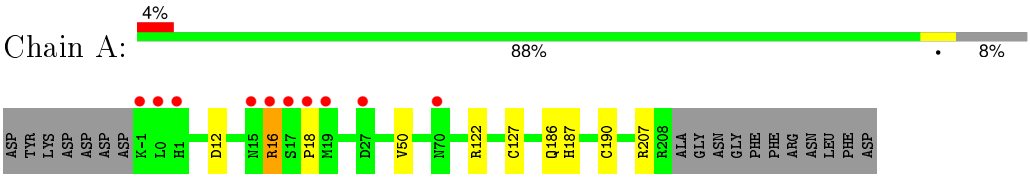
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	93	Total O 93 93	0	0
4	B	88	Total O 88 88	0	0
4	C	91	Total O 91 91	0	0
4	D	79	Total O 79 79	0	0
4	E	108	Total O 108 108	0	0
4	F	81	Total O 81 81	0	0
4	G	118	Total O 118 118	0	0
4	H	102	Total O 102 102	0	0
4	I	74	Total O 74 74	0	0
4	J	94	Total O 94 94	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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.

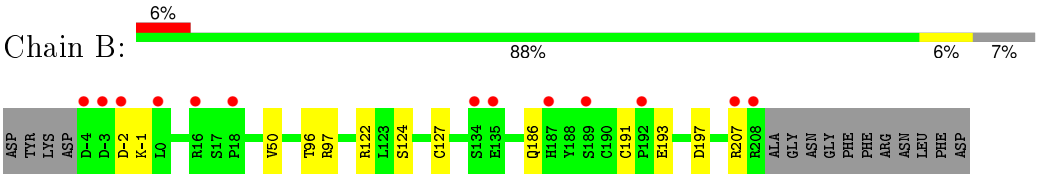
- Molecule 1: Soluble acetylcholine receptor

Chain A:



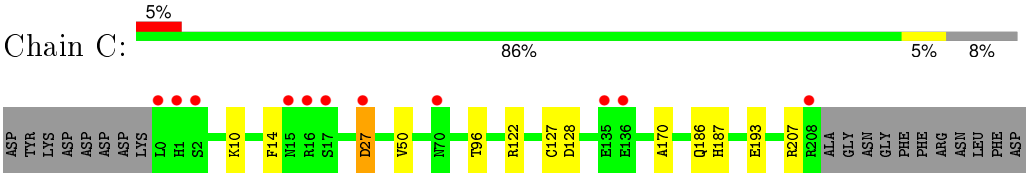
- Molecule 1: Soluble acetylcholine receptor

Chain B:



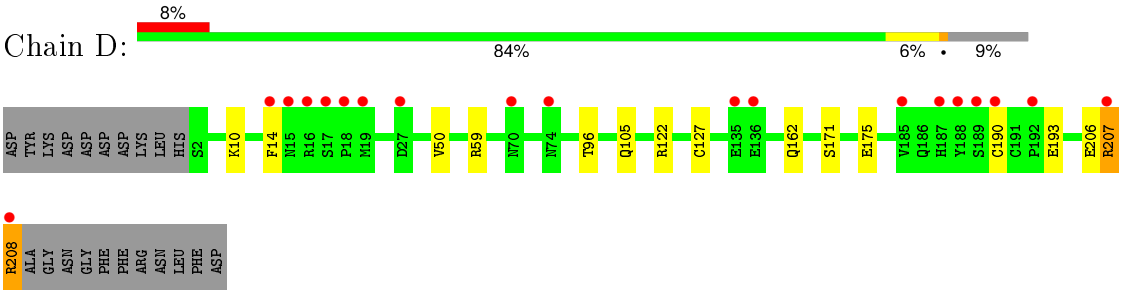
- Molecule 1: Soluble acetylcholine receptor

Chain C:



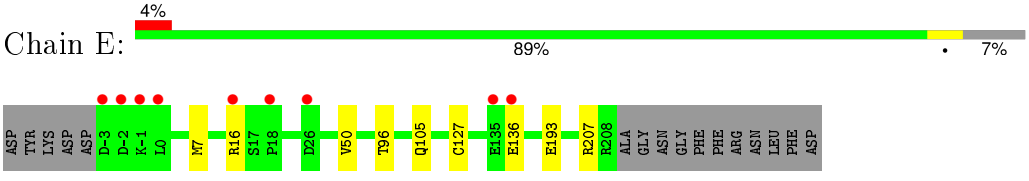
- Molecule 1: Soluble acetylcholine receptor

Chain D:



