



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:45 am BST

PDB ID : 2XZ6
Title : MTSET-modified Y53C mutant of Aplysia AChBP
Authors : Brams, M.; Gay, E.A.; Colon Saez, J.; Guskov, A.; Van Elk, R.; Van Der Schors, R.C.; Peigneur, S.; Tytgat, J.; Strelkov, S.V.; Smit, A.B.; Yakel, J.L.; Ulens, C.
Deposited on : 2010-11-23
Resolution : 3.14 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

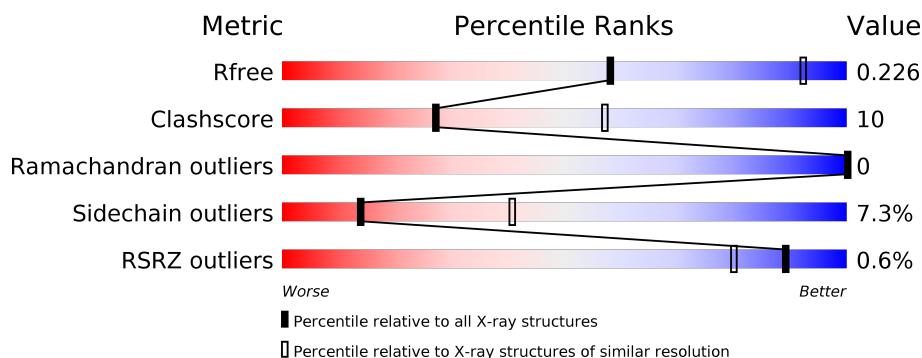
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.14 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}	130704	1626 (3.18-3.10)
Clashscore	141614	1735 (3.18-3.10)
Ramachandran outliers	138981	1677 (3.18-3.10)
Sidechain outliers	138945	1677 (3.18-3.10)
RSRZ outliers	127900	1588 (3.18-3.10)

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 respectively. 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	217	
1	B	217	
1	C	217	
1	D	217	
1	E	217	
1	F	217	

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Mol	Chain	Length	Quality of chain
1	G	217	
1	H	217	
1	I	217	
1	J	217	

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	ETM	E	1206	-	-	-	X
2	ETM	G	1206	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16380 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	206	Total	C	N	O	S	0	0	1
			1631	1030	267	324	10			
1	B	206	Total	C	N	O	S	0	0	1
			1631	1030	267	324	10			
1	C	206	Total	C	N	O	S	0	0	1
			1631	1030	267	324	10			
1	D	206	Total	C	N	O	S	0	0	1
			1631	1030	267	324	10			
1	E	206	Total	C	N	O	S	0	0	1
			1631	1030	267	324	10			
1	F	206	Total	C	N	O	S	0	0	1
			1631	1030	267	324	10			
1	G	206	Total	C	N	O	S	0	0	1
			1631	1030	267	324	10			
1	H	206	Total	C	N	O	S	0	0	1
			1631	1030	267	324	10			
1	I	206	Total	C	N	O	S	0	0	1
			1631	1030	267	324	10			
1	J	206	Total	C	N	O	S	0	0	1
			1631	1030	267	324	10			

There are 30 discrepancies between the modelled and reference sequences:

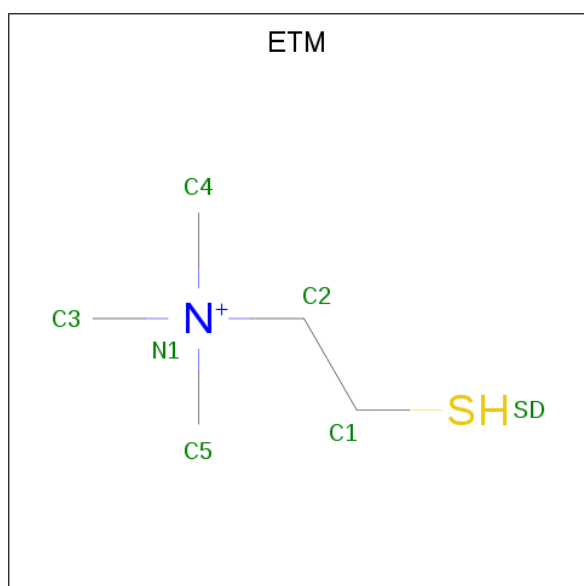
Chain	Residue	Modelled	Actual	Comment	Reference
A	41	VAL	ALA	conflict	UNP Q8WSF8
A	53	CYS	TYR	engineered mutation	UNP Q8WSF8
A	136	VAL	ALA	conflict	UNP Q8WSF8
B	41	VAL	ALA	conflict	UNP Q8WSF8
B	53	CYS	TYR	engineered mutation	UNP Q8WSF8
B	136	VAL	ALA	conflict	UNP Q8WSF8
C	41	VAL	ALA	conflict	UNP Q8WSF8
C	53	CYS	TYR	engineered mutation	UNP Q8WSF8
C	136	VAL	ALA	conflict	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	41	VAL	ALA	conflict	UNP Q8WSF8
D	53	CYS	TYR	engineered mutation	UNP Q8WSF8
D	136	VAL	ALA	conflict	UNP Q8WSF8
E	41	VAL	ALA	conflict	UNP Q8WSF8
E	53	CYS	TYR	engineered mutation	UNP Q8WSF8
E	136	VAL	ALA	conflict	UNP Q8WSF8
F	41	VAL	ALA	conflict	UNP Q8WSF8
F	53	CYS	TYR	engineered mutation	UNP Q8WSF8
F	136	VAL	ALA	conflict	UNP Q8WSF8
G	41	VAL	ALA	conflict	UNP Q8WSF8
G	53	CYS	TYR	engineered mutation	UNP Q8WSF8
G	136	VAL	ALA	conflict	UNP Q8WSF8
H	41	VAL	ALA	conflict	UNP Q8WSF8
H	53	CYS	TYR	engineered mutation	UNP Q8WSF8
H	136	VAL	ALA	conflict	UNP Q8WSF8
I	41	VAL	ALA	conflict	UNP Q8WSF8
I	53	CYS	TYR	engineered mutation	UNP Q8WSF8
I	136	VAL	ALA	conflict	UNP Q8WSF8
J	41	VAL	ALA	conflict	UNP Q8WSF8
J	53	CYS	TYR	engineered mutation	UNP Q8WSF8
J	136	VAL	ALA	conflict	UNP Q8WSF8

- Molecule 2 is 2-(TRIMETHYLAMMONIUM)ETHYL THIOL (three-letter code: ETM) (formula: C₅H₁₄NS).



