



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:45 PM GMT

PDB ID : 1UX2  
Title : X-RAY STRUCTURE OF ACETYLCHOLINE BINDING PROTEIN (ACHBP)  
Authors : Celie, P.H.N.; Van Rossum-Fikkert, S.E.; Van Dijk, W.J.; Brejc, K.; Smit, A.B.; Sixma, T.K.  
Deposited on : 2004-02-18  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

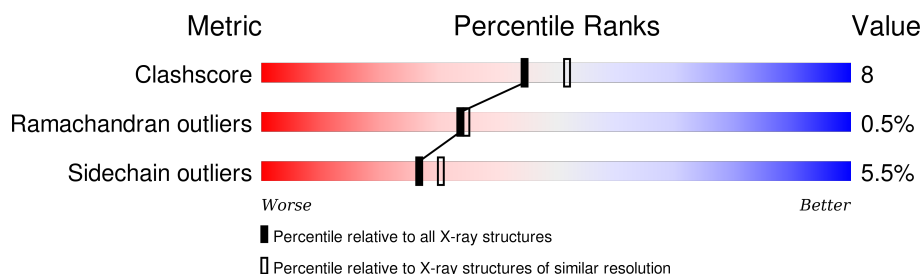
# 1 Overall quality at a glance

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))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	212	
1	B	212	
1	C	212	
1	D	212	
1	E	212	
1	F	212	
1	G	212	

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Mol	Chain	Length	Quality of chain
1	H	212	 77%18% . .
1	I	212	 76%18% . .
1	J	212	 79%17% . .

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	EPE	C	1206	-	-	X	-
2	EPE	J	1206	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18194 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 ACETYLCHOLINE BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1655	1036	282	332	5			
1	B	206	Total	C	N	O	S	0	0	0
			1648	1031	281	331	5			
1	C	207	Total	C	N	O	S	0	0	0
			1655	1036	282	332	5			
1	D	207	Total	C	N	O	S	0	0	0
			1655	1036	282	332	5			
1	E	206	Total	C	N	O	S	0	0	0
			1648	1031	281	331	5			
1	F	207	Total	C	N	O	S	0	0	0
			1655	1036	282	332	5			
1	G	206	Total	C	N	O	S	0	0	0
			1648	1031	281	331	5			
1	H	207	Total	C	N	O	S	0	0	0
			1655	1036	282	332	5			
1	I	206	Total	C	N	O	S	0	0	0
			1648	1031	281	331	5			
1	J	206	Total	C	N	O	S	0	0	0
			1648	1031	281	331	5			

There are 30 discrepancies between the modelled and reference sequences:

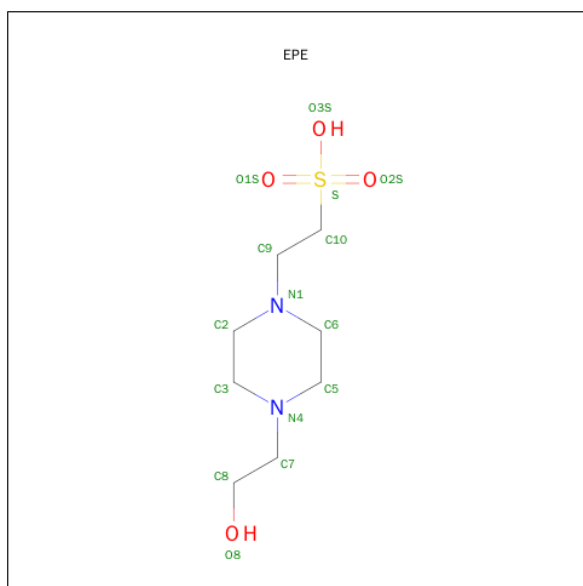
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	VAL	LEU	CONFLICT	UNP P58154
A	0	GLU	SER	CONFLICT	UNP P58154
A	1	PHE	LEU	CONFLICT	UNP P58154
B	-1	VAL	LEU	CONFLICT	UNP P58154
B	0	GLU	SER	CONFLICT	UNP P58154
B	1	PHE	LEU	CONFLICT	UNP P58154
C	-1	VAL	LEU	CONFLICT	UNP P58154
C	0	GLU	SER	CONFLICT	UNP P58154
C	1	PHE	LEU	CONFLICT	UNP P58154

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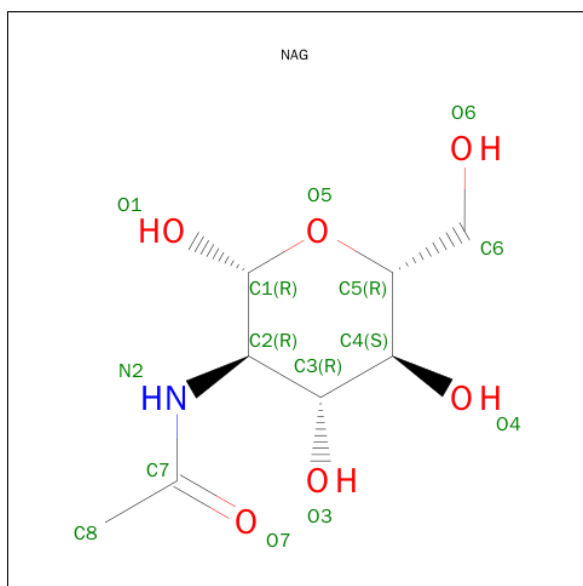
Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	VAL	LEU	CONFLICT	UNP P58154
D	0	GLU	SER	CONFLICT	UNP P58154
D	1	PHE	LEU	CONFLICT	UNP P58154
E	-1	VAL	LEU	CONFLICT	UNP P58154
E	0	GLU	SER	CONFLICT	UNP P58154
E	1	PHE	LEU	CONFLICT	UNP P58154
F	-1	VAL	LEU	CONFLICT	UNP P58154
F	0	GLU	SER	CONFLICT	UNP P58154
F	1	PHE	LEU	CONFLICT	UNP P58154
G	-1	VAL	LEU	CONFLICT	UNP P58154
G	0	GLU	SER	CONFLICT	UNP P58154
G	1	PHE	LEU	CONFLICT	UNP P58154
H	-1	VAL	LEU	CONFLICT	UNP P58154
H	0	GLU	SER	CONFLICT	UNP P58154
H	1	PHE	LEU	CONFLICT	UNP P58154
I	-1	VAL	LEU	CONFLICT	UNP P58154
I	0	GLU	SER	CONFLICT	UNP P58154
I	1	PHE	LEU	CONFLICT	UNP P58154
J	-1	VAL	LEU	CONFLICT	UNP P58154
J	0	GLU	SER	CONFLICT	UNP P58154
J	1	PHE	LEU	CONFLICT	UNP P58154

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	H	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	I	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	J	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		