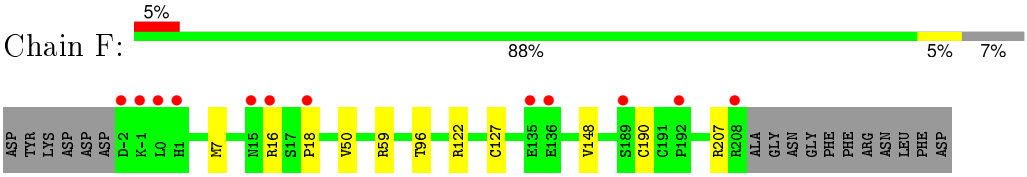
- Molecule 1: Soluble acetylcholine receptor

Chain E:



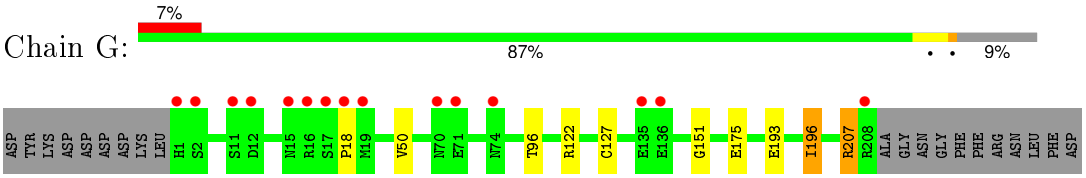
- Molecule 1: Soluble acetylcholine receptor

Chain F:



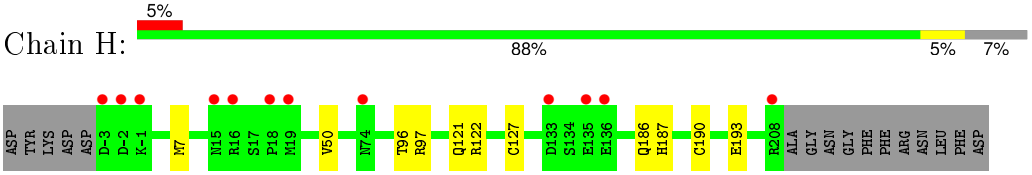
- Molecule 1: Soluble acetylcholine receptor

Chain G:



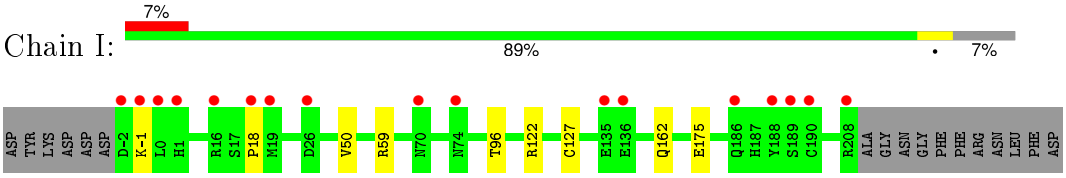
- Molecule 1: Soluble acetylcholine receptor

Chain H:



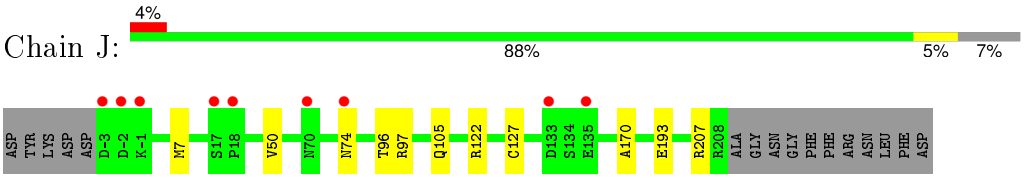
- Molecule 1: Soluble acetylcholine receptor

Chain I:



- Molecule 1: Soluble acetylcholine receptor

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	184.84Å 142.92Å 142.13Å 90.00° 126.48° 90.00°	Depositor
Resolution (Å)	34.00 – 2.20 33.62 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (34.00-2.20) 99.6 (33.62-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.199 , 0.211 0.211 , 0.224	Depositor DCC
R_{free} test set	7513 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	31.8	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	3 of 149549 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18268	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.95 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.2007e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 41J, CL

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	0.48	0/1724	0.79	3/2351 (0.1%)
1	B	0.49	0/1749	0.75	1/2386 (0.0%)
1	C	0.50	0/1716	0.81	1/2340 (0.0%)
1	D	0.58	3/1700 (0.2%)	0.87	7/2318 (0.3%)
1	E	0.50	0/1735	0.77	2/2366 (0.1%)
1	F	0.46	0/1736	0.78	4/2366 (0.2%)
1	G	0.51	0/1705	0.80	4/2326 (0.2%)
1	H	0.50	0/1737	0.76	1/2368 (0.0%)
1	I	0.50	0/1730	0.81	4/2359 (0.2%)
1	J	0.47	0/1746	0.75	0/2380
All	All	0.50	3/17278 (0.0%)	0.79	27/23560 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
1	F	0	1
1	H	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	206	GLU	CD-OE2	-7.70	1.17	1.25
1	D	206	GLU	CD-OE1	7.02	1.33	1.25
1	D	193	GLU	CD-OE1	-6.69	1.18	1.25

