



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 8, 2021 – 10:03 PM EDT

PDB ID : 3UQR
Title : Crystal structure of BACE1 with its inhibitor
Authors : Chen, T.T.; Chen, W.Y.; Li, L.; Xu, Y.C.
Deposited on : 2011-11-21
Resolution : 3.06 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 : 2.23.1
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) : 2.23.1

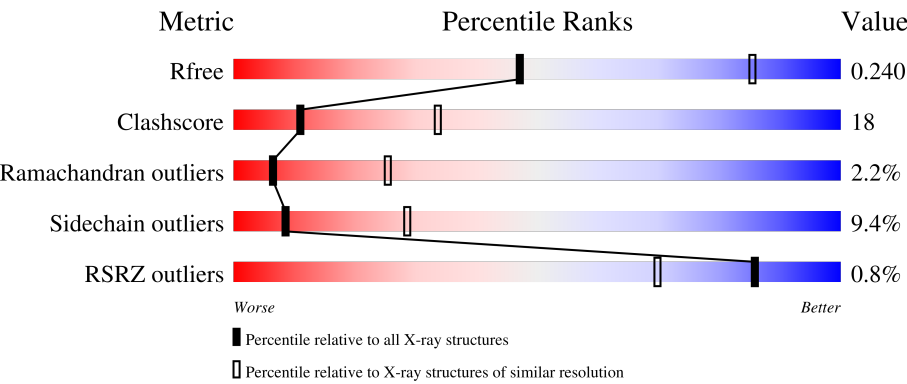
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.06 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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 of 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	433	<div><div>%</div><div><div></div><div>59%</div><div>24%</div><div>•</div><div>13%</div></div></div>
1	B	433	<div><div>%</div><div><div></div><div>57%</div><div>25%</div><div>•</div><div>14%</div></div></div>
1	C	433	<div><div></div><div><div></div><div>54%</div><div>28%</div><div>5%</div><div>13%</div></div></div>
2	D	7	<div><div></div><div><div>14%</div><div>57%</div><div>14%</div><div>14%</div></div></div>
2	E	7	<div><div></div><div><div>14%</div><div>57%</div><div>14%</div><div>14%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	F	7	

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	PSA	F	3	-	X	-	-
2	ZAE	F	6	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8971 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 Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	1	0
			2900	1865	483	538	14			
1	B	374	Total	C	N	O	S	0	0	0
			2868	1842	473	539	14			
1	C	377	Total	C	N	O	S	0	0	0
			2901	1858	480	549	14			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-39	MET	-	expression tag	UNP P56817
A	-38	GLY	-	expression tag	UNP P56817
A	-37	SER	-	expression tag	UNP P56817
A	-36	SER	-	expression tag	UNP P56817
A	-35	HIS	-	expression tag	UNP P56817
A	-34	HIS	-	expression tag	UNP P56817
A	-33	HIS	-	expression tag	UNP P56817
A	-32	HIS	-	expression tag	UNP P56817
A	-31	HIS	-	expression tag	UNP P56817
A	-30	HIS	-	expression tag	UNP P56817
A	-29	SER	-	expression tag	UNP P56817
A	-28	ALA	-	expression tag	UNP P56817
A	-27	GLY	-	expression tag	UNP P56817
A	-26	GLU	-	expression tag	UNP P56817
A	-25	ASN	-	expression tag	UNP P56817
A	-24	LEU	-	expression tag	UNP P56817
A	-23	TYR	-	expression tag	UNP P56817
A	-22	PHE	-	expression tag	UNP P56817
A	-21	GLN	-	expression tag	UNP P56817
A	-20	GLY	-	expression tag	UNP P56817
A	-19	THR	-	expression tag	UNP P56817
B	-39	MET	-	expression tag	UNP P56817
B	-38	GLY	-	expression tag	UNP P56817