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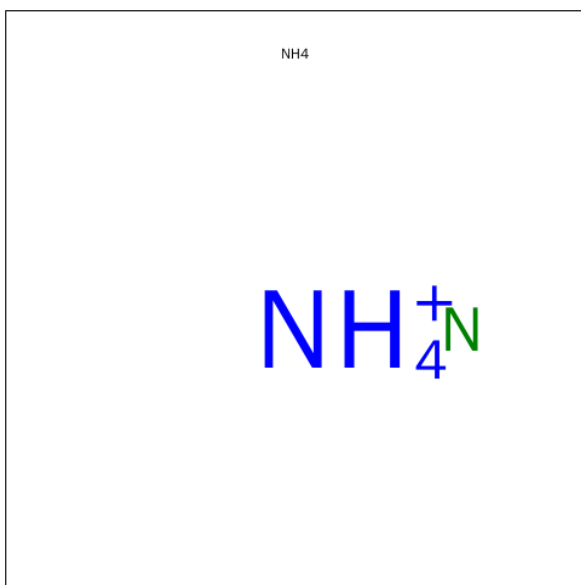
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		
3	I	1	Total	C	N	O	0	0
			14	8	1	5		
3	J	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is AMMONIUM ION (three-letter code: NH4) (formula: H<sub>4</sub>N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total N 1 1	0	0
5	B	1	Total N 1 1	0	0
5	G	1	Total N 1 1	0	0
5	G	1	Total N 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	133	Total O 133 133	0	0
6	B	138	Total O 138 138	0	0
6	C	147	Total O 147 147	0	0
6	D	142	Total O 142 142	0	0
6	E	131	Total O 131 131	0	0
6	F	147	Total O 147 147	0	0
6	G	163	Total O 163 163	0	0
6	H	142	Total O 142 142	0	0

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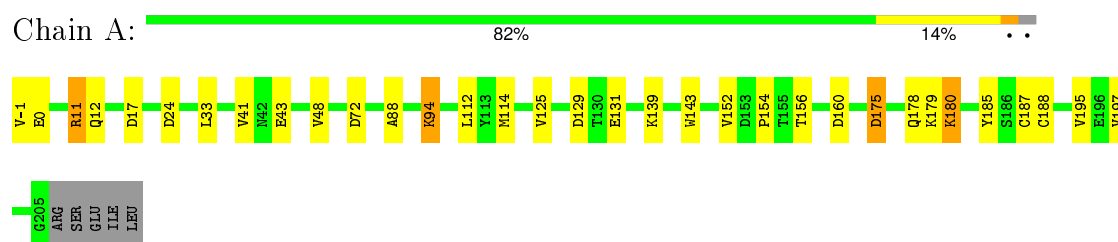
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	138	Total 138	O 138	0	0
6	J	124	Total 124	O 124	0	0

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

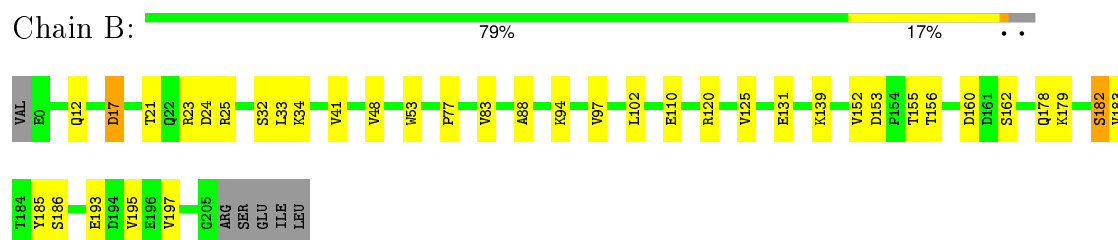
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

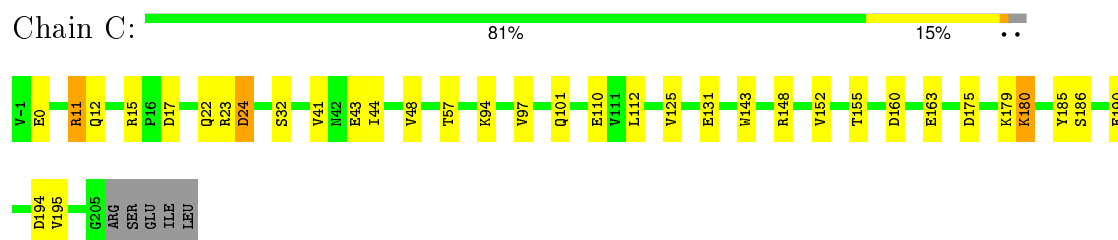
#### • Molecule 1: ACETYLCHOLINE BINDING PROTEIN



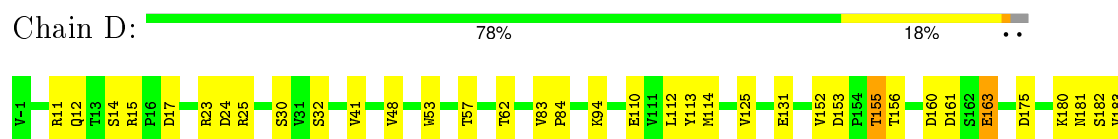
#### • Molecule 1: ACETYLCHOLINE BINDING PROTEIN



#### • Molecule 1: ACETYLCHOLINE BINDING PROTEIN



#### • Molecule 1: ACETYLCHOLINE BINDING PROTEIN





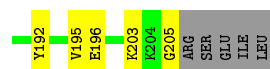
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain E: 78% 17%



• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain F: 79% 17%



• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain G: 77% 18%



• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain H: 77% 18%



• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain I: 76% 18%



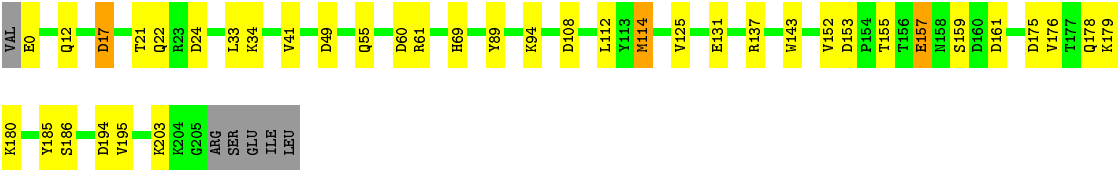
● Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain J: 

79%

17%

••



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.64Å 140.64Å 238.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.20	Depositor
% Data completeness (in resolution range)	84.2 (12.00-2.20)	Depositor
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.236 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18194	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NH4, EPE, NAG, SO4

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	0.59	0/1692	0.79	5/2309 (0.2%)
1	B	0.59	0/1685	0.81	2/2299 (0.1%)
1	C	0.61	0/1692	0.81	4/2309 (0.2%)
1	D	0.58	0/1692	0.79	3/2309 (0.1%)
1	E	0.59	0/1685	0.83	7/2299 (0.3%)
1	F	0.61	0/1692	0.85	7/2309 (0.3%)
1	G	0.63	0/1685	0.84	7/2299 (0.3%)
1	H	0.61	0/1692	0.84	5/2309 (0.2%)
1	I	0.58	0/1685	0.79	4/2299 (0.2%)
1	J	0.58	0/1685	0.84	6/2299 (0.3%)
All	All	0.60	0/16885	0.82	50/23040 (0.2%)

There are no bond length outliers.