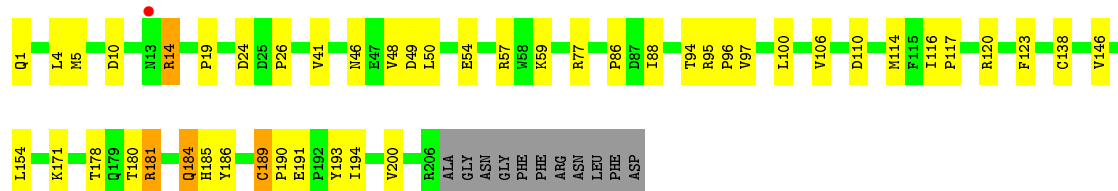
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	S	0	0
			7	5	1	1		
2	B	1	Total	C	N	S	0	0
			7	5	1	1		
2	C	1	Total	C	N	S	0	0
			7	5	1	1		
2	D	1	Total	C	N	S	0	0
			7	5	1	1		
2	E	1	Total	C	N	S	0	0
			7	5	1	1		
2	F	1	Total	C	N	S	0	0
			7	5	1	1		
2	G	1	Total	C	N	S	0	0
			7	5	1	1		
2	H	1	Total	C	N	S	0	0
			7	5	1	1		
2	I	1	Total	C	N	S	0	0
			7	5	1	1		
2	J	1	Total	C	N	S	0	0
			7	5	1	1		

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.

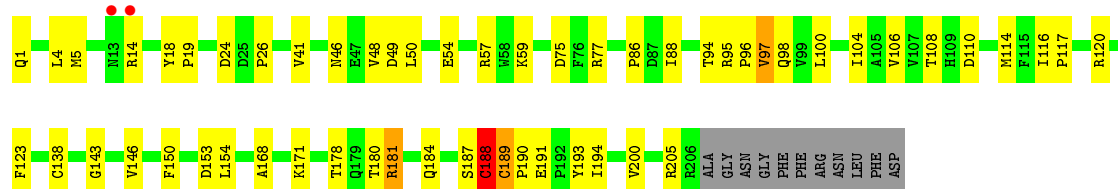
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain A: 



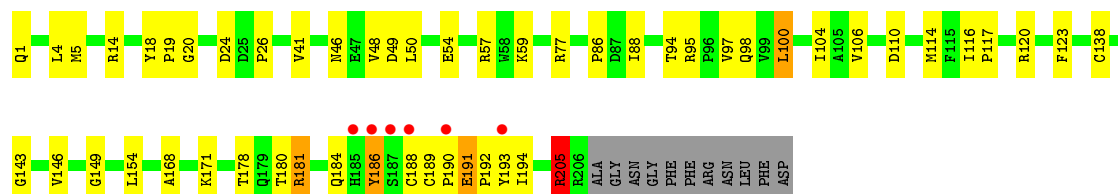
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain B: 



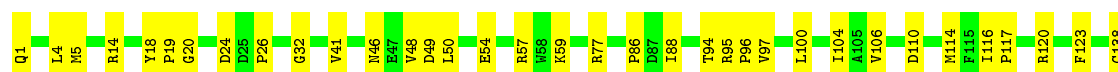
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

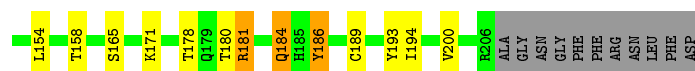
Chain C: 



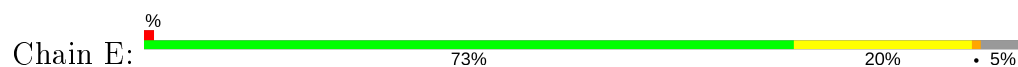
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain D: 

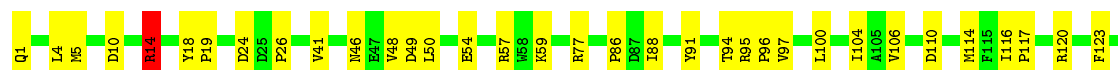




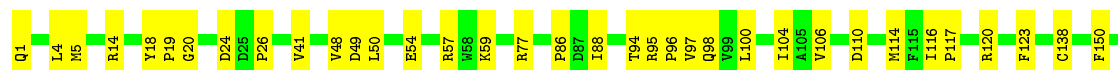
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR



• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR



• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

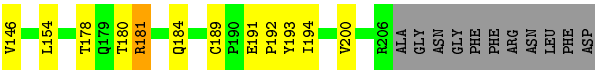


• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR



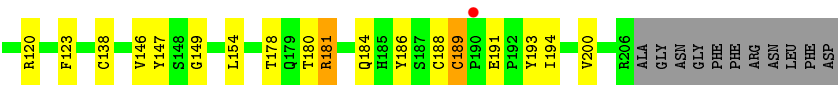
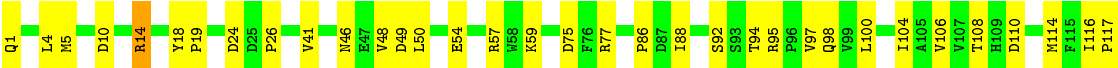
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR





● Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain J: 71% 23% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	144.82Å 144.82Å 274.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.95 – 3.14 95.95 – 3.14	Depositor EDS
% Data completeness (in resolution range)	95.8 (95.95-3.14) 97.7 (95.95-3.14)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 3.13Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.186 , 0.236 0.177 , 0.226	Depositor DCC
R_{free} test set	2571 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 62.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16380	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.98% 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

5.1 Standard geometry

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

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	0.42	0/1670	0.59	0/2279
1	B	0.43	0/1670	0.60	0/2279
1	C	0.48	0/1670	0.83	3/2279 (0.1%)
1	D	0.44	0/1670	0.59	1/2279 (0.0%)
1	E	0.43	0/1670	0.82	4/2279 (0.2%)
1	F	0.46	0/1670	0.87	3/2279 (0.1%)
1	G	0.43	0/1670	0.59	0/2279
1	H	0.45	0/1670	0.63	1/2279 (0.0%)
1	I	0.43	0/1670	0.60	1/2279 (0.0%)
1	J	0.44	0/1670	0.59	0/2279
All	All	0.44	0/16700	0.68	13/22790 (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	B	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	14	ARG	NE-CZ-NH2	-21.62	109.49	120.30
1	F	14	ARG	NE-CZ-NH1	19.62	130.11	120.30
1	C	205	ARG	NE-CZ-NH2	-18.34	111.13	120.30
1	C	205	ARG	NE-CZ-NH1	17.79	129.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	205	ARG	NE-CZ-NH2	-17.48	111.56	120.30
1	E	205	ARG	NE-CZ-NH1	16.81	128.71	120.30
1	F	14	ARG	CD-NE-CZ	8.88	136.03	123.60
1	C	205	ARG	CD-NE-CZ	7.46	134.04	123.60
1	I	32	GLY	N-CA-C	-6.42	97.04	113.10
1	E	205	ARG	CD-NE-CZ	6.29	132.41	123.60
1	E	205	ARG	CG-CD-NE	6.03	124.45	111.80
1	H	186	TYR	N-CA-C	5.87	126.84	111.00
1	D	32	GLY	N-CA-C	-5.24	100.01	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	188	CYS	Peptide
1	C	188	CYS	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	1631	0	1567	36	0
1	B	1631	0	1567	43	0
1	C	1631	0	1567	47	0
1	D	1631	0	1567	35	0
1	E	1631	0	1567	38	0
1	F	1631	0	1567	41	0
1	G	1631	0	1567	40	0
1	H	1631	0	1567	38	0
1	I	1631	0	1567	32	0
1	J	1631	0	1567	40	0
2	A	7	0	13	1	0
2	B	7	0	13	0	0
2	C	7	0	13	0	0
2	D	7	0	13	4	0
2	E	7	0	13	0	0
2	F	7	0	13	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	7	0	13	0	0
2	H	7	0	13	0	0
2	I	7	0	13	0	0
2	J	7	0	13	0	0
All	All	16380	0	15800	324	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 10.