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-37	SER	-	expression tag	UNP P56817
B	-36	SER	-	expression tag	UNP P56817
B	-35	HIS	-	expression tag	UNP P56817
B	-34	HIS	-	expression tag	UNP P56817
B	-33	HIS	-	expression tag	UNP P56817
B	-32	HIS	-	expression tag	UNP P56817
B	-31	HIS	-	expression tag	UNP P56817
B	-30	HIS	-	expression tag	UNP P56817
B	-29	SER	-	expression tag	UNP P56817
B	-28	ALA	-	expression tag	UNP P56817
B	-27	GLY	-	expression tag	UNP P56817
B	-26	GLU	-	expression tag	UNP P56817
B	-25	ASN	-	expression tag	UNP P56817
B	-24	LEU	-	expression tag	UNP P56817
B	-23	TYR	-	expression tag	UNP P56817
B	-22	PHE	-	expression tag	UNP P56817
B	-21	GLN	-	expression tag	UNP P56817
B	-20	GLY	-	expression tag	UNP P56817
B	-19	THR	-	expression tag	UNP P56817
C	-39	MET	-	expression tag	UNP P56817
C	-38	GLY	-	expression tag	UNP P56817
C	-37	SER	-	expression tag	UNP P56817
C	-36	SER	-	expression tag	UNP P56817
C	-35	HIS	-	expression tag	UNP P56817
C	-34	HIS	-	expression tag	UNP P56817
C	-33	HIS	-	expression tag	UNP P56817
C	-32	HIS	-	expression tag	UNP P56817
C	-31	HIS	-	expression tag	UNP P56817
C	-30	HIS	-	expression tag	UNP P56817
C	-29	SER	-	expression tag	UNP P56817
C	-28	ALA	-	expression tag	UNP P56817
C	-27	GLY	-	expression tag	UNP P56817
C	-26	GLU	-	expression tag	UNP P56817
C	-25	ASN	-	expression tag	UNP P56817
C	-24	LEU	-	expression tag	UNP P56817
C	-23	TYR	-	expression tag	UNP P56817
C	-22	PHE	-	expression tag	UNP P56817
C	-21	GLN	-	expression tag	UNP P56817
C	-20	GLY	-	expression tag	UNP P56817
C	-19	THR	-	expression tag	UNP P56817

- Molecule 2 is a protein called METHYL (2S)-1-[(2R,5S,8S,12S,13S)-2,13-DIBENZYL-12-HYDROXY-3,5-DIMETHYL-15-(3-[METHYL(METHYLSULFONYL)AMINO]-5-[[[(1R)-1-P

HENYLETHYL]CARBAMOYL}PHENYL)-8-(2-METHYLPROPYL)-4,7,10,15-TETRAOXO-3,6,9,14-TETRAAZAPENTADECAN-1-OYL]PYRROLIDINE-2-CARBOXYLATE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	7	Total	C	N	O	S	0	0	0
			73	54	7	11	1			
2	E	7	Total	C	N	O	S	0	0	0
			73	54	7	11	1			
2	F	7	Total	C	N	O	S	0	0	0
			73	54	7	11	1			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	29	Total	O	0	0
			29	29		
3	B	21	Total	O	0	0
			21	21		
3	C	31	Total	O	0	0
			31	31		
3	D	1	Total	O	0	0
			1	1		
3	E	1	Total	O	0	0
			1	1		



Chain F: 43% 43% 14%

QSC1	ZSC2	F3	L4	A5	2AE6	PLJ7
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.51Å 132.12Å 163.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.06 – 3.06 74.28 – 3.06	Depositor EDS
% Data completeness (in resolution range)	91.7 (66.06-3.06) 96.5 (74.28-3.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.7_650	Depositor
R, R_{free}	0.192 , 0.242 0.190 , 0.240	Depositor DCC
R_{free} test set	2177 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	1.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8971	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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: QSC, PLJ, ZAE, PSA, ZSC

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	0.45	0/2978	0.60	0/4059
1	B	0.43	0/2942	0.61	0/4013
1	C	0.45	0/2975	0.62	0/4055
2	D	1.37	0/12	1.28	0/15
2	E	1.45	0/12	1.58	0/15
2	F	1.51	0/12	2.08	0/15
All	All	0.45	0/8931	0.62	0/12172

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
2	D	0	2
2	E	0	2
2	F	0	2
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	3	PSA	Mainchain,Peptide
2	E	3	PSA	Mainchain,Peptide
2	F	3	PSA	Mainchain,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	2900	0	2760	82	0
1	B	2868	0	2706	102	0
1	C	2901	0	2739	121	0
2	D	73	0	68	4	0
2	E	73	0	69	5	0
2	F	73	0	67	14	0
3	A	29	0	0	1	0
3	B	21	0	0	0	0
3	C	31	0	0	1	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
All	All	8971	0	8409	313	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 18.