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	160	ASP	CB-CG-OD2	8.16	125.65	118.30
1	F	160	ASP	CB-CG-OD2	7.24	124.81	118.30
1	J	153	ASP	CB-CG-OD2	6.79	124.41	118.30
1	G	17	ASP	CB-CG-OD2	6.67	124.30	118.30
1	C	17	ASP	CB-CG-OD2	6.52	124.17	118.30
1	H	17	ASP	CB-CG-OD2	6.23	123.91	118.30
1	F	60	ASP	CB-CG-OD2	6.11	123.80	118.30
1	J	60	ASP	CB-CG-OD2	6.09	123.78	118.30
1	G	161	ASP	CB-CG-OD2	6.09	123.78	118.30
1	G	153	ASP	CB-CG-OD2	6.07	123.76	118.30
1	J	108	ASP	CB-CG-OD2	5.97	123.67	118.30
1	B	17	ASP	CB-CG-OD2	5.95	123.66	118.30
1	E	60	ASP	CB-CG-OD2	5.79	123.52	118.30
1	A	160	ASP	CB-CG-OD2	5.71	123.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	175	ASP	CB-CG-OD2	5.70	123.42	118.30
1	F	175	ASP	CB-CG-OD2	5.67	123.40	118.30
1	C	194	ASP	CB-CG-OD2	5.63	123.37	118.30
1	H	60	ASP	CB-CG-OD2	5.62	123.36	118.30
1	J	194	ASP	CB-CG-OD2	5.62	123.35	118.30
1	D	175	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	72	ASP	CB-CG-OD2	5.56	123.30	118.30
1	J	49	ASP	CB-CG-OD2	5.55	123.30	118.30
1	E	108	ASP	CB-CG-OD2	5.53	123.28	118.30
1	E	153	ASP	CB-CG-OD2	5.53	123.28	118.30
1	C	160	ASP	CB-CG-OD2	5.50	123.25	118.30
1	D	160	ASP	CB-CG-OD2	5.44	123.20	118.30
1	F	161	ASP	CB-CG-OD2	5.43	123.19	118.30
1	E	194	ASP	CB-CG-OD2	5.42	123.18	118.30
1	G	160	ASP	CB-CG-OD2	5.42	123.18	118.30
1	I	17	ASP	CB-CG-OD2	5.42	123.17	118.30
1	I	161	ASP	CB-CG-OD2	5.34	123.11	118.30
1	E	175	ASP	CB-CG-OD2	5.34	123.11	118.30
1	H	72	ASP	CB-CG-OD2	5.33	123.10	118.30
1	F	72	ASP	CB-CG-OD2	5.32	123.09	118.30
1	H	161	ASP	CB-CG-OD2	5.30	123.07	118.30
1	D	161	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	129	ASP	CB-CG-OD2	5.28	123.05	118.30
1	I	194	ASP	CB-CG-OD2	5.28	123.05	118.30
1	F	153	ASP	CB-CG-OD2	5.27	123.05	118.30
1	E	72	ASP	CB-CG-OD2	5.22	123.00	118.30
1	F	104	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	H	153	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	17	ASP	CB-CG-OD2	5.14	122.92	118.30
1	G	49	ASP	CB-CG-OD2	5.11	122.90	118.30
1	I	153	ASP	CB-CG-OD2	5.09	122.88	118.30
1	J	175	ASP	CB-CG-OD2	5.08	122.87	118.30
1	G	72	ASP	CB-CG-OD2	5.07	122.87	118.30
1	C	175	ASP	CB-CG-OD2	5.04	122.83	118.30
1	A	175	ASP	CB-CG-OD2	5.01	122.81	118.30
1	B	160	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	1655	0	1593	19	0
1	B	1648	0	1584	25	1
1	C	1655	0	1593	27	0
1	D	1655	0	1593	30	1
1	E	1648	0	1584	23	1
1	F	1655	0	1593	28	0
1	G	1648	0	1584	27	1
1	H	1655	0	1593	39	0
1	I	1648	0	1584	32	1
1	J	1648	0	1584	20	0
2	A	15	0	17	4	0
2	C	15	0	17	9	0
2	D	15	0	17	1	0
2	E	15	0	17	1	0
2	F	15	0	17	5	0
2	H	15	0	17	5	0
2	I	15	0	17	1	0
2	J	15	0	17	7	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	C	14	0	13	0	0
3	D	14	0	13	0	0
3	E	14	0	13	0	0
3	F	14	0	13	0	0
3	G	14	0	13	0	0
3	H	14	0	13	0	0
3	I	14	0	13	0	0
3	J	14	0	13	2	0
4	B	5	0	0	0	0
4	G	5	0	0	0	0
5	B	2	0	0	0	0
5	G	2	0	0	0	0
6	A	133	0	0	5	0
6	B	138	0	0	6	0
6	C	147	0	0	10	0
6	D	142	0	0	10	0
6	E	131	0	0	6	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	147	0	0	10	0
6	G	163	0	0	13	0
6	H	142	0	0	13	0
6	I	138	0	0	11	0
6	J	124	0	0	10	0
All	All	18194	0	16151	259	4

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 8.