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	27	ASP	CB-CG-OD2	10.29	127.56	118.30
1	G	207	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	D	206	GLU	CG-CD-OE1	8.34	134.99	118.30
1	D	206	GLU	CG-CD-OE2	-7.96	102.37	118.30
1	B	-2	ASP	CB-CG-OD1	7.74	125.26	118.30
1	A	16	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	F	16	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	D	207	ARG	N-CA-CB	-6.42	99.05	110.60
1	A	16	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	D	193	GLU	CG-CD-OE2	6.16	130.61	118.30
1	I	-1	LYS	CD-CE-NZ	5.90	125.27	111.70
1	G	175	GLU	CA-CB-CG	5.70	125.93	113.40
1	I	175	GLU	CA-CB-CG	5.68	125.89	113.40
1	D	175	GLU	CA-CB-CG	5.61	125.75	113.40
1	E	207	ARG	CG-CD-NE	5.57	123.51	111.80
1	F	207	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	G	207	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	F	16	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	H	97	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	I	162	GLN	CG-CD-OE1	-5.38	110.84	121.60
1	D	59	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	D	162	GLN	CG-CD-OE1	-5.34	110.92	121.60
1	G	196	ILE	CG1-CB-CG2	-5.30	99.74	111.40
1	E	16	ARG	CG-CD-NE	-5.27	100.74	111.80
1	F	59	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	A	207	ARG	CG-CD-NE	5.19	122.69	111.80
1	I	59	ARG	NE-CZ-NH1	-5.13	117.73	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	190	CYS	Peptide
1	D	190	CYS	Peptide
1	F	190	CYS	Peptide
1	H	190	CYS	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1680	0	1615	5	0
1	B	1702	0	1632	14	0
1	C	1672	0	1604	10	0
1	D	1657	0	1592	8	0
1	E	1691	0	1621	5	0
1	F	1692	0	1630	7	0
1	G	1661	0	1591	8	0
1	H	1693	0	1628	6	0
1	I	1686	0	1619	4	0
1	J	1699	0	1634	10	0
2	A	50	0	63	0	0
2	B	50	0	63	0	0
2	C	50	0	63	0	0
2	D	50	0	63	0	0
2	E	50	0	63	0	0
2	F	50	0	63	1	0
2	G	50	0	63	0	0
2	H	50	0	63	0	0
2	I	50	0	63	0	0
2	J	50	0	63	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	J	1	0	0	0	0
4	A	93	0	0	0	0
4	B	88	0	0	0	0
4	C	91	0	0	0	0
4	D	79	0	0	0	0
4	E	108	0	0	0	0
4	F	81	0	0	0	0
4	G	118	0	0	1	0
4	H	102	0	0	1	0
4	I	74	0	0	0	0
4	J	94	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	18268	0	16796	60	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 2.