All (313) 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:B:253:SER:HB2	1:B:254:THR:C	1.78	1.04
1:B:255:GLU:CB	1:B:257:PHE:HE1	1.76	0.97
1:B:246:LYS:H	1:B:246:LYS:HD2	1.36	0.91
1:A:307[B]:ARG:HG3	1:A:323:ALA:HB2	1.54	0.86
1:C:-2:SER:HA	1:C:-1:PHE:CB	2.06	0.85
1:B:188:LEU:HB3	1:B:355:ALA:HB2	1.55	0.85
1:C:188:LEU:HD23	1:C:355:ALA:HB2	1.57	0.85
1:C:-2:SER:HA	1:C:-1:PHE:HB2	1.60	0.83
1:A:190:TYR:HD2	1:A:351:ARG:HG3	1.45	0.82
1:C:-4:ARG:HG3	1:C:-4:ARG:HH11	1.43	0.82
1:B:257:PHE:HD1	1:B:257:PHE:H	1.27	0.81
1:C:113:SER:HB2	1:C:115:TRP:CD1	2.16	0.80
1:C:194:ARG:HD2	1:C:202:ILE:HD11	1.66	0.78
1:B:8:GLY:C	1:B:10:SER:H	1.89	0.75
1:B:250:ALA:HA	1:B:254:THR:CB	2.17	0.74
1:A:190:TYR:CD2	1:A:351:ARG:HG3	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:PHE:CE1	1:B:111:ASN:HB2	2.23	0.73
1:B:8:GLY:O	1:B:170:VAL:HB	1.89	0.73
1:A:241:PHE:O	1:A:245:VAL:HG23	1.89	0.72
1:C:9:LYS:O	1:C:10:SER:HB3	1.88	0.72
1:C:193:ILE:HG12	1:C:352:ILE:CD1	2.20	0.72
2:F:4:LEU:HD11	2:F:7:PLJ:HG3	1.71	0.71
1:C:10:SER:O	1:C:12:GLN:HG2	1.91	0.71
1:C:93:VAL:HG21	1:C:140:LEU:HD11	1.70	0.71
1:B:149:LEU:HD13	1:B:178:GLY:HA2	1.73	0.71
1:A:32:ASP:OD2	1:A:35:SER:HB3	1.91	0.70
1:B:360:HIS:CE1	1:B:362:HIS:HD2	2.10	0.70
1:B:385:ASN:O	1:B:386:ILE:HB	1.91	0.70
1:B:255:GLU:CB	1:B:257:PHE:CE1	2.68	0.70
1:B:125:GLU:O	1:B:125:GLU:HG3	1.92	0.69
1:B:253:SER:HB2	1:B:254:THR:O	1.90	0.69
1:C:-2:SER:HA	1:C:-1:PHE:CD1	2.28	0.69
1:C:82:THR:O	1:C:83:ASP:HB2	1.91	0.68
1:B:257:PHE:N	1:B:257:PHE:CD1	2.59	0.68
1:A:71:TYR:CD1	2:D:3:PSA:HB2	2.29	0.68
1:C:91:PRO:HB2	1:C:93:VAL:HG22	1.77	0.67
1:B:149:LEU:HD23	1:B:346:ASP:HA	1.76	0.67
1:B:276:PRO:O	1:B:279:ILE:HG12	1.95	0.67
1:B:45:HIS:HB3	1:B:48:LEU:HG	1.77	0.66
1:B:75:LYS:HE2	1:B:106:ASP:HB3	1.77	0.66
1:C:218:LYS:HE2	1:C:381:ASP:O	1.96	0.66
1:C:42:ALA:HB2	1:C:101:ALA:HB1	1.79	0.65
1:A:61:ARG:HH21	1:C:3:VAL:HG13	1.60	0.64
1:C:113:SER:HB2	1:C:115:TRP:NE1	2.11	0.64
2:F:4:LEU:CD1	2:F:4:LEU:C	2.66	0.64
1:A:147:PRO:HG2	1:A:177:GLY:O	1.97	0.64
1:C:22:SER:HA	1:C:23:PRO:C	2.19	0.64
1:A:236:LEU:HD23	1:A:331:THR:HG23	1.80	0.64
1:B:246:LYS:HD2	1:B:246:LYS:N	2.07	0.64
1:C:-2:SER:HA	1:C:-1:PHE:CG	2.33	0.63
1:B:10:SER:HA	1:B:170:VAL:HG21	1.81	0.63
1:B:253:SER:HB2	1:B:255:GLU:N	2.13	0.63