All (324) 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:F:1206:ETM:H51	1:J:186:TYR:CE2	2.06	0.90
1:H:19:PRO:HG3	1:I:5:MET:HG3	1.60	0.84
2:F:1206:ETM:H51	1:J:186:TYR:HE2	1.44	0.80
1:C:46:ASN:ND2	1:D:171:LYS:HG2	1.95	0.80
1:F:19:PRO:HG3	1:G:5:MET:HG3	1.60	0.80
1:C:189:CYS:HB3	1:C:191:GLU:OE2	1.86	0.75
1:I:19:PRO:HG3	1:J:5:MET:HG3	1.67	0.74
1:C:189:CYS:CB	1:C:191:GLU:OE2	2.35	0.74
1:D:19:PRO:HB2	1:E:4:LEU:HD23	1.70	0.74
1:F:5:MET:HG3	1:J:19:PRO:HG3	1.70	0.73
1:G:19:PRO:HB2	1:H:4:LEU:HD23	1.71	0.71
1:F:77:ARG:HD2	1:F:106:VAL:HG22	1.71	0.71
1:B:19:PRO:HG3	1:C:5:MET:HG3	1.72	0.71
1:E:168:ALA:O	1:E:205:ARG:NH2	2.23	0.71
1:A:4:LEU:HD23	1:E:19:PRO:HB2	1.72	0.70
1:B:94:THR:O	1:C:120:ARG:HD2	1.94	0.68
1:G:184:GLN:HG3	1:G:184:GLN:O	1.90	0.68
1:C:41:VAL:HG22	1:C:48:VAL:HG22	1.76	0.68
1:B:50:LEU:HG	1:B:123:PHE:HE1	1.59	0.67
1:I:77:ARG:HD2	1:I:106:VAL:HG22	1.76	0.67
1:C:77:ARG:HD2	1:C:106:VAL:HG22	1.75	0.67
1:B:41:VAL:HG22	1:B:48:VAL:HG22	1.75	0.67
1:A:19:PRO:HG3	1:B:5:MET:HG3	1.77	0.67
1:G:50:LEU:HG	1:G:123:PHE:HE1	1.58	0.67
1:J:41:VAL:HG22	1:J:48:VAL:HG22	1.77	0.67
1:B:77:ARG:HD2	1:B:106:VAL:HG22	1.76	0.67
1:H:41:VAL:HG22	1:H:48:VAL:HG22	1.77	0.67
1:H:154:LEU:HB2	1:H:194:ILE:CG2	2.26	0.66
1:C:94:THR:O	1:D:120:ARG:HD2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:154:LEU:HB2	1:J:194:ILE:CG2	2.25	0.66
1:E:50:LEU:HG	1:E:123:PHE:HE1	1.60	0.66
1:G:77:ARG:HD2	1:G:106:VAL:HG22	1.76	0.66
1:G:41:VAL:HG22	1:G:48:VAL:HG22	1.76	0.65
1:G:19:PRO:HG3	1:H:5:MET:HG3	1.78	0.65
1:A:154:LEU:HB2	1:A:194:ILE:CG2	2.27	0.65
1:B:193:TYR:C	1:B:194:ILE:HD12	2.17	0.65
1:F:50:LEU:HG	1:F:123:PHE:HE1	1.61	0.65
1:A:50:LEU:HG	1:A:123:PHE:HE1	1.62	0.65
1:F:41:VAL:HG22	1:F:48:VAL:HG22	1.78	0.65
1:J:50:LEU:HG	1:J:123:PHE:HE1	1.62	0.64
1:J:77:ARG:HD2	1:J:106:VAL:HG22	1.77	0.64
1:E:77:ARG:HD2	1:E:106:VAL:HG22	1.79	0.64
1:E:41:VAL:HG22	1:E:48:VAL:HG22	1.78	0.64
1:D:41:VAL:HG22	1:D:48:VAL:HG22	1.79	0.64
1:C:154:LEU:HB2	1:C:194:ILE:CG2	2.28	0.64
1:I:154:LEU:HB2	1:I:194:ILE:CG2	2.28	0.64
1:I:94:THR:O	1:J:120:ARG:HD2	1.99	0.63
1:A:77:ARG:HD2	1:A:106:VAL:HG22	1.81	0.63
1:B:19:PRO:HB2	1:C:4:LEU:HD23	1.80	0.63
1:H:50:LEU:HG	1:H:123:PHE:HE1	1.63	0.63
1:D:154:LEU:HB2	1:D:194:ILE:CG2	2.29	0.63
1:C:50:LEU:HG	1:C:123:PHE:HE1	1.63	0.62
1:F:4:LEU:HD23	1:J:19:PRO:HB2	1.82	0.62
1:C:168:ALA:O	1:C:205:ARG:NH2	2.33	0.62
1:D:96:PRO:CG	1:E:98:GLN:HB3	2.29	0.62
1:I:50:LEU:HG	1:I:123:PHE:HE1	1.65	0.62
1:A:41:VAL:HG22	1:A:48:VAL:HG22	1.80	0.62
1:C:19:PRO:HB2	1:D:4:LEU:HD23	1.82	0.62
1:H:186:TYR:O	1:H:187:SER:HB3	2.00	0.62
1:H:188:CYS:SG	1:H:189:CYS:N	2.73	0.62
1:H:77:ARG:HD2	1:H:106:VAL:HG22	1.82	0.62
1:I:193:TYR:C	1:I:194:ILE:HD12	2.20	0.61
1:E:193:TYR:C	1:E:194:ILE:HD12	2.20	0.61
1:D:165:SER:CB	2:D:1206:ETM:H51	2.31	0.61
1:D:94:THR:O	1:E:120:ARG:HD2	2.00	0.61
1:F:193:TYR:C	1:F:194:ILE:HD12	2.20	0.61
1:H:19:PRO:HB2	1:I:4:LEU:HD23	1.81	0.61
1:D:77:ARG:HD2	1:D:106:VAL:HG22	1.81	0.60
1:F:104:ILE:HG21	1:J:146:VAL:HG21	1.83	0.60
1:J:188:CYS:SG	1:J:189:CYS:N	2.74	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:LEU:HB2	1:B:194:ILE:CG2	2.32	0.60
1:H:193:TYR:C	1:H:194:ILE:HD12	2.22	0.60
1:I:41:VAL:HG22	1:I:48:VAL:HG22	1.83	0.60
1:C:54:GLU:O	1:C:117:PRO:HD2	2.02	0.59
1:D:193:TYR:C	1:D:194:ILE:HD12	2.22	0.59
1:F:146:VAL:HG21	1:G:104:ILE:HG21	1.84	0.59
1:D:50:LEU:HG	1:D:123:PHE:HE1	1.68	0.59
1:A:10:ASP:O	1:A:14:ARG:NE	2.36	0.59
1:F:154:LEU:HB2	1:F:194:ILE:CG2	2.32	0.59
1:H:153:ASP:OD1	1:H:181:ARG:NH2	2.36	0.59
1:H:154:LEU:HB2	1:H:194:ILE:HG21	1.85	0.59
1:G:193:TYR:C	1:G:194:ILE:HD12	2.23	0.59
1:C:189:CYS:HB2	1:C:191:GLU:OE2	2.03	0.58
1:D:19:PRO:HG3	1:E:5:MET:HG3	1.84	0.58
1:J:154:LEU:HB2	1:J:194:ILE:HG22	1.85	0.58
1:A:19:PRO:HB2	1:B:4:LEU:HD23	1.86	0.58
1:H:185:HIS:CD2	1:H:192:PRO:HA	2.39	0.58
1:A:184:GLN:HG2	1:A:186:TYR:OH	2.04	0.58
1:F:94:THR:O	1:G:120:ARG:HD2	2.02	0.58
1:I:96:PRO:CG	1:J:98:GLN:HB3	2.34	0.58
1:A:94:THR:O	1:B:120:ARG:HD2	2.04	0.57
1:E:154:LEU:HB2	1:E:194:ILE:CG2	2.34	0.57
1:B:191:GLU:OE2	1:B:193:TYR:OH	2.18	0.57
1:E:169:SER:HA	1:E:205:ARG:NH2	2.19	0.57
1:G:194:ILE:HD12	1:G:194:ILE:N	2.19	0.57
1:A:193:TYR:C	1:A:194:ILE:HD12	2.25	0.57
1:H:146:VAL:HG21	1:I:104:ILE:HG21	1.86	0.56
1:B:50:LEU:HG	1:B:123:PHE:CE1	2.40	0.56
1:D:19:PRO:HB2	1:E:4:LEU:CD2	2.34	0.56
1:F:120:ARG:HD2	1:J:94:THR:O	2.05	0.56
1:C:59:LYS:HE3	1:C:110:ASP:O	2.05	0.56
1:F:185:HIS:C	1:F:186:TYR:CD1	2.78	0.56
1:I:146:VAL:HG21	1:J:104:ILE:HG21	1.87	0.56
1:B:96:PRO:CG	1:C:98:GLN:HB3	2.36	0.56
1:I:19:PRO:HB2	1:J:4:LEU:HD23	1.88	0.56
2:D:1206:ETM:H42	2:D:1206:ETM:SD	2.46	0.56
1:I:154:LEU:HB2	1:I:194:ILE:HG22	1.87	0.55
1:A:46:ASN:ND2	1:B:171:LYS:HG2	2.21	0.55
1:G:95:ARG:HG2	1:G:95:ARG:HH11	1.71	0.55
1:F:54:GLU:O	1:F:117:PRO:HD2	2.06	0.55
1:A:154:LEU:HB2	1:A:194:ILE:HG22	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:59:LYS:HE3	1:F:110:ASP:O	2.06	0.55
1:H:184:GLN:HB3	1:H:186:TYR:CZ	2.42	0.55
1:G:19:PRO:HB2	1:H:4:LEU:CD2	2.35	0.55
1:G:54:GLU:O	1:G:117:PRO:HD2	2.07	0.55