All (60) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:ALA:O	1:C:207:ARG:NH1	1.90	1.05
1:J:97[B]:ARG:HH11	1:J:97[B]:ARG:HG2	1.41	0.85
1:J:97[B]:ARG:HH11	1:J:97[B]:ARG:CG	1.97	0.77
1:J:170:ALA:O	1:J:207[B]:ARG:NH1	2.20	0.75
1:F:7:MET:CE	1:G:18:PRO:HB2	2.21	0.70
1:F:7:MET:HE3	1:G:18:PRO:HB2	1.73	0.70
1:B:97[B]:ARG:NH2	1:B:124:SER:OG	2.25	0.69
1:B:-1:LYS:HA	1:C:27:ASP:OD2	1.93	0.68
1:C:170:ALA:C	1:C:207:ARG:HH12	1.98	0.67
1:B:191:CYS:HB3	1:B:193:GLU:OE1	1.95	0.66
1:D:171:SER:HA	1:D:207:ARG:HH22	1.62	0.65
1:B:207:ARG:NH2	1:C:128:ASP:OD2	2.32	0.61
1:B:207:ARG:HH22	1:C:128:ASP:CG	2.05	0.60
1:H:7:MET:SD	1:I:18:PRO:HB2	2.43	0.59
1:A:18:PRO:HB2	1:E:7:MET:SD	2.44	0.57
1:J:97[B]:ARG:NH1	1:J:97[B]:ARG:CG	2.67	0.54
1:A:122:ARG:HD2	1:B:96:THR:O	2.06	0.54
1:B:97[B]:ARG:HH21	1:B:97[B]:ARG:CG	2.20	0.53
1:B:97[B]:ARG:NH2	1:B:124:SER:CB	2.73	0.52
1:G:207:ARG:HD3	4:G:507:HOH:O	2.08	0.52
1:D:122:ARG:HD2	1:E:96:THR:O	2.09	0.52
1:B:97[B]:ARG:HG3	1:B:97[B]:ARG:NH2	2.25	0.52
1:B:97[B]:ARG:HH22	1:B:124:SER:CB	2.23	0.51
1:H:122:ARG:HD2	1:I:96:THR:O	2.11	0.51
1:D:207:ARG:HD3	1:D:208:ARG:HB3	1.92	0.50
1:F:18:PRO:HB2	1:J:7:MET:SD	2.53	0.48
1:I:50:VAL:HG21	1:I:127:CYS:SG	2.54	0.48
1:D:10:LYS:O	1:D:14:PHE:HD1	1.97	0.48
1:I:122:ARG:HD2	1:J:96:THR:O	2.14	0.48
1:J:50:VAL:HG21	1:J:127:CYS:SG	2.54	0.47
1:A:12:ASP:OD1	1:A:16:ARG:NH1	2.47	0.47
1:G:50:VAL:HG21	1:G:127:CYS:SG	2.54	0.47
1:F:50:VAL:HG21	1:F:127:CYS:SG	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:VAL:HG21	1:C:127:CYS:SG	2.55	0.47
1:G:122:ARG:HD2	1:H:96:THR:O	2.14	0.47
1:A:50:VAL:HG21	1:A:127:CYS:SG	2.54	0.47
1:B:122:ARG:HD2	1:C:96:THR:O	2.15	0.47
1:B:50:VAL:HG21	1:B:127:CYS:SG	2.55	0.47
1:F:122:ARG:HD2	1:G:96:THR:O	2.14	0.47
1:D:50:VAL:HG21	1:D:127:CYS:SG	2.54	0.47
1:H:50:VAL:HG21	1:H:127:CYS:SG	2.55	0.46
1:H:186:GLN:HG3	1:H:187:HIS:N	2.29	0.46
1:D:105:GLN:HE21	1:D:105:GLN:HA	1.80	0.46
1:C:186:GLN:HG3	1:C:187:HIS:N	2.31	0.46
1:E:50:VAL:HG21	1:E:127:CYS:SG	2.56	0.46
1:C:10:LYS:O	1:C:14:PHE:HD1	1.98	0.46
1:F:96:THR:O	1:J:122:ARG:HD2	2.16	0.45
1:A:186:GLN:HG3	1:A:187:HIS:N	2.31	0.44
1:J:105:GLN:HA	1:J:105:GLN:HE21	1.83	0.44
1:E:105:GLN:HE21	1:E:105:GLN:HA	1.82	0.44
1:B:186:GLN:OE1	1:B:197:ASP:OD2	2.36	0.44
1:B:97[B]:ARG:HH21	1:B:97[B]:ARG:HG3	1.80	0.43
1:H:121:GLN:OE1	4:H:401:HOH:O	2.21	0.43
1:G:151:GLY:HA3	1:G:196:ILE:CD1	2.48	0.43
1:F:148:VAL:HG12	2:F:301:41J:H48	2.00	0.43
1:G:151:GLY:CA	1:G:196:ILE:CD1	2.97	0.42
1:D:105:GLN:HA	1:D:105:GLN:NE2	2.36	0.41
1:J:97[B]:ARG:NH1	1:J:97[B]:ARG:HG2	2.21	0.41
1:C:122:ARG:HD2	1:D:96:THR:O	2.21	0.40
1:E:105:GLN:NE2	1:E:105:GLN:HA	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	209/228 (92%)	206 (99%)	3 (1%)	0	100	100
1	B	213/228 (93%)	211 (99%)	2 (1%)	0	100	100
1	C	208/228 (91%)	205 (99%)	3 (1%)	0	100	100
1	D	206/228 (90%)	203 (98%)	3 (2%)	0	100	100
1	E	211/228 (92%)	208 (99%)	3 (1%)	0	100	100
1	F	210/228 (92%)	207 (99%)	3 (1%)	0	100	100
1	G	207/228 (91%)	204 (99%)	3 (1%)	0	100	100
1	H	211/228 (92%)	207 (98%)	4 (2%)	0	100	100
1	I	210/228 (92%)	207 (99%)	3 (1%)	0	100	100
1	J	212/228 (93%)	209 (99%)	3 (1%)	0	100	100
All	All	2097/2280 (92%)	2067 (99%)	30 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	191/206 (93%)	191 (100%)	0	100	100
1	B	193/206 (94%)	193 (100%)	0	100	100
1	C	190/206 (92%)	189 (100%)	1 (0%)	92	96
1	D	189/206 (92%)	188 (100%)	1 (0%)	92	96
1	E	192/206 (93%)	190 (99%)	2 (1%)	82	91
1	F	193/206 (94%)	193 (100%)	0	100	100
1	G	189/206 (92%)	188 (100%)	1 (0%)	92	96
1	H	193/206 (94%)	192 (100%)	1 (0%)	92	96
1	I	192/206 (93%)	192 (100%)	0	100	100
1	J	193/206 (94%)	191 (99%)	2 (1%)	82	91
All	All	1915/2060 (93%)	1907 (100%)	8 (0%)	93	97