1:C:12:GLN:O	2:F:1:QSC:HAE	1.99	0.63
1:A:26:THR:HG22	1:A:50:ARG:NH2	2.14	0.63
1:B:292:THR:HG22	1:B:293:ASN:HD22	1.64	0.62
1:B:152:LEU:HD21	1:B:174:MET:HG3	1.81	0.62
1:C:-2:SER:CA	1:C:-1:PHE:HB2	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:GLY:HA2	1:C:107:LYS:HB2	1.80	0.62
1:B:238:LYS:O	1:B:242:GLU:HG2	2.00	0.62
1:A:225:SER:HB3	1:A:331:THR:HB	1.83	0.61
1:A:230:GLY:O	2:D:1:QSC:HBF	2.01	0.61
1:A:77:GLU:HG2	1:A:104:GLU:HB2	1.82	0.61
1:B:179:ILE:HG23	1:B:342:TYR:HE2	1.65	0.61
1:A:277:TRP:CZ3	1:A:303:GLN:HG3	2.36	0.60
1:A:300:ILE:HG21	1:A:337:ILE:HD13	1.83	0.60
1:B:40:VAL:HG21	1:B:52:TYR:HB2	1.83	0.60
1:B:270:TRP:CE3	1:B:275:THR:HG23	2.37	0.60
1:C:-4:ARG:HH11	1:C:-4:ARG:CG	2.14	0.60
1:B:243:ALA:HA	1:B:246:LYS:HD3	1.83	0.59
1:B:253:SER:CB	1:B:254:THR:C	2.64	0.59
1:C:190:TYR:CD2	1:C:351:ARG:HG3	2.37	0.59
2:F:4:LEU:C	2:F:4:LEU:HD13	2.22	0.59
1:C:357:SER:HB3	1:C:360:HIS:HB3	1.83	0.59
1:C:261:PHE:CE1	1:C:268:VAL:HG22	2.38	0.59
1:C:74:GLY:HA2	1:C:107:LYS:CB	2.33	0.59
1:C:292:THR:HG22	1:C:293:ASN:HD22	1.68	0.59
1:A:69:VAL:HG22	1:A:128:ARG:HG3	1.85	0.59
1:B:360:HIS:O	1:B:361:VAL:C	2.41	0.59
1:C:38:PHE:CD1	1:C:99:ILE:HG12	2.37	0.59
1:A:270:TRP:CE3	1:A:275:THR:HG23	2.38	0.58
1:B:152:LEU:CD2	1:B:174:MET:HG3	2.33	0.58
1:B:149:LEU:CD1	1:B:178:GLY:HA2	2.34	0.57
1:C:230:GLY:O	2:F:1:QSC:HBF	2.04	0.57
1:C:335:ALA:HB1	1:C:339:GLU:OE1	2.04	0.57
1:B:242:GLU:HB3	1:B:246:LYS:HE2	1.85	0.57
1:B:36:SER:HB3	1:B:122:ALA:O	2.04	0.57
1:A:189:TRP:O	1:A:353:GLY:HA2	2.05	0.57
1:B:257:PHE:CB	1:B:258:PRO:CD	2.82	0.57
1:C:78:GLY:HA3	1:C:101:ALA:O	2.05	0.57
1:C:292:THR:HG22	1:C:293:ASN:ND2	2.20	0.57
1:B:241:PHE:CD2	1:B:326:GLN:HB3	2.40	0.57
1:C:21:GLY:HA2	1:C:83:ASP:OD1	2.03	0.56
1:B:8:GLY:C	1:B:10:SER:N	2.59	0.56
1:B:47:PHE:CZ	1:B:111:ASN:HB2	2.40	0.56
1:B:40:VAL:CG2	1:B:52:TYR:HB2	2.35	0.56
1:C:193:ILE:HG12	1:C:352:ILE:HD12	1.87	0.56
1:B:74:GLY:C	1:B:75:LYS:HG3	2.25	0.56
1:B:267:LEU:HD23	1:B:267:LEU:N	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:TYR:HD2	1:C:351:ARG:HG3	1.71	0.55
1:A:45:HIS:ND1	1:A:46:PRO:HD2	2.22	0.55
1:C:45:HIS:HE1	1:C:47:PHE:CD1	2.25	0.55
1:C:20:VAL:HG12	1:C:85:VAL:HG22	1.88	0.55
1:C:261:PHE:HE1	1:C:268:VAL:HG22	1.72	0.55