1:B:59:LYS:HE3	1:B:110:ASP:O	2.07	0.55
1:C:95:ARG:HG2	1:C:95:ARG:HH11	1.72	0.55
1:E:191:GLU:O	1:E:191:GLU:HG2	2.07	0.55
1:J:154:LEU:HB2	1:J:194:ILE:HG21	1.89	0.55
1:J:193:TYR:C	1:J:194:ILE:HD12	2.27	0.54
1:B:150:PHE:CD2	1:B:191:GLU:HB2	2.42	0.54
1:A:120:ARG:HD2	1:E:94:THR:O	2.08	0.54
1:F:19:PRO:HB2	1:G:4:LEU:HD23	1.90	0.54
1:A:194:ILE:HD12	1:A:194:ILE:N	2.23	0.54
1:E:194:ILE:HD12	1:E:194:ILE:N	2.22	0.54
1:F:86:PRO:HB2	1:F:88:ILE:HG12	1.88	0.54
1:G:186:TYR:HD2	1:G:193:TYR:CE1	2.26	0.54
1:A:95:ARG:HH11	1:A:95:ARG:HG2	1.73	0.54
1:B:194:ILE:HD12	1:B:194:ILE:N	2.22	0.54
1:A:5:MET:HG3	1:E:19:PRO:HG3	1.89	0.54
1:E:95:ARG:HG2	1:E:95:ARG:HH11	1.73	0.54
1:H:194:ILE:HD12	1:H:194:ILE:N	2.23	0.54
1:G:154:LEU:HB2	1:G:194:ILE:CG2	2.37	0.54
1:G:86:PRO:HB2	1:G:88:ILE:HG12	1.89	0.54
1:C:154:LEU:HB2	1:C:194:ILE:HG21	1.90	0.53
1:C:154:LEU:HB2	1:C:194:ILE:HG22	1.89	0.53
1:E:154:LEU:O	1:E:181:ARG:HD2	2.07	0.53
1:A:54:GLU:O	1:A:117:PRO:HD2	2.08	0.53
1:E:168:ALA:C	1:E:205:ARG:HH22	2.11	0.53
1:I:54:GLU:O	1:I:117:PRO:HD2	2.09	0.53
1:J:59:LYS:HE3	1:J:110:ASP:O	2.08	0.53
1:H:19:PRO:HB2	1:I:4:LEU:CD2	2.37	0.53
1:B:54:GLU:O	1:B:117:PRO:HD2	2.08	0.53
1:H:59:LYS:HE3	1:H:110:ASP:O	2.09	0.53
1:B:95:ARG:HH11	1:B:95:ARG:HG2	1.74	0.53
1:E:50:LEU:HG	1:E:123:PHE:CE1	2.43	0.53
1:H:154:LEU:HB2	1:H:194:ILE:HG22	1.90	0.53
1:G:50:LEU:HG	1:G:123:PHE:CE1	2.42	0.53
1:D:154:LEU:HB2	1:D:194:ILE:HG21	1.90	0.53
1:H:147:TYR:CE1	1:I:77:ARG:HG3	2.44	0.52
1:A:154:LEU:HB2	1:A:194:ILE:HG21	1.91	0.52
1:C:24:ASP:O	1:C:26:PRO:HD3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:TYR:C	1:C:186:TYR:CD1	2.83	0.52
1:C:86:PRO:HB2	1:C:88:ILE:HG12	1.91	0.52
1:F:4:LEU:CD2	1:J:19:PRO:HB2	2.40	0.52
1:I:194:ILE:HD12	1:I:194:ILE:N	2.25	0.52
1:A:24:ASP:O	1:A:26:PRO:HD3	2.10	0.52
1:E:59:LYS:HE3	1:E:110:ASP:O	2.10	0.52
1:G:59:LYS:HE3	1:G:110:ASP:O	2.10	0.52
1:I:86:PRO:HB2	1:I:88:ILE:HG12	1.92	0.52
1:J:86:PRO:HB2	1:J:88:ILE:HG12	1.92	0.52
1:J:95:ARG:HH11	1:J:95:ARG:HG2	1.75	0.52
1:J:191:GLU:HG2	1:J:193:TYR:CE1	2.45	0.52
1:C:186:TYR:HD1	1:C:186:TYR:C	2.14	0.52
1:E:189:CYS:HB3	1:E:191:GLU:OE2	2.09	0.52
1:E:54:GLU:O	1:E:117:PRO:HD2	2.10	0.52
1:I:154:LEU:HB2	1:I:194:ILE:HG21	1.91	0.52
1:I:50:LEU:HG	1:I:123:PHE:CE1	2.44	0.52
1:F:96:PRO:CG	1:G:98:GLN:HB3	2.40	0.51
1:D:154:LEU:O	1:D:181:ARG:HD2	2.10	0.51
1:B:154:LEU:O	1:B:181:ARG:HD2	2.10	0.51
1:C:46:ASN:HD21	1:D:171:LYS:HG2	1.70	0.51
1:D:186:TYR:CD1	1:D:186:TYR:N	2.78	0.51
1:H:54:GLU:O	1:H:117:PRO:HD2	2.10	0.51
1:J:50:LEU:HG	1:J:123:PHE:CE1	2.45	0.51
1:A:59:LYS:HE3	1:A:110:ASP:O	2.10	0.51
1:A:154:LEU:O	1:A:181:ARG:HD2	2.11	0.51
1:D:154:LEU:HB2	1:D:194:ILE:HG22	1.90	0.51
1:D:95:ARG:HH11	1:D:95:ARG:HG2	1.76	0.51
1:H:86:PRO:HB2	1:H:88:ILE:HG12	1.92	0.51
1:F:154:LEU:HB2	1:F:194:ILE:HG22	1.93	0.51
1:I:154:LEU:O	1:I:181:ARG:HD2	2.10	0.51
1:B:154:LEU:HB2	1:B:194:ILE:HG22	1.92	0.51
1:C:50:LEU:HG	1:C:123:PHE:CE1	2.45	0.51
1:C:19:PRO:HG3	1:D:5:MET:HG3	1.91	0.50
1:D:194:ILE:N	1:D:194:ILE:HD12	2.25	0.50
1:F:186:TYR:CD1	1:F:186:TYR:N	2.78	0.50
1:J:54:GLU:O	1:J:117:PRO:HD2	2.10	0.50
1:F:154:LEU:HB2	1:F:194:ILE:HG21	1.93	0.50
1:B:86:PRO:HB2	1:B:88:ILE:HG12	1.94	0.50
1:D:59:LYS:HE3	1:D:110:ASP:O	2.12	0.50
1:E:154:LEU:HB2	1:E:194:ILE:HG22	1.94	0.50
1:F:194:ILE:N	1:F:194:ILE:HD12	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ARG:HH11	1:A:114:MET:HE2	1.77	0.50
1:B:57:ARG:HH11	1:B:114:MET:HE2	1.77	0.50
1:C:190:PRO:HD2	1:C:191:GLU:OE2	2.11	0.50
1:D:86:PRO:HB2	1:D:88:ILE:HG12	1.94	0.49
1:A:191:GLU:HG3	1:A:193:TYR:OH	2.12	0.49
1:F:50:LEU:HG	1:F:123:PHE:CE1	2.44	0.49
1:G:183:VAL:HG12	1:G:183:VAL:O	2.12	0.49
1:E:189:CYS:CB	1:E:191:GLU:OE2	2.60	0.49
1:J:194:ILE:HD12	1:J:194:ILE:N	2.27	0.49
1:C:193:TYR:C	1:C:194:ILE:HD12	2.32	0.49
1:D:165:SER:HB3	2:D:1206:ETM:H51	1.95	0.49
1:F:77:ARG:HG3	1:J:147:TYR:CE1	2.48	0.49
1:B:154:LEU:HB2	1:B:194:ILE:HG21	1.94	0.49
1:C:146:VAL:HG21	1:D:104:ILE:HG21	1.93	0.49
1:D:50:LEU:HG	1:D:123:PHE:CE1	2.47	0.49
1:E:86:PRO:HB2	1:E:88:ILE:HG12	1.94	0.49
1:A:4:LEU:CD2	1:E:19:PRO:HB2	2.40	0.49
1:A:50:LEU:HG	1:A:123:PHE:CE1	2.45	0.49
1:D:24:ASP:O	1:D:26:PRO:HD3	2.13	0.49
1:C:191:GLU:HG2	1:C:193:TYR:CE1	2.48	0.48
1:G:154:LEU:O	1:G:181:ARG:HD2	2.13	0.48
1:F:95:ARG:HH11	1:F:95:ARG:HG2	1.78	0.48
1:F:10:ASP:O	1:F:14:ARG:HD3	2.12	0.48
1:H:94:THR:O	1:I:120:ARG:HD2	2.13	0.48
1:A:171:LYS:HG2	1:E:46:ASN:ND2	2.29	0.48
1:H:24:ASP:O	1:H:26:PRO:HD3	2.14	0.48
1:G:154:LEU:HB2	1:G:194:ILE:HG22	1.96	0.48
1:A:86:PRO:HB2	1:A:88:ILE:HG12	1.95	0.48
1:H:50:LEU:HG	1:H:123:PHE:CE1	2.46	0.48
1:E:154:LEU:HB2	1:E:194:ILE:HG21	1.96	0.47
1:F:190:PRO:HD2	1:F:191:GLU:OE1	2.15	0.47
1:A:189:CYS:HB2	1:A:191:GLU:OE2	2.15	0.47
1:C:57:ARG:HH11	1:C:114:MET:HE2	1.79	0.47
1:D:96:PRO:HG2	1:E:98:GLN:HB3	1.96	0.47
1:G:24:ASP:O	1:G:26:PRO:HD3	2.15	0.47
1:I:95:ARG:HH11	1:I:95:ARG:HG2	1.78	0.47
1:B:24:ASP:O	1:B:26:PRO:HD3	2.15	0.47
1:B:46:ASN:ND2	1:C:171:LYS:HG2	2.30	0.47
1:D:54:GLU:O	1:D:117:PRO:HD2	2.14	0.47
1:F:46:ASN:ND2	1:G:171:LYS:HG2	2.30	0.47