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	193	GLU
1	D	208	ARG
1	E	136	GLU
1	E	193	GLU
1	G	193	GLU
1	H	193	GLU
1	J	74	ASN
1	J	193	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	57	GLN
1	B	186	GLN
1	D	105	GLN
1	E	105	GLN
1	G	187	HIS
1	H	15	ASN
1	J	74	ASN
1	J	105	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 7 are monoatomic - leaving 10 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	41J	A	301	-	53,57,57	1.84	2 (3%)	48,91,91	1.62	8 (16%)
2	41J	B	301	-	53,57,57	1.83	4 (7%)	48,91,91	1.61	9 (18%)
2	41J	C	301	-	53,57,57	1.82	5 (9%)	48,91,91	1.69	7 (14%)
2	41J	D	301	-	53,57,57	1.84	5 (9%)	48,91,91	1.65	9 (18%)
2	41J	E	301	-	53,57,57	1.84	2 (3%)	48,91,91	1.58	8 (16%)
2	41J	F	301	-	53,57,57	1.86	3 (5%)	48,91,91	1.56	7 (14%)
2	41J	G	301	-	53,57,57	1.80	2 (3%)	48,91,91	1.61	7 (14%)
2	41J	H	301	-	53,57,57	1.82	2 (3%)	48,91,91	1.62	8 (16%)
2	41J	I	301	-	53,57,57	1.89	5 (9%)	48,91,91	1.75	7 (14%)
2	41J	J	301	-	53,57,57	1.79	2 (3%)	48,91,91	1.55	8 (16%)

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	41J	A	301	-	-	0/16/129/129	0/0/8/8
2	41J	B	301	-	-	0/16/129/129	0/0/8/8
2	41J	C	301	-	-	0/16/129/129	0/0/8/8
2	41J	D	301	-	-	0/16/129/129	0/0/8/8
2	41J	E	301	-	-	0/16/129/129	0/0/8/8
2	41J	F	301	-	-	0/16/129/129	0/0/8/8
2	41J	G	301	-	-	0/16/129/129	0/0/8/8
2	41J	H	301	-	-	0/16/129/129	0/0/8/8
2	41J	I	301	-	-	0/16/129/129	0/0/8/8
2	41J	J	301	-	-	0/16/129/129	0/0/8/8

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	41J	C38-C36	-7.72	1.32	1.50
2	E	301	41J	C38-C36	-7.51	1.32	1.50
2	F	301	41J	C38-C36	-7.42	1.32	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	301	41J	C38-C36	-7.31	1.33	1.50
2	H	301	41J	C38-C36	-7.30	1.33	1.50
2	C	301	41J	C38-C36	-7.21	1.33	1.50
2	B	301	41J	C38-C36	-7.19	1.33	1.50
2	G	301	41J	C38-C36	-7.17	1.33	1.50
2	J	301	41J	C38-C36	-7.16	1.33	1.50
2	D	301	41J	C38-C36	-7.15	1.33	1.50
2	B	301	41J	C12-C13	2.01	1.53	1.50
2	D	301	41J	C9-C8	2.02	1.52	1.50
2	D	301	41J	C12-C13	2.04	1.53	1.50
2	C	301	41J	C12-C15	2.05	1.55	1.53
2	B	301	41J	C9-C8	2.13	1.52	1.50
2	D	301	41J	C12-C15	2.14	1.56	1.53
2	I	301	41J	C12-C13	2.20	1.53	1.50
2	F	301	41J	C12-C15	2.22	1.56	1.53
2	I	301	41J	C13-C8	2.23	1.35	1.33
2	C	301	41J	C12-C13	2.25	1.53	1.50
2	I	301	41J	C12-C15	2.31	1.56	1.53
2	C	301	41J	C13-C8	2.45	1.36	1.33
2	C	301	41J	C35-C36	9.47	1.51	1.33
2	B	301	41J	C35-C36	9.59	1.51	1.33
2	J	301	41J	C35-C36	9.65	1.51	1.33
2	A	301	41J	C35-C36	9.73	1.52	1.33
2	H	301	41J	C35-C36	9.76	1.52	1.33
2	D	301	41J	C35-C36	9.77	1.52	1.33
2	F	301	41J	C35-C36	9.78	1.52	1.33
2	G	301	41J	C35-C36	9.80	1.52	1.33
2	I	301	41J	C35-C36	9.91	1.52	1.33
2	E	301	41J	C35-C36	9.99	1.52	1.33