All (259) 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:F:17:ASP:HB3	6:G:2013:HOH:O	1.46	1.11
1:C:57:THR:HB	6:C:2094:HOH:O	1.65	0.95
1:I:112:LEU:HG	6:I:2089:HOH:O	1.65	0.94
1:E:33:LEU:H	1:E:178:GLN:HE22	1.06	0.94
1:A:152:VAL:HG12	1:A:195:VAL:HG23	1.50	0.91
1:D:152:VAL:HG12	1:D:195:VAL:HG23	1.53	0.90
1:J:152:VAL:HG12	1:J:195:VAL:HG23	1.53	0.88
1:H:152:VAL:HG12	1:H:195:VAL:HG23	1.55	0.88
1:I:152:VAL:HG12	1:I:195:VAL:HG23	1.54	0.88
1:I:188:CYS:SG	6:I:2137:HOH:O	2.32	0.87
1:F:152:VAL:HG12	1:F:195:VAL:HG23	1.54	0.87
1:C:152:VAL:HG12	1:C:195:VAL:HG23	1.57	0.86
1:D:17:ASP:HB3	6:D:2026:HOH:O	1.74	0.85
1:B:152:VAL:HG12	1:B:195:VAL:HG23	1.56	0.85
1:E:152:VAL:HG12	1:E:195:VAL:HG23	1.57	0.84
1:I:114:MET:HB2	6:I:2089:HOH:O	1.78	0.83
1:G:152:VAL:HG12	1:G:195:VAL:HG23	1.62	0.82
1:H:61:ARG:CZ	6:H:2050:HOH:O	2.25	0.82
1:C:15:ARG:N	6:C:2024:HOH:O	2.13	0.80
1:H:189:PRO:HG2	1:H:190:GLU:OE2	1.82	0.79
1:F:113:TYR:OH	6:F:2090:HOH:O	2.00	0.78
1:B:25:ARG:HG2	6:B:2035:HOH:O	1.82	0.77
1:E:180:LYS:NZ	1:E:193:GLU:OE1	2.18	0.77
1:J:55:GLN:OE1	6:J:2045:HOH:O	2.02	0.77
1:E:33:LEU:N	1:E:178:GLN:HE22	1.82	0.76
1:I:185:TYR:HE2	1:I:192:TYR:HB2	1.50	0.76
1:H:5:ASP:OD2	6:H:2008:HOH:O	2.04	0.76
1:J:185:TYR:CE1	2:J:1206:EPE:H101	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:34:LYS:HE2	1:H:164:TYR:CE2	2.22	0.75
1:A:11:ARG:HD2	6:A:2014:HOH:O	1.86	0.74
1:A:43:GLU:OE2	6:A:2047:HOH:O	2.04	0.73
1:E:33:LEU:H	1:E:178:GLN:NE2	1.85	0.72
2:A:1206:EPE:H102	1:B:53:TRP:HH2	1.54	0.71
1:D:15:ARG:N	6:D:2023:HOH:O	2.01	0.70
1:J:69:HIS:ND1	6:J:2061:HOH:O	2.24	0.69
1:F:188:CYS:SG	2:F:1206:EPE:H52	2.33	0.69
2:F:1206:EPE:H32	1:G:114:MET:HE3	1.73	0.69
1:H:53:TRP:CZ3	1:H:164:TYR:CD1	2.82	0.67
1:D:205:GLY:O	6:D:2137:HOH:O	2.12	0.67
1:G:3:ARG:HB3	6:G:2034:HOH:O	1.95	0.67
1:A:112:LEU:HD23	6:E:2129:HOH:O	1.95	0.67
1:E:190:GLU:HG2	6:E:2096:HOH:O	1.95	0.67
1:H:17:ASP:OD2	1:I:11:ARG:NH2	2.29	0.66
1:I:15:ARG:N	6:I:2019:HOH:O	2.19	0.65
1:H:53:TRP:CZ3	1:H:164:TYR:CE1	2.85	0.65
1:F:33:LEU:H	1:F:178:GLN:HE22	1.45	0.65
1:F:155:THR:HG22	1:F:156:THR:H	1.62	0.64
1:I:25:ARG:HD2	6:I:2032:HOH:O	1.96	0.64
1:F:178:GLN:HG3	6:F:2120:HOH:O	1.98	0.64
1:I:183:VAL:HB	1:I:185:TYR:CZ	2.33	0.64
1:I:89:TYR:OH	6:I:2077:HOH:O	2.12	0.63
1:C:32:SER:HB2	1:C:155:THR:HB	1.80	0.63
1:F:170:ARG:HD3	6:F:2118:HOH:O	1.99	0.63
1:D:62:THR:HG23	6:D:2029:HOH:O	1.97	0.62
1:J:152:VAL:CG1	1:J:195:VAL:HG23	2.28	0.62
1:F:53:TRP:HH2	2:J:1206:EPE:H102	1.64	0.62
1:D:14:SER:O	6:D:2022:HOH:O	2.16	0.60
1:D:11:ARG:HD3	6:D:2017:HOH:O	2.02	0.60
1:C:110:GLU:HG3	6:C:2094:HOH:O	2.01	0.59
1:J:17:ASP:HB3	6:J:2020:HOH:O	2.02	0.59
1:C:43:GLU:OE2	6:C:2048:HOH:O	2.17	0.59
1:C:22:GLN:HB2	6:C:2033:HOH:O	2.02	0.59
1:B:23:ARG:NH1	6:B:2032:HOH:O	2.31	0.58
6:A:2002:HOH:O	1:H:22:GLN:HG3	2.03	0.58
1:A:152:VAL:CG1	1:A:195:VAL:HG23	2.31	0.58
2:C:1206:EPE:H102	1:D:53:TRP:HH2	1.68	0.58
1:F:94:LYS:HD3	1:G:97:VAL:O	2.06	0.56
2:J:1206:EPE:H31	6:J:2075:HOH:O	2.05	0.56
2:H:1206:EPE:H102	1:I:53:TRP:HH2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:181:ASN:HD21	1:F:196:GLU:HB2	1.70	0.56
1:D:23:ARG:HE	1:D:25:ARG:HH21	1.54	0.55
1:G:189:PRO:HD2	6:G:2148:HOH:O	2.06	0.55
1:H:53:TRP:HZ3	1:H:164:TYR:CE1	2.24	0.55
1:C:185:TYR:CE1	2:C:1206:EPE:H101	2.42	0.55
1:A:185:TYR:CE1	2:A:1206:EPE:H101	2.41	0.55
1:B:32:SER:HB2	1:B:155:THR:HG22	1.87	0.55
1:H:110:GLU:HG3	6:H:2081:HOH:O	2.07	0.55
1:F:23:ARG:HB2	6:F:2028:HOH:O	2.06	0.55
1:H:190:GLU:H	1:H:190:GLU:CD	2.10	0.54
1:F:22:GLN:HG2	1:F:23:ARG:HG2	1.89	0.54
1:J:33:LEU:H	1:J:178:GLN:HE22	1.55	0.54
1:G:129:ASP:HB3	6:G:2113:HOH:O	2.08	0.54
1:I:32:SER:HB2	1:I:155:THR:OG1	2.07	0.53
1:H:53:TRP:HZ3	1:H:164:TYR:HE1	1.57	0.53
1:D:153:ASP:HB2	6:D:2111:HOH:O	2.08	0.53
1:G:137:ARG:NH2	6:G:2117:HOH:O	2.16	0.53
1:G:17:ASP:OD2	1:H:11:ARG:NH2	2.41	0.53
1:D:41:VAL:HG13	1:D:125:VAL:HG11	1.89	0.53
2:A:1206:EPE:H102	1:B:53:TRP:CH2	2.40	0.53
2:D:1206:EPE:H102	1:E:114:MET:HE3	1.91	0.52
1:J:17:ASP:CB	6:J:2020:HOH:O	2.57	0.52
2:C:1206:EPE:H61	1:D:53:TRP:CH2	2.44	0.52
1:H:160:ASP:OD1	1:H:161:ASP:N	2.43	0.52
1:E:41:VAL:HG13	1:E:125:VAL:HG11	1.91	0.51
1:J:41:VAL:HG13	1:J:125:VAL:HG11	1.91	0.51
1:B:83:VAL:HG21	6:B:2008:HOH:O	2.10	0.51
6:D:2138:HOH:O	1:E:112:LEU:HB3	2.10	0.51
1:G:41:VAL:HG13	1:G:125:VAL:HG11	1.91	0.51
1:G:205:GLY:C	6:G:2161:HOH:O	2.48	0.51
1:B:94:LYS:NZ	6:B:2081:HOH:O	2.43	0.51
1:H:185:TYR:CE1	2:H:1206:EPE:H101	2.46	0.51
1:A:-1:VAL:N	6:A:2001:HOH:O	2.42	0.51
1:F:11:ARG:CZ	6:F:2016:HOH:O	2.59	0.51
3:J:1207:NAG:H81	6:J:2124:HOH:O	2.10	0.51
1:H:41:VAL:HG13	1:H:125:VAL:HG11	1.93	0.50
1:D:113:TYR:OH	6:D:2087:HOH:O	2.19	0.50
2:C:1206:EPE:H22	1:D:53:TRP:CZ2	2.46	0.50
1:F:101:GLN:HG2	6:F:2090:HOH:O	2.10	0.50
1:D:32:SER:HB2	1:D:155:THR:OG1	2.12	0.50
1:E:12:GLN:NE2	6:E:2015:HOH:O	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:40:GLU:HB2	6:I:2043:HOH:O	2.12	0.50
1:C:15:ARG:NE	6:C:2022:HOH:O	2.45	0.49
1:A:143:TRP:CZ3	2:A:1206:EPE:H21	2.47	0.49
1:I:41:VAL:HG13	1:I:125:VAL:HG11	1.92	0.49
1:H:61:ARG:NH2	6:H:2050:HOH:O	2.41	0.49
1:J:203:LYS:HE2	6:J:2121:HOH:O	2.11	0.49
1:H:41:VAL:HG22	1:H:48:VAL:HG12	1.93	0.49
1:H:53:TRP:CZ3	1:H:164:TYR:HD1	2.31	0.49
1:G:203:LYS:HE3	6:G:2137:HOH:O	2.13	0.49
2:C:1206:EPE:H61	1:D:53:TRP:HH2	1.78	0.49
1:H:129:ASP:HB2	6:H:2092:HOH:O	2.11	0.49
1:A:41:VAL:HG13	1:A:125:VAL:HG11	1.95	0.49
2:C:1206:EPE:H22	1:D:53:TRP:CH2	2.48	0.48
1:F:181:ASN:ND2	1:F:196:GLU:HB2	2.28	0.48
1:H:94:LYS:HG2	1:I:98:LEU:HA	1.96	0.48
2:C:1206:EPE:H102	1:D:53:TRP:CH2	2.47	0.48
1:E:148:ARG:HD3	6:E:2098:HOH:O	2.13	0.48
1:C:148:ARG:NH2	1:C:190:GLU:OE2	2.46	0.48
1:I:152:VAL:CG1	1:I:195:VAL:HG23	2.35	0.48
1:F:152:VAL:CG1	1:F:195:VAL:HG23	2.36	0.48
1:E:185:TYR:CE1	2:E:1206:EPE:H101	2.49	0.48