1:J:154:LEU:O	1:J:181:ARG:HD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:59:LYS:HE3	1:I:110:ASP:O	2.14	0.46
1:G:18:TYR:HA	1:G:19:PRO:HD3	1.76	0.46
1:H:95:ARG:HG2	1:H:95:ARG:HH11	1.79	0.46
1:F:171:LYS:HG2	1:J:46:ASN:ND2	2.30	0.46
1:C:18:TYR:HA	1:C:19:PRO:HD3	1.78	0.46
1:H:147:TYR:CE1	1:I:77:ARG:CG	2.99	0.46
1:J:14:ARG:HD2	1:J:14:ARG:HA	1.68	0.46
1:I:19:PRO:HB2	1:J:4:LEU:CD2	2.45	0.46
1:I:95:ARG:NH2	1:J:120:ARG:NH2	2.64	0.46
1:A:10:ASP:O	1:A:14:ARG:CD	2.63	0.46
1:C:189:CYS:HB3	1:C:190:PRO:CD	2.46	0.46
1:D:18:TYR:CE2	1:D:20:GLY:HA2	2.51	0.46
1:G:94:THR:O	1:H:120:ARG:HD2	2.15	0.46
1:B:187:SER:HB2	1:G:182:GLN:HB3	1.98	0.45
1:B:19:PRO:HB2	1:C:4:LEU:CD2	2.46	0.45
1:A:96:PRO:CG	1:B:98:GLN:HB3	2.45	0.45
1:D:165:SER:HB2	2:D:1206:ETM:H41	1.98	0.45
1:F:77:ARG:CD	1:F:106:VAL:HG22	2.44	0.45
1:G:150:PHE:CE2	1:G:191:GLU:HB3	2.51	0.45
1:A:191:GLU:HG3	1:A:193:TYR:CZ	2.51	0.45
1:F:19:PRO:HB2	1:G:4:LEU:CD2	2.46	0.45
1:G:186:TYR:CD2	1:G:193:TYR:CE1	3.05	0.45
1:D:46:ASN:ND2	1:E:171:LYS:HG2	2.31	0.45
1:G:189:CYS:HA	1:G:190:PRO:HD3	1.62	0.45
1:J:57:ARG:HH11	1:J:114:MET:HE2	1.81	0.45
1:B:189:CYS:HA	1:B:190:PRO:HD3	1.64	0.45
1:C:154:LEU:O	1:C:181:ARG:HD2	2.17	0.45
1:C:189:CYS:HB3	1:C:190:PRO:HD3	1.98	0.45
1:F:18:TYR:HA	1:F:19:PRO:HD3	1.76	0.45
1:I:57:ARG:HH11	1:I:114:MET:HE2	1.82	0.44
1:J:24:ASP:O	1:J:26:PRO:HD3	2.16	0.44
1:F:24:ASP:O	1:F:26:PRO:HD3	2.17	0.44
1:B:18:TYR:HA	1:B:19:PRO:HD3	1.74	0.44
1:B:95:ARG:NH2	1:C:120:ARG:NH2	2.66	0.44
1:H:57:ARG:HH11	1:H:114:MET:HE2	1.83	0.44
1:B:150:PHE:CE2	1:B:191:GLU:CB	3.01	0.44
1:A:10:ASP:O	1:A:14:ARG:HD3	2.18	0.43
1:G:96:PRO:CG	1:H:98:GLN:HB3	2.48	0.43
1:I:24:ASP:O	1:I:26:PRO:HD3	2.18	0.43
1:B:191:GLU:OE2	1:B:193:TYR:CZ	2.71	0.43
1:F:189:CYS:HA	1:F:190:PRO:HD3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:85:THR:HA	1:H:86:PRO:HD3	1.85	0.43
1:G:18:TYR:CE2	1:G:20:GLY:HA2	2.53	0.43
1:H:150:PHE:CE2	1:H:191:GLU:HB3	2.54	0.43
1:I:191:GLU:HA	1:I:192:PRO:HD3	1.77	0.43
1:F:154:LEU:O	1:F:181:ARG:HD2	2.19	0.43
1:A:146:VAL:HG21	1:B:104:ILE:HG21	1.99	0.43
1:B:188:CYS:C	1:B:189:CYS:SG	2.96	0.43
1:B:143:GLY:HA2	1:B:154:LEU:HD11	2.01	0.43
1:G:150:PHE:CD2	1:G:191:GLU:HB3	2.54	0.42
1:G:154:LEU:HB2	1:G:194:ILE:HG21	2.00	0.42
1:J:149:GLY:CA	1:J:194:ILE:HD13	2.49	0.42
1:J:18:TYR:HA	1:J:19:PRO:HD3	1.79	0.42
1:F:77:ARG:CG	1:J:147:TYR:CE1	3.02	0.42
2:A:1206:ETM:H53	1:E:186:TYR:OH	2.20	0.42
1:J:75:ASP:HB3	1:J:108:THR:HG23	2.02	0.42
1:H:31:LEU:HA	1:H:31:LEU:HD12	1.87	0.42
1:F:153:ASP:OD1	1:F:181:ARG:NH1	2.52	0.42
1:D:184:GLN:HB3	1:D:186:TYR:CE1	2.55	0.42
1:A:184:GLN:HG2	1:A:186:TYR:CZ	2.54	0.42
1:I:18:TYR:HA	1:I:19:PRO:HD3	1.81	0.42
1:B:146:VAL:HG21	1:C:104:ILE:HG21	2.02	0.42
1:C:191:GLU:HB2	1:C:192:PRO:HD2	2.01	0.42
1:E:24:ASP:O	1:E:26:PRO:HD3	2.20	0.42
1:C:149:GLY:CA	1:C:194:ILE:HD13	2.49	0.41
1:C:149:GLY:HA3	1:C:194:ILE:HD13	2.03	0.41
1:F:57:ARG:HH11	1:F:114:MET:HE2	1.85	0.41
1:G:95:ARG:HH11	1:G:95:ARG:CG	2.33	0.41
1:B:153:ASP:OD1	1:B:181:ARG:NH1	2.53	0.41
1:H:191:GLU:HA	1:H:192:PRO:HD3	1.87	0.41
1:A:190:PRO:HD2	1:A:191:GLU:OE1	2.21	0.41
1:B:97:VAL:H	1:B:97:VAL:HG12	1.56	0.41
1:C:18:TYR:CE2	1:C:20:GLY:HA2	2.56	0.41
1:E:57:ARG:HH11	1:E:114:MET:HE2	1.86	0.41
1:E:169:SER:CA	1:E:205:ARG:NH2	2.82	0.41
1:H:190:PRO:HD2	1:H:191:GLU:OE1	2.20	0.41
1:E:149:GLY:CA	1:E:194:ILE:HD13	2.51	0.41
1:F:91:TYR:CD1	1:F:91:TYR:N	2.88	0.41
1:G:57:ARG:HH11	1:G:114:MET:HE2	1.85	0.41
1:G:191:GLU:HA	1:G:192:PRO:HD3	1.95	0.41
1:B:168:ALA:O	1:B:205:ARG:NH1	2.54	0.41
1:C:143:GLY:HA2	1:C:154:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:ARG:HH11	1:D:114:MET:HE2	1.86	0.41
1:J:10:ASP:O	1:J:14:ARG:HG2	2.20	0.41
1:E:149:GLY:HA3	1:E:194:ILE:HD13	2.02	0.40
1:F:191:GLU:HA	1:F:192:PRO:HD3	1.73	0.40
1:H:18:TYR:HA	1:H:19:PRO:HD3	1.81	0.40
1:C:100:LEU:HD12	1:C:100:LEU:HA	1.84	0.40
1:B:75:ASP:HB3	1:B:108:THR:HG23	2.04	0.40
1:C:77:ARG:CD	1:C:106:VAL:HG22	2.49	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	204/217 (94%)	200 (98%)	4 (2%)	0	100	100
1	B	204/217 (94%)	197 (97%)	7 (3%)	0	100	100
1	C	204/217 (94%)	195 (96%)	9 (4%)	0	100	100
1	D	204/217 (94%)	201 (98%)	3 (2%)	0	100	100
1	E	204/217 (94%)	195 (96%)	9 (4%)	0	100	100
1	F	204/217 (94%)	199 (98%)	5 (2%)	0	100	100
1	G	204/217 (94%)	199 (98%)	5 (2%)	0	100	100
1	H	204/217 (94%)	197 (97%)	7 (3%)	0	100	100
1	I	204/217 (94%)	199 (98%)	5 (2%)	0	100	100
1	J	204/217 (94%)	198 (97%)	6 (3%)	0	100	100
All	All	2040/2170 (94%)	1980 (97%)	60 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	188/197 (95%)	174 (93%)	14 (7%)	13	40
1	B	188/197 (95%)	174 (93%)	14 (7%)	13	40
1	C	188/197 (95%)	174 (93%)	14 (7%)	13	40
1	D	188/197 (95%)	173 (92%)	15 (8%)	12	37
1	E	188/197 (95%)	175 (93%)	13 (7%)	15	43
1	F	188/197 (95%)	174 (93%)	14 (7%)	13	40
1	G	188/197 (95%)	176 (94%)	12 (6%)	17	46
1	H	188/197 (95%)	175 (93%)	13 (7%)	15	43
1	I	188/197 (95%)	174 (93%)	14 (7%)	13	40
1	J	188/197 (95%)	174 (93%)	14 (7%)	13	40
All	All	1880/1970 (95%)	1743 (93%)	137 (7%)	14	41