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	41J	C34-C35-C36	-5.69	115.38	127.76
2	G	301	41J	C34-C35-C36	-5.68	115.41	127.76
2	J	301	41J	C34-C35-C36	-5.67	115.44	127.76
2	A	301	41J	C34-C35-C36	-5.61	115.57	127.76
2	D	301	41J	C34-C35-C36	-5.58	115.63	127.76
2	B	301	41J	C34-C35-C36	-5.43	115.96	127.76
2	I	301	41J	C34-C35-C36	-5.31	116.22	127.76
2	F	301	41J	C34-C35-C36	-5.26	116.33	127.76
2	E	301	41J	C34-C35-C36	-5.08	116.72	127.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	301	41J	C34-C35-C36	-5.06	116.76	127.76
2	I	301	41J	C17-O65-C61	-2.58	102.85	107.67
2	E	301	41J	C17-O65-C61	-2.48	103.04	107.67
2	G	301	41J	C17-O65-C61	-2.43	103.13	107.67
2	D	301	41J	C17-O65-C61	-2.26	103.45	107.67
2	A	301	41J	C17-O65-C61	-2.26	103.46	107.67
2	H	301	41J	C17-O65-C61	-2.24	103.49	107.67
2	F	301	41J	C17-O65-C61	-2.18	103.60	107.67
2	C	301	41J	C17-O65-C61	-2.18	103.60	107.67
2	B	301	41J	C17-O65-C61	-2.15	103.66	107.67
2	B	301	41J	C34-C33-C32	2.01	117.43	112.92
2	E	301	41J	C42-C55-C23	2.07	105.77	103.24
2	H	301	41J	C34-C33-C32	2.08	117.60	112.92
2	A	301	41J	C43-O47-C48	2.09	116.34	113.06
2	A	301	41J	C38-C36-C37	2.11	118.51	115.50
2	J	301	41J	C43-O47-C48	2.12	116.40	113.06
2	H	301	41J	C23-O48-C21	2.13	118.05	114.14
2	G	301	41J	C23-O48-C21	2.15	118.08	114.14
2	D	301	41J	C23-O48-C21	2.15	118.08	114.14
2	F	301	41J	C38-C36-C37	2.15	118.57	115.50
2	E	301	41J	C43-O47-C48	2.16	116.45	113.06
2	A	301	41J	C23-O48-C21	2.21	118.21	114.14
2	G	301	41J	C38-C36-C37	2.22	118.67	115.50
2	F	301	41J	C43-O47-C48	2.24	116.58	113.06
2	D	301	41J	C43-O47-C48	2.24	116.59	113.06
2	G	301	41J	C42-C55-C23	2.25	106.00	103.24
2	C	301	41J	O47-C48-C37	2.27	108.01	106.02
2	D	301	41J	C38-C36-C37	2.34	118.84	115.50
2	B	301	41J	C38-C36-C37	2.35	118.86	115.50
2	A	301	41J	C42-C55-C23	2.36	106.12	103.24
2	B	301	41J	C42-C55-C23	2.37	106.14	103.24
2	J	301	41J	C23-O48-C21	2.40	118.55	114.14
2	H	301	41J	C38-C36-C37	2.40	118.93	115.50
2	B	301	41J	O47-C48-C37	2.44	108.16	106.02
2	F	301	41J	C42-C55-C23	2.50	106.30	103.24
2	J	301	41J	C42-C55-C23	2.52	106.33	103.24
2	E	301	41J	C38-C36-C37	2.53	119.11	115.50
2	B	301	41J	C43-O47-C48	2.55	117.07	113.06
2	I	301	41J	C42-C55-C23	2.58	106.40	103.24
2	C	301	41J	C42-C55-C23	2.58	106.40	103.24
2	D	301	41J	C42-C55-C23	2.62	106.44	103.24
2	J	301	41J	O47-C48-C37	2.62	108.32	106.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	41J	C38-C36-C37	2.71	119.36	115.50
2	J	301	41J	C38-C36-C37	2.72	119.38	115.50
2	H	301	41J	C42-C55-C23	2.73	106.58	103.24
2	I	301	41J	C38-C36-C37	2.81	119.51	115.50
2	J	301	41J	O16-C17-C18	2.85	114.47	109.36
2	D	301	41J	O47-C48-C37	2.88	108.55	106.02
2	D	301	41J	O16-C17-C18	3.11	114.94	109.36
2	F	301	41J	O16-C17-C18	3.19	115.08	109.36
2	E	301	41J	O16-C17-C18	3.30	115.28	109.36
2	G	301	41J	O16-C17-C18	3.39	115.44	109.36
2	H	301	41J	O16-C17-C18	3.62	115.85	109.36
2	B	301	41J	O16-C17-C18	3.70	116.00	109.36
2	E	301	41J	O47-C48-C37	3.75	109.31	106.02
2	E	301	41J	O16-C15-C12	3.81	114.63	109.00
2	I	301	41J	O16-C17-C18	3.81	116.20	109.36
2	A	301	41J	O16-C17-C18	3.84	116.25	109.36
2	J	301	41J	O16-C15-C12	3.85	114.69	109.00
2	C	301	41J	O16-C17-C18	4.23	116.96	109.36
2	D	301	41J	O16-C15-C12	4.52	115.69	109.00
2	A	301	41J	O16-C15-C12	4.55	115.72	109.00
2	G	301	41J	O16-C15-C12	4.60	115.80	109.00
2	I	301	41J	O16-C15-C12	4.62	115.84	109.00
2	F	301	41J	O16-C15-C12	4.66	115.89	109.00
2	B	301	41J	O16-C15-C12	4.82	116.13	109.00
2	I	301	41J	O47-C48-C37	4.84	110.27	106.02
2	H	301	41J	O16-C15-C12	5.01	116.41	109.00
2	C	301	41J	O16-C15-C12	5.20	116.69	109.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	41J	1	0