1:A:187:CYS:SG	6:B:2117:HOH:O	2.60	0.48
1:B:17:ASP:OD2	1:C:11:ARG:NH2	2.47	0.48
1:G:184:THR:HG21	6:G:2147:HOH:O	2.13	0.48
1:J:34:LYS:HD3	1:J:157:GLU:OE2	2.14	0.48
1:B:41:VAL:HG13	1:B:125:VAL:HG11	1.96	0.47
1:G:34:LYS:HE2	1:G:164:TYR:HE2	1.79	0.47
1:I:83:VAL:CG1	1:I:84:PRO:HD2	2.43	0.47
1:F:-1:VAL:N	6:F:2001:HOH:O	2.47	0.47
1:A:12:GLN:HB3	1:H:12:GLN:HB3	1.97	0.47
1:I:157:GLU:HB3	6:I:2113:HOH:O	2.14	0.47
1:C:44:ILE:HG12	6:C:2046:HOH:O	2.13	0.47
1:B:152:VAL:CG1	1:B:195:VAL:HG23	2.35	0.47
1:C:41:VAL:HG13	1:C:125:VAL:HG11	1.96	0.47
1:I:25:ARG:CD	6:I:2032:HOH:O	2.61	0.47
1:D:41:VAL:HG22	1:D:48:VAL:HG12	1.97	0.47
1:C:180:LYS:HE2	6:C:2140:HOH:O	2.15	0.47
1:C:143:TRP:CZ3	2:C:1206:EPE:H21	2.50	0.47
1:B:183:VAL:HB	1:B:185:TYR:CE1	2.50	0.46
1:G:161:ASP:HB3	1:G:176:VAL:HG23	1.96	0.46
1:B:41:VAL:HG22	1:B:48:VAL:HG12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:179:LYS:HE3	6:H:2140:HOH:O	2.14	0.46
1:C:185:TYR:CE2	2:C:1206:EPE:H51	2.49	0.46
2:F:1206:EPE:C3	1:G:114:MET:HE3	2.45	0.46
1:B:12:GLN:HB3	1:G:12:GLN:HB3	1.97	0.46
1:D:183:VAL:HB	1:D:185:TYR:CZ	2.50	0.46
1:G:41:VAL:HG22	1:G:48:VAL:HG12	1.98	0.46
1:D:152:VAL:CG1	1:D:195:VAL:HG23	2.36	0.46
1:G:15:ARG:NH2	6:G:2020:HOH:O	2.26	0.46
1:H:186:SER:HB2	1:I:163:GLU:OE1	2.16	0.45
1:G:93:SER:HA	6:H:2073:HOH:O	2.15	0.45
1:J:137:ARG:HD3	6:J:2096:HOH:O	2.15	0.45
1:A:188:CYS:HB3	6:A:2123:HOH:O	2.15	0.45
1:C:186:SER:HB3	1:D:163:GLU:OE1	2.17	0.45
1:B:182:SER:HB2	1:B:193:GLU:HG2	1.98	0.45
1:A:88:ALA:HA	1:A:139:LYS:O	2.17	0.45
1:E:152:VAL:CG1	1:E:195:VAL:HG23	2.38	0.45
1:F:192:TYR:CZ	2:F:1206:EPE:H51	2.52	0.45
1:H:111:VAL:C	1:H:112:LEU:HG	2.37	0.45
1:G:11:ARG:NH1	6:G:2014:HOH:O	2.50	0.45
1:H:179:LYS:HE2	6:H:2124:HOH:O	2.17	0.45
1:C:186:SER:CB	1:D:163:GLU:OE1	2.65	0.45
1:C:97:VAL:HG11	1:C:101:GLN:OE1	2.17	0.45
1:I:17:ASP:HB2	6:J:2014:HOH:O	2.16	0.45
1:J:33:LEU:H	1:J:178:GLN:NE2	2.14	0.45
1:A:41:VAL:HG22	1:A:48:VAL:HG12	1.98	0.45
1:E:41:VAL:HG13	1:E:125:VAL:CG1	2.47	0.44
1:H:132:SER:HA	6:H:2093:HOH:O	2.15	0.44
1:G:203:LYS:CE	6:G:2137:HOH:O	2.65	0.44
1:H:185:TYR:CE2	2:H:1206:EPE:H51	2.52	0.44
1:A:187:CYS:SG	1:A:188:CYS:N	2.90	0.44
1:A:33:LEU:HG	1:A:197:VAL:HG21	1.99	0.44
3:J:1207:NAG:H82	6:J:2058:HOH:O	2.18	0.44
1:C:94:LYS:HD2	6:C:2085:HOH:O	2.18	0.44
1:I:41:VAL:HG13	1:I:125:VAL:CG1	2.48	0.44
1:C:41:VAL:HG22	1:C:48:VAL:HG12	2.00	0.44
1:B:185:TYR:N	1:B:185:TYR:CD1	2.86	0.44
1:F:205:GLY:C	6:F:2141:HOH:O	2.55	0.44
1:I:118:ARG:CZ	6:I:2092:HOH:O	2.65	0.44
1:I:30:SER:HB2	1:I:57:THR:OG1	2.18	0.44
1:I:180:LYS:NZ	1:I:193:GLU:OE1	2.35	0.44
1:B:41:VAL:HG13	1:B:125:VAL:CG1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:34:LYS:HE2	1:G:164:TYR:CE2	2.53	0.43
1:B:120:ARG:HG3	1:B:120:ARG:HH11	1.83	0.43
1:I:155:THR:HG22	6:I:2111:HOH:O	2.17	0.43
1:H:41:VAL:HG13	1:H:125:VAL:CG1	2.49	0.43
1:F:53:TRP:CH2	2:J:1206:EPE:H102	2.50	0.43
1:D:83:VAL:CG2	1:D:84:PRO:HD2	2.49	0.43
1:C:152:VAL:CG1	1:C:195:VAL:HG23	2.40	0.43
1:D:41:VAL:HG13	1:D:125:VAL:CG1	2.48	0.43
1:H:94:LYS:CG	1:I:97:VAL:O	2.66	0.43
1:C:11:ARG:CZ	6:C:2015:HOH:O	2.67	0.43
1:G:41:VAL:HG13	1:G:125:VAL:CG1	2.48	0.43
2:H:1206:EPE:H22	1:I:53:TRP:CH2	2.53	0.43
1:F:41:VAL:HG22	1:F:48:VAL:HG12	2.01	0.43
1:H:139:LYS:HD2	6:H:2098:HOH:O	2.18	0.43
1:J:143:TRP:CZ3	2:J:1206:EPE:H21	2.54	0.42
1:B:33:LEU:H	1:B:178:GLN:HE22	1.67	0.42
1:I:154:PRO:HD3	1:I:195:VAL:HG22	2.01	0.42
1:E:188:CYS:HA	1:E:189:PRO:HD3	1.90	0.42
1:H:32:SER:HB2	1:H:155:THR:OG1	2.18	0.42
2:I:1206:EPE:H102	1:J:114:MET:HE3	2.02	0.42
1:J:161:ASP:HB3	1:J:176:VAL:HG23	2.01	0.42
1:C:22:GLN:O	1:C:24:ASP:N	2.53	0.42
2:H:1206:EPE:H102	1:I:53:TRP:CH2	2.53	0.42
1:J:185:TYR:CZ	2:J:1206:EPE:H101	2.55	0.42
1:B:120:ARG:NH1	1:B:120:ARG:HG3	2.34	0.42
1:F:203:LYS:HE2	6:F:2140:HOH:O	2.19	0.42
1:E:203:LYS:HE2	6:E:2113:HOH:O	2.20	0.42
1:C:179:LYS:HG3	1:C:180:LYS:N	2.34	0.42
1:E:120:ARG:HG3	1:E:120:ARG:NH1	2.35	0.42
1:E:25:ARG:CZ	6:E:2030:HOH:O	2.67	0.42
1:G:146:HIS:HD2	6:G:2150:HOH:O	2.02	0.42
1:F:23:ARG:NE	1:F:25:ARG:HE	2.18	0.42
1:G:151:SER:HB3	6:G:2152:HOH:O	2.20	0.42
1:B:33:LEU:HG	1:B:197:VAL:HG21	2.02	0.42
1:E:120:ARG:HG3	1:E:120:ARG:HH11	1.84	0.42
1:F:41:VAL:HG13	1:F:125:VAL:HG11	2.02	0.41
1:E:155:THR:HG22	1:E:156:THR:H	1.85	0.41
1:J:41:VAL:HG13	1:J:125:VAL:CG1	2.50	0.41
1:F:125:VAL:HG12	1:F:125:VAL:O	2.21	0.41
1:D:30:SER:HB2	1:D:57:THR:OG1	2.21	0.41
1:B:34:LYS:HG2	6:B:2051:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:152:VAL:CG1	1:H:195:VAL:HG23	2.39	0.41
1:H:34:LYS:CE	1:H:164:TYR:CE2	3.00	0.41
1:J:89:TYR:CD2	2:J:1206:EPE:H92	2.55	0.41
1:D:125:VAL:O	1:D:125:VAL:HG12	2.21	0.41
1:E:41:VAL:HG22	1:E:48:VAL:HG12	2.02	0.41
1:F:120:ARG:HD2	6:F:2047:HOH:O	2.21	0.41
1:B:77:PRO:HA	1:B:102:LEU:HD23	2.03	0.41
1:A:152:VAL:O	1:A:180:LYS:HE3	2.20	0.41
1:A:41:VAL:HG13	1:A:125:VAL:CG1	2.51	0.41
1:H:88:ALA:HA	1:H:139:LYS:O	2.20	0.41
1:D:181:ASN:O	1:D:193:GLU:HA	2.20	0.41
1:C:12:GLN:HB3	1:F:12:GLN:HB3	2.03	0.41
1:G:33:LEU:HG	1:G:197:VAL:HG21	2.03	0.41
1:I:181:ASN:HB2	1:I:194:ASP:OD2	2.21	0.41
2:F:1206:EPE:O3S	1:G:53:TRP:HH2	2.04	0.41
1:D:12:GLN:HB3	1:J:12:GLN:HB3	2.02	0.41
1:B:88:ALA:HA	1:B:139:LYS:O	2.21	0.41
1:C:41:VAL:HG13	1:C:125:VAL:CG1	2.50	0.40
1:I:33:LEU:HG	1:I:197:VAL:HG21	2.03	0.40
1:D:14:SER:HA	6:D:2023:HOH:O	2.21	0.40
1:E:30:SER:HB2	1:E:57:THR:OG1	2.22	0.40
1:H:57:THR:HB	6:H:2081:HOH:O	2.21	0.40
1:E:33:LEU:HG	1:E:197:VAL:HG21	2.04	0.40
1:H:189:PRO:HD3	6:H:2133:HOH:O	2.22	0.40
1:A:94:LYS:HD3	1:B:97:VAL:O	2.21	0.40
1:H:163:GLU:N	6:H:2114:HOH:O	2.53	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:2053:HOH:O	6:E:2053:HOH:O[8_665]	1.35	0.85
1:G:129:ASP:OD2	1:G:129:ASP:OD2[7_556]	2.05	0.15
1:D:25:ARG:NH1	1:I:24:ASP:OD2[8_665]	2.09	0.11
1:B:25:ARG:NH2	1:E:132:SER:CB[5_545]	2.16	0.04