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	14	ARG
1	A	49	ASP
1	A	97	VAL
1	A	100	LEU
1	A	116	ILE
1	A	138	CYS
1	A	178	THR
1	A	180	THR
1	A	181	ARG
1	A	184	GLN
1	A	185	HIS
1	A	189	CYS
1	A	200	VAL
1	B	1	GLN
1	B	14	ARG

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Mol	Chain	Res	Type
1	B	49	ASP
1	B	97	VAL
1	B	100	LEU
1	B	116	ILE
1	B	138	CYS
1	B	178	THR
1	B	180	THR
1	B	181	ARG
1	B	184	GLN
1	B	188	CYS
1	B	189	CYS
1	B	200	VAL
1	C	1	GLN
1	C	14	ARG
1	C	49	ASP
1	C	97	VAL
1	C	100	LEU
1	C	116	ILE
1	C	138	CYS
1	C	178	THR
1	C	180	THR
1	C	181	ARG
1	C	184	GLN
1	C	186	TYR
1	C	191	GLU
1	C	205	ARG
1	D	1	GLN
1	D	14	ARG
1	D	49	ASP
1	D	97	VAL
1	D	100	LEU
1	D	116	ILE
1	D	138	CYS
1	D	158	THR
1	D	178	THR
1	D	180	THR
1	D	181	ARG
1	D	184	GLN
1	D	186	TYR
1	D	189	CYS
1	D	200	VAL
1	E	1	GLN