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, 95^{th} 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	210/228 (92%)	0.04	10 (4%)	34 34	25, 44, 98, 138	0
1	B	213/228 (93%)	0.18	13 (6%)	25 24	28, 46, 86, 103	0
1	C	209/228 (91%)	0.05	11 (5%)	30 29	27, 46, 86, 113	0
1	D	207/228 (90%)	0.36	19 (9%)	11 10	26, 50, 90, 122	0
1	E	212/228 (92%)	-0.08	9 (4%)	40 39	24, 39, 75, 106	0
1	F	211/228 (92%)	0.24	12 (5%)	27 27	25, 50, 95, 132	0
1	G	208/228 (91%)	0.13	15 (7%)	18 18	24, 40, 87, 128	0
1	H	212/228 (92%)	-0.00	12 (5%)	27 27	26, 45, 78, 109	0
1	I	211/228 (92%)	0.27	17 (8%)	15 14	27, 51, 96, 140	0
1	J	212/228 (92%)	0.06	9 (4%)	40 39	26, 43, 82, 106	0
All	All	2105/2280 (92%)	0.13	127 (6%)	25 25	24, 46, 89, 140	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	0	LEU	7.3
1	I	-1	LYS	7.1
1	G	1	HIS	6.3
1	D	208	ARG	6.1
1	I	18	PRO	6.1
1	I	-2	ASP	6.0
1	G	18	PRO	5.7
1	A	-1	LYS	5.7
1	D	18	PRO	5.7
1	I	0	LEU	5.6
1	H	208	ARG	5.5
1	F	-2	ASP	5.3
1	C	1	HIS	5.3