## 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	205/212 (97%)	201 (98%)	3 (2%)	1 (0%)	34	35
1	B	204/212 (96%)	200 (98%)	4 (2%)	0	100	100
1	C	205/212 (97%)	200 (98%)	4 (2%)	1 (0%)	34	35
1	D	205/212 (97%)	204 (100%)	1 (0%)	0	100	100
1	E	204/212 (96%)	201 (98%)	3 (2%)	0	100	100
1	F	205/212 (97%)	201 (98%)	3 (2%)	1 (0%)	34	35
1	G	204/212 (96%)	200 (98%)	3 (2%)	1 (0%)	34	35
1	H	205/212 (97%)	196 (96%)	6 (3%)	3 (2%)	13	9
1	I	204/212 (96%)	203 (100%)	0	1 (0%)	34	35
1	J	204/212 (96%)	200 (98%)	2 (1%)	2 (1%)	19	16
All	All	2045/2120 (96%)	2006 (98%)	29 (1%)	10 (0%)	34	35

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	23	ARG
1	F	23	ARG
1	H	157	GLU
1	J	159	SER
1	H	156	THR
1	J	157	GLU
1	G	157	GLU
1	I	155	THR
1	H	159	SER
1	A	154	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	193/198 (98%)	182 (94%)	11 (6%)	25	29
1	B	192/198 (97%)	182 (95%)	10 (5%)	29	33
1	C	193/198 (98%)	186 (96%)	7 (4%)	42	52
1	D	193/198 (98%)	181 (94%)	12 (6%)	23	25
1	E	192/198 (97%)	180 (94%)	12 (6%)	22	24
1	F	193/198 (98%)	184 (95%)	9 (5%)	32	39
1	G	192/198 (97%)	182 (95%)	10 (5%)	29	33
1	H	193/198 (98%)	184 (95%)	9 (5%)	32	39
1	I	192/198 (97%)	180 (94%)	12 (6%)	22	24
1	J	192/198 (97%)	178 (93%)	14 (7%)	17	18
All	All	1925/1980 (97%)	1819 (94%)	106 (6%)	27	30