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Mol	Chain	Res	Type
1	E	14	ARG
1	E	49	ASP
1	E	97	VAL
1	E	100	LEU
1	E	116	ILE
1	E	138	CYS
1	E	178	THR
1	E	180	THR
1	E	181	ARG
1	E	184	GLN
1	E	189	CYS
1	E	200	VAL
1	F	1	GLN
1	F	14	ARG
1	F	49	ASP
1	F	97	VAL
1	F	100	LEU
1	F	116	ILE
1	F	138	CYS
1	F	178	THR
1	F	180	THR
1	F	181	ARG
1	F	184	GLN
1	F	186	TYR
1	F	189	CYS
1	F	200	VAL
1	G	1	GLN
1	G	14	ARG
1	G	49	ASP
1	G	97	VAL
1	G	100	LEU
1	G	116	ILE
1	G	138	CYS
1	G	178	THR
1	G	180	THR
1	G	181	ARG
1	G	184	GLN
1	G	189	CYS
1	H	1	GLN
1	H	14	ARG
1	H	49	ASP
1	H	92	SER

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Mol	Chain	Res	Type
1	H	97	VAL
1	H	100	LEU
1	H	116	ILE
1	H	138	CYS
1	H	178	THR
1	H	180	THR
1	H	185	HIS
1	H	189	CYS
1	H	200	VAL
1	I	1	GLN
1	I	14	ARG
1	I	49	ASP
1	I	92	SER
1	I	97	VAL
1	I	100	LEU
1	I	116	ILE
1	I	138	CYS
1	I	178	THR
1	I	180	THR
1	I	181	ARG
1	I	184	GLN
1	I	189	CYS
1	I	200	VAL
1	J	1	GLN
1	J	14	ARG
1	J	49	ASP
1	J	92	SER
1	J	97	VAL
1	J	100	LEU
1	J	116	ILE
1	J	138	CYS
1	J	178	THR
1	J	180	THR
1	J	181	ARG
1	J	184	GLN
1	J	189	CYS
1	J	200	VAL

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

Mol	Chain	Res	Type
1	J	1	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](#)