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Mol	Chain	Res	Type	RSRZ
1	G	16	ARG	5.3
1	A	0	LEU	5.2
1	D	70	ASN	5.2
1	B	-3	ASP	5.2
1	D	17	SER	5.2
1	B	-2	ASP	5.1
1	G	70	ASN	5.0
1	E	-3	ASP	4.9
1	B	208	ARG	4.9
1	D	16	ARG	4.8
1	H	-3	ASP	4.7
1	G	17	SER	4.5
1	A	1	HIS	4.4
1	D	15	ASN	4.2
1	F	-1	LYS	4.2
1	A	16	ARG	4.2
1	A	70	ASN	4.2
1	F	208	ARG	4.1
1	F	1	HIS	4.0
1	A	15	ASN	4.0
1	I	16	ARG	3.9
1	E	136	GLU	3.8
1	F	16	ARG	3.8
1	A	17	SER	3.8
1	E	0	LEU	3.8
1	G	15	ASN	3.6
1	I	189	SER	3.6
1	J	18	PRO	3.6
1	B	18	PRO	3.5
1	B	-4	ASP	3.5
1	I	190	CYS	3.5
1	J	-3	ASP	3.5
1	G	135	GLU	3.4
1	G	11	SER	3.3
1	G	74	ASN	3.3
1	H	-2	ASP	3.3
1	B	135	GLU	3.3
1	I	1	HIS	3.3
1	E	-2	ASP	3.3
1	D	207	ARG	3.2
1	D	74	ASN	3.2
1	D	189	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	-1	LYS	3.1
1	C	70	ASN	3.1
1	D	19	MET	3.1
1	D	136	GLU	3.1
1	G	136	GLU	3.1
1	D	192	PRO	3.1
1	E	-1	LYS	3.0
1	H	16	ARG	3.0
1	B	0	LEU	3.0
1	I	26	ASP	3.0
1	J	-2	ASP	3.0
1	C	2	SER	3.0
1	I	186	GLN	2.9
1	F	189	SER	2.9
1	I	74	ASN	2.9
1	I	135	GLU	2.9
1	A	27	ASP	2.8
1	C	135	GLU	2.8
1	H	135	GLU	2.8
1	I	70	ASN	2.8
1	J	70	ASN	2.8
1	F	135	GLU	2.8
1	D	135	GLU	2.7
1	G	71	GLU	2.7
1	H	19	MET	2.7
1	E	18	PRO	2.7
1	F	15	ASN	2.7
1	G	19	MET	2.6
1	G	2	SER	2.6
1	C	0	LEU	2.6
1	H	18	PRO	2.5
1	E	135	GLU	2.5
1	J	74	ASN	2.5
1	I	19	MET	2.5
1	C	15	ASN	2.5
1	D	190	CYS	2.5
1	C	208	ARG	2.5
1	E	16	ARG	2.5
1	J	133	ASP	2.4
1	H	136	GLU	2.4
1	C	16	ARG	2.4
1	H	15	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	134	SER	2.3
1	D	188	TYR	2.3
1	D	14	PHE	2.3
1	J	135	GLU	2.3
1	F	136	GLU	2.3
1	I	208	ARG	2.3
1	I	136	GLU	2.3
1	B	187	HIS	2.2
1	D	187	HIS	2.2
1	E	26	ASP	2.2
1	A	19	MET	2.2
1	J	-1	LYS	2.2
1	G	208	ARG	2.2
1	C	17	SER	2.2
1	J	17	SER	2.2
1	F	192	PRO	2.2
1	G	12	ASP	2.1
1	H	133	ASP	2.1
1	B	16	ARG	2.1
1	H	74	ASN	2.1
1	D	185	VAL	2.1
1	B	207	ARG	2.1
1	A	18	PRO	2.1
1	F	18	PRO	2.1
1	I	188	TYR	2.1
1	D	27	ASP	2.1
1	B	189	SER	2.1
1	B	192	PRO	2.1
1	C	136	GLU	2.0
1	C	27	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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
3	CL	C	302	1/1	0.94	0.11	-0.56	45,45,45,45	0
3	CL	A	302	1/1	0.90	0.11	-0.64	48,48,48,48	0
2	41J	D	301	50/50	0.95	0.10	-1.13	28,31,33,34	0
2	41J	H	301	50/50	0.95	0.09	-1.13	20,22,23,24	0
2	41J	A	301	50/50	0.96	0.10	-1.16	20,22,23,24	0
2	41J	I	301	50/50	0.94	0.10	-1.25	28,32,33,34	0
2	41J	B	301	50/50	0.94	0.11	-1.29	27,29,31,32	0
2	41J	C	301	50/50	0.96	0.09	-1.37	21,23,26,27	0
2	41J	G	301	50/50	0.96	0.09	-1.43	22,24,26,26	0
3	CL	H	302	1/1	0.99	0.04	-1.64	35,35,35,35	0
2	41J	F	301	50/50	0.95	0.09	-1.65	23,28,29,31	0
3	CL	G	302	1/1	0.96	0.05	-1.75	44,44,44,44	0
3	CL	J	302	1/1	0.97	0.05	-1.87	40,40,40,40	0
2	41J	J	301	50/50	0.96	0.09	-2.13	23,24,27,28	0
2	41J	E	301	50/50	0.97	0.07	-2.14	22,24,25,26	0
3	CL	B	302	1/1	0.98	0.04	-2.23	39,39,39,39	0
3	CL	E	302	1/1	0.98	0.03	-3.14	34,34,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.