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	GLU
1	A	11	ARG
1	A	24	ASP
1	A	94	LYS
1	A	114	MET
1	A	131	GLU
1	A	156	THR
1	A	175	ASP
1	A	178	GLN
1	A	179	LYS
1	A	180	LYS
1	B	21	THR
1	B	24	ASP
1	B	110	GLU
1	B	131	GLU
1	B	153	ASP

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Mol	Chain	Res	Type
1	B	156	THR
1	B	162	SER
1	B	179	LYS
1	B	182	SER
1	B	186	SER
1	C	0	GLU
1	C	11	ARG
1	C	24	ASP
1	C	112	LEU
1	C	131	GLU
1	C	163	GLU
1	C	180	LYS
1	D	24	ASP
1	D	94	LYS
1	D	110	GLU
1	D	112	LEU
1	D	114	MET
1	D	131	GLU
1	D	155	THR
1	D	156	THR
1	D	163	GLU
1	D	180	LYS
1	D	182	SER
1	D	188	CYS
1	E	0	GLU
1	E	11	ARG
1	E	24	ASP
1	E	94	LYS
1	E	131	GLU
1	E	156	THR
1	E	175	ASP
1	E	180	LYS
1	E	182	SER
1	E	186	SER
1	E	188	CYS
1	E	190	GLU
1	F	11	ARG
1	F	17	ASP
1	F	21	THR
1	F	24	ASP
1	F	94	LYS
1	F	114	MET

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Mol	Chain	Res	Type
1	F	131	GLU
1	F	160	ASP
1	F	186	SER
1	G	23	ARG
1	G	24	ASP
1	G	94	LYS
1	G	112	LEU
1	G	131	GLU
1	G	155	THR
1	G	161	ASP
1	G	163	GLU
1	G	175	ASP
1	G	180	LYS
1	H	11	ARG
1	H	21	THR
1	H	24	ASP
1	H	94	LYS
1	H	110	GLU
1	H	112	LEU
1	H	131	GLU
1	H	162	SER
1	H	180	LYS
1	I	0	GLU
1	I	11	ARG
1	I	24	ASP
1	I	61	ARG
1	I	94	LYS
1	I	131	GLU
1	I	153	ASP
1	I	155	THR
1	I	160	ASP
1	I	179	LYS
1	I	180	LYS
1	I	186	SER
1	J	0	GLU
1	J	17	ASP
1	J	21	THR
1	J	22	GLN
1	J	24	ASP
1	J	61	ARG
1	J	94	LYS
1	J	112	LEU

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Mol	Chain	Res	Type
1	J	114	MET
1	J	131	GLU
1	J	155	THR
1	J	179	LYS
1	J	180	LYS
1	J	186	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	178	GLN
1	J	178	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 24 ligands modelled in this entry, 4 are modelled with single atom - leaving 20 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	EPE	A	1206	-	14,15,15	0.52	0	18,20,20	2.30	7 (38%)
3	NAG	A	1207	1	14,14,15	0.64	0	15,19,21	1.53	4 (26%)
4	SO4	B	1206	-	4,4,4	0.17	0	6,6,6	0.16	0
3	NAG	B	1209	1	14,14,15	0.70	0	15,19,21	1.85	3 (20%)
2	EPE	C	1206	-	14,15,15	0.47	0	18,20,20	2.42	7 (38%)
3	NAG	C	1207	1	14,14,15	0.36	0	15,19,21	1.63	3 (20%)
2	EPE	D	1206	-	14,15,15	0.46	0	18,20,20	2.06	4 (22%)
3	NAG	D	1207	1	14,14,15	0.62	0	15,19,21	1.04	0
2	EPE	E	1206	-	14,15,15	0.49	0	18,20,20	2.02	5 (27%)
3	NAG	E	1207	1	14,14,15	0.66	0	15,19,21	1.30	3 (20%)
2	EPE	F	1206	-	14,15,15	0.34	0	18,20,20	2.20	5 (27%)
3	NAG	F	1207	1	14,14,15	0.53	0	15,19,21	1.47	3 (20%)
4	SO4	G	1206	-	4,4,4	0.11	0	6,6,6	0.19	0
3	NAG	G	1209	1	14,14,15	0.53	0	15,19,21	0.89	1 (6%)
2	EPE	H	1206	-	14,15,15	0.45	0	18,20,20	2.33	7 (38%)
3	NAG	H	1207	1	14,14,15	0.58	0	15,19,21	1.32	1 (6%)
2	EPE	I	1206	-	14,15,15	0.48	0	18,20,20	2.13	5 (27%)
3	NAG	I	1207	1	14,14,15	0.58	0	15,19,21	1.36	1 (6%)
2	EPE	J	1206	-	14,15,15	0.52	0	18,20,20	2.33	7 (38%)
3	NAG	J	1207	1	14,14,15	0.44	0	15,19,21	1.55	2 (13%)