10 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	ETM	B	1206	1	6,6,6	0.87	0	7,8,8	3.33	3 (42%)
2	ETM	J	1206	1	6,6,6	1.00	0	7,8,8	3.37	3 (42%)
2	ETM	H	1206	1	6,6,6	0.94	0	7,8,8	3.09	3 (42%)
2	ETM	G	1206	1	6,6,6	1.03	0	7,8,8	3.26	3 (42%)
2	ETM	E	1206	1	6,6,6	0.81	0	7,8,8	3.09	3 (42%)
2	ETM	C	1206	1	6,6,6	0.92	0	7,8,8	3.14	3 (42%)
2	ETM	A	1206	1	6,6,6	0.90	0	7,8,8	3.20	3 (42%)
2	ETM	I	1206	1	6,6,6	0.91	0	7,8,8	3.42	3 (42%)
2	ETM	F	1206	1	6,6,6	0.91	0	7,8,8	3.07	3 (42%)
2	ETM	D	1206	1	6,6,6	1.05	0	7,8,8	2.89	2 (28%)

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	ETM	B	1206	1	-	4/4/4/4	-
2	ETM	J	1206	1	-	0/4/4/4	-
2	ETM	H	1206	1	-	2/4/4/4	-
2	ETM	G	1206	1	-	1/4/4/4	-
2	ETM	E	1206	1	-	2/4/4/4	-
2	ETM	C	1206	1	-	0/4/4/4	-
2	ETM	A	1206	1	-	0/4/4/4	-
2	ETM	I	1206	1	-	2/4/4/4	-
2	ETM	F	1206	1	-	0/4/4/4	-
2	ETM	D	1206	1	-	2/4/4/4	-

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1206	ETM	C4-N1-C3	7.57	128.45	108.97
2	I	1206	ETM	C4-N1-C3	7.54	128.35	108.97
2	G	1206	ETM	C4-N1-C3	7.38	127.94	108.97
2	A	1206	ETM	C4-N1-C3	7.14	127.34	108.97
2	C	1206	ETM	C4-N1-C3	7.02	127.03	108.97
2	B	1206	ETM	C4-N1-C3	6.88	126.65	108.97
2	D	1206	ETM	C4-N1-C3	6.76	126.35	108.97
2	F	1206	ETM	C4-N1-C3	6.70	126.20	108.97
2	E	1206	ETM	C4-N1-C3	6.60	125.94	108.97
2	H	1206	ETM	C4-N1-C3	6.31	125.20	108.97
2	H	1206	ETM	C5-N1-C3	-3.92	98.89	108.97
2	B	1206	ETM	C5-N1-C3	-3.75	99.34	108.97
2	F	1206	ETM	C5-N1-C3	-3.66	99.57	108.97
2	C	1206	ETM	C5-N1-C3	-3.53	99.90	108.97
2	B	1206	ETM	C5-N1-C4	-3.43	100.15	108.97
2	I	1206	ETM	C5-N1-C4	-3.36	100.33	108.97
2	E	1206	ETM	C5-N1-C3	-3.19	100.77	108.97
2	A	1206	ETM	C5-N1-C4	-3.14	100.90	108.97
2	J	1206	ETM	C5-N1-C4	-3.12	100.95	108.97
2	G	1206	ETM	C5-N1-C4	-3.06	101.10	108.97
2	I	1206	ETM	C5-N1-C3	-2.97	101.33	108.97
2	H	1206	ETM	C5-N1-C4	-2.96	101.36	108.97
2	J	1206	ETM	C5-N1-C3	-2.93	101.44	108.97
2	E	1206	ETM	C5-N1-C4	-2.82	101.72	108.97
2	A	1206	ETM	C5-N1-C3	-2.70	102.03	108.97
2	D	1206	ETM	C5-N1-C3	-2.68	102.09	108.97
2	F	1206	ETM	C5-N1-C4	-2.43	102.74	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1206	ETM	C5-N1-C3	-2.35	102.94	108.97
2	C	1206	ETM	C5-N1-C4	-2.20	103.31	108.97

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1206	ETM	SD-C1-C2-N1
2	G	1206	ETM	SD-C1-C2-N1
2	I	1206	ETM	SD-C1-C2-N1
2	E	1206	ETM	C1-C2-N1-C5
2	D	1206	ETM	SD-C1-C2-N1
2	B	1206	ETM	C1-C2-N1-C3
2	B	1206	ETM	C1-C2-N1-C4
2	B	1206	ETM	C1-C2-N1-C5
2	H	1206	ETM	C1-C2-N1-C3
2	H	1206	ETM	C1-C2-N1-C4
2	E	1206	ETM	C1-C2-N1-C4
2	D	1206	ETM	C1-C2-N1-C3
2	I	1206	ETM	C1-C2-N1-C3

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1206	ETM	1	0
2	F	1206	ETM	2	0
2	D	1206	ETM	4	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, 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	206/217 (94%)	-0.00	1 (0%) 91 83	40, 64, 98, 157	0
1	B	206/217 (94%)	-0.14	2 (0%) 82 70	42, 62, 97, 156	0
1	C	206/217 (94%)	-0.11	6 (2%) 51 30	41, 64, 114, 157	0
1	D	206/217 (94%)	-0.06	0 100 100	44, 65, 104, 156	0
1	E	206/217 (94%)	0.04	2 (0%) 82 70	38, 63, 102, 156	0
1	F	206/217 (94%)	-0.13	0 100 100	34, 60, 95, 158	0
1	G	206/217 (94%)	-0.16	0 100 100	36, 60, 96, 156	0
1	H	206/217 (94%)	-0.07	1 (0%) 91 83	39, 60, 95, 156	0
1	I	206/217 (94%)	-0.02	0 100 100	36, 62, 97, 156	0
1	J	206/217 (94%)	-0.07	1 (0%) 91 83	40, 62, 100, 168	0
All	All	2060/2170 (94%)	-0.07	13 (0%) 89 80	34, 63, 105, 168	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	187	SER	5.0
1	E	16	PRO	3.0
1	C	188	CYS	2.7
1	H	184	GLN	2.6
1	C	186	TYR	2.6
1	C	185	HIS	2.6
1	B	13	ASN	2.6
1	C	193	TYR	2.6
1	J	190	PRO	2.5
1	B	14	ARG	2.4
1	A	13	ASN	2.4
1	E	15	SER	2.1
1	C	190	PRO	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. 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	B-factors(\AA^2)	Q<0.9
2	ETM	E	1206	7/7	0.40	0.45	75,97,126,127	7
2	ETM	B	1206	7/7	0.75	0.34	41,71,103,106	7
2	ETM	I	1206	7/7	0.77	0.38	66,94,118,122	7
2	ETM	C	1206	7/7	0.78	0.30	61,112,130,135	0
2	ETM	G	1206	7/7	0.79	0.49	94,110,118,123	7
2	ETM	A	1206	7/7	0.80	0.31	65,109,141,146	0
2	ETM	J	1206	7/7	0.82	0.43	74,115,151,161	0
2	ETM	F	1206	7/7	0.82	0.35	94,113,161,165	0
2	ETM	H	1206	7/7	0.84	0.29	20,93,116,120	7
2	ETM	D	1206	7/7	0.87	0.35	76,107,116,132	7

6.5 Other polymers [i](#)

There are no such residues in this entry.