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	EPE	A	1206	-	-	0/9/19/19	0/1/1/1
3	NAG	A	1207	1	-	0/6/23/26	0/1/1/1
4	SO4	B	1206	-	-	0/0/0/0	0/0/0/0
3	NAG	B	1209	1	-	0/6/23/26	0/1/1/1
2	EPE	C	1206	-	-	0/9/19/19	0/1/1/1
3	NAG	C	1207	1	-	0/6/23/26	0/1/1/1
2	EPE	D	1206	-	-	0/9/19/19	0/1/1/1
3	NAG	D	1207	1	-	0/6/23/26	0/1/1/1
2	EPE	E	1206	-	-	0/9/19/19	0/1/1/1
3	NAG	E	1207	1	-	1/6/23/26	0/1/1/1
2	EPE	F	1206	-	-	0/9/19/19	0/1/1/1
3	NAG	F	1207	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	G	1206	-	-	0/0/0/0	0/0/0/0
3	NAG	G	1209	1	-	0/6/23/26	0/1/1/1
2	EPE	H	1206	-	-	0/9/19/19	0/1/1/1
3	NAG	H	1207	1	-	0/6/23/26	0/1/1/1
2	EPE	I	1206	-	-	0/9/19/19	0/1/1/1
3	NAG	I	1207	1	-	1/6/23/26	0/1/1/1
2	EPE	J	1206	-	-	0/9/19/19	0/1/1/1
3	NAG	J	1207	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1207	NAG	C4-C3-C2	-2.74	106.96	111.23
3	F	1207	NAG	C2-N2-C7	-2.61	119.69	123.04
3	G	1209	NAG	C2-N2-C7	-2.50	119.83	123.04
3	E	1207	NAG	O3-C3-C4	-2.33	105.09	110.34
3	F	1207	NAG	C4-C3-C2	-2.32	107.62	111.23
3	A	1207	NAG	O7-C7-C8	-2.08	118.25	122.06
2	E	1206	EPE	O2S-S-C10	2.01	108.62	106.91
3	E	1207	NAG	O5-C5-C6	2.11	111.92	107.35
2	I	1206	EPE	C7-N4-C5	2.16	116.80	111.27
2	J	1206	EPE	C6-C5-N4	2.21	114.59	110.63
2	D	1206	EPE	C7-N4-C5	2.22	116.97	111.27
2	A	1206	EPE	C2-C3-N4	2.22	114.61	110.63
2	D	1206	EPE	C7-N4-C3	2.23	116.98	111.27
3	H	1207	NAG	C8-C7-N2	2.23	120.38	116.11
2	H	1206	EPE	C6-C5-N4	2.25	114.66	110.63
2	I	1206	EPE	C7-N4-C3	2.29	117.15	111.27
3	A	1207	NAG	C3-C4-C5	2.33	114.26	110.20
2	J	1206	EPE	O1S-S-C10	2.39	108.94	106.91
3	A	1207	NAG	C1-O5-C5	2.41	115.31	112.25
2	J	1206	EPE	C2-C3-N4	2.42	114.97	110.63
3	F	1207	NAG	C1-O5-C5	2.50	115.42	112.25
2	A	1206	EPE	C7-N4-C5	2.51	117.70	111.27
2	I	1206	EPE	C6-C5-N4	2.52	115.15	110.63
3	C	1207	NAG	C4-C3-C2	2.53	115.17	111.23
2	A	1206	EPE	C6-C5-N4	2.53	115.16	110.63
3	A	1207	NAG	C2-N2-C7	2.54	126.31	123.04
2	C	1206	EPE	C2-C3-N4	2.55	115.19	110.63
2	H	1206	EPE	C7-N4-C5	2.65	118.06	111.27
2	F	1206	EPE	O1S-S-C10	2.65	109.17	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1207	NAG	C1-O5-C5	2.66	115.63	112.25
2	J	1206	EPE	C7-N4-C5	2.72	118.23	111.27
2	E	1206	EPE	C7-N4-C3	2.73	118.28	111.27
2	J	1206	EPE	C7-N4-C3	2.79	118.41	111.27
2	A	1206	EPE	O2S-S-C10	2.79	109.29	106.91
2	H	1206	EPE	O1S-S-C10	2.80	109.29	106.91
2	C	1206	EPE	C7-N4-C5	2.80	118.45	111.27
3	E	1207	NAG	C4-C3-C2	2.91	115.76	111.23
2	F	1206	EPE	C2-C3-N4	2.92	115.85	110.63
2	C	1206	EPE	C6-C5-N4	3.00	116.00	110.63
2	H	1206	EPE	C2-C3-N4	3.03	116.05	110.63
3	C	1207	NAG	C3-C4-C5	3.05	115.51	110.20
3	B	1209	NAG	C4-C3-C2	3.06	115.98	111.23
2	H	1206	EPE	C7-N4-C3	3.07	119.14	111.27
2	F	1206	EPE	C7-N4-C3	3.08	119.17	111.27
2	C	1206	EPE	C7-N4-C3	3.16	119.37	111.27
2	A	1206	EPE	C7-N4-C3	3.18	119.42	111.27
3	B	1209	NAG	C3-C4-C5	3.33	116.00	110.20
2	C	1206	EPE	O2S-S-C10	3.40	109.81	106.91
3	C	1207	NAG	C1-O5-C5	3.42	116.59	112.25
2	F	1206	EPE	C6-C5-N4	3.44	116.79	110.63
2	E	1206	EPE	C7-N4-C5	3.56	120.39	111.27
2	C	1206	EPE	O1S-S-C10	3.66	110.03	106.91
2	E	1206	EPE	O1S-S-C10	3.93	110.26	106.91
2	H	1206	EPE	O2S-S-C10	4.00	110.31	106.91
2	A	1206	EPE	O1S-S-C10	4.03	110.35	106.91
3	J	1207	NAG	C1-O5-C5	4.11	117.47	112.25
2	J	1206	EPE	O2S-S-C10	4.15	110.45	106.91
3	B	1209	NAG	C2-N2-C7	4.33	128.60	123.04
2	E	1206	EPE	C5-N4-C3	4.85	119.39	108.90
2	I	1206	EPE	C5-N4-C3	4.93	119.59	108.90
2	D	1206	EPE	C5-N4-C3	4.99	119.70	108.90
2	I	1206	EPE	O1S-S-C10	5.39	111.50	106.91
2	D	1206	EPE	O1S-S-C10	5.54	111.63	106.91
2	H	1206	EPE	C5-N4-C3	5.71	121.26	108.90
2	F	1206	EPE	C5-N4-C3	5.89	121.66	108.90
2	A	1206	EPE	C5-N4-C3	5.92	121.71	108.90
2	C	1206	EPE	C5-N4-C3	6.04	121.99	108.90
2	J	1206	EPE	C5-N4-C3	6.22	122.38	108.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1207	NAG	O7-C7-N2-C2
3	I	1207	NAG	O7-C7-N2-C2

There are no ring outliers.

9 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1206	EPE	4	0
2	C	1206	EPE	9	0
2	D	1206	EPE	1	0
2	E	1206	EPE	1	0
2	F	1206	EPE	5	0
2	H	1206	EPE	5	0
2	I	1206	EPE	1	0
2	J	1206	EPE	7	0
3	J	1207	NAG	2	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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.