1:B:257:PHE:HB3	1:B:258:PRO:CD	2.37	0.55
1:A:110:ILE:HB	1:A:113:SER:HB3	1.88	0.54
1:A:314:THR:O	1:A:315:SER:CB	2.54	0.54
1:C:205:ARG:HB3	1:C:286:TYR:HB2	1.88	0.54
1:B:55:GLN:O	1:B:56:LEU:HD23	2.07	0.54
1:C:-3:GLY:O	1:C:-2:SER:CB	2.56	0.54
1:C:188:LEU:HD23	1:C:355:ALA:CB	2.35	0.54
1:C:8:GLY:O	1:C:170:VAL:HB	2.07	0.54
1:A:82:THR:O	1:A:83:ASP:HB2	2.07	0.53
1:A:188:LEU:HD23	1:A:355:ALA:HB2	1.90	0.53
1:C:131:ASP:OD1	1:C:131:ASP:N	2.40	0.53
1:C:9:LYS:O	1:C:10:SER:CB	2.54	0.53
1:C:74:GLY:C	1:C:75:LYS:HG3	2.28	0.53
1:B:188:LEU:CB	1:B:355:ALA:HB2	2.33	0.53
1:C:2:MET:HG2	1:C:90:GLY:HA2	1.90	0.53
1:C:71:TYR:HD1	2:F:4:LEU:HA	1.74	0.53
1:B:26:THR:HG22	1:B:50:ARG:HH12	1.72	0.53
1:B:209:ASN:HB2	1:B:281:PRO:HB3	1.90	0.53
1:C:74:GLY:HA3	1:C:107:LYS:O	2.09	0.53
1:B:71:TYR:CD1	2:E:3:PSA:HB2	2.44	0.53
1:B:310:GLU:O	1:B:311:ASP:CB	2.57	0.53
1:B:385:ASN:OD1	1:B:385:ASN:N	2.42	0.52
1:A:175:ILE:O	1:A:175:ILE:HG22	2.08	0.52
2:D:4:LEU:HG	2:D:5:ALA:N	2.23	0.52
1:C:42:ALA:CB	1:C:101:ALA:HB1	2.38	0.52
1:C:198:TYR:CE2	1:C:224:LYS:HE3	2.44	0.52
1:B:376:THR:HG22	1:B:379:MET:HG2	1.91	0.52
1:C:386:ILE:O	1:C:386:ILE:HG12	2.09	0.52
1:C:241:PHE:O	1:C:245:VAL:HG23	2.10	0.51
1:A:261:PHE:CE1	1:A:268:VAL:CG2	2.94	0.51
1:C:36:SER:OG	1:C:126:ILE:HG13	2.11	0.51
1:C:204:VAL:HG12	1:C:382:CYS:SG	2.51	0.51
1:A:222:TYR:O	1:A:223:ASP:HB2	2.10	0.51
1:B:148:ASN:HB3	1:B:348:ALA:HB2	1.93	0.51
1:B:244:ALA:O	1:B:248:ILE:HG13	2.12	0.50
1:C:93:VAL:CG1	1:C:144:THR:HG21	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:TYR:OH	1:A:297:ARG:NH1	2.45	0.50
1:B:2:MET:HG2	1:B:90:GLY:HA2	1.92	0.50
1:C:22:SER:HG	1:C:59:THR:HG1	1.59	0.50
1:B:267:LEU:O	1:B:268:VAL:HG23	2.12	0.50
1:C:26:THR:HG22	1:C:50:ARG:NH1	2.26	0.50
1:C:73:GLN:O	2:F:3:PSA:HE1	2.11	0.50
1:A:291:VAL:O	1:A:294:GLN:HB3	2.12	0.50
1:B:14:TYR:O	1:B:30:LEU:HD12	2.12	0.49
1:C:197:TRP:N	1:C:197:TRP:CD1	2.79	0.49
1:C:335:ALA:HB2	2:F:1:QSC:HAT	1.93	0.49
1:A:205:ARG:HD3	1:A:286:TYR:CE1	2.48	0.49
1:A:228:ASP:C	1:A:228:ASP:OD1	2.48	0.49
1:B:198:TYR:CE2	1:B:224:LYS:HE3	2.48	0.49
2:E:3:PSA:N	2:E:3:PSA:CD2	2.73	0.49
1:A:280:PHE:HB2	1:A:302:PRO:HG3	1.95	0.49
1:B:149:LEU:CD2	1:B:346:ASP:HA	2.40	0.49
1:A:277:TRP:HE3	1:A:302:PRO:HB2	1.77	0.49
1:B:197:TRP:CG	1:B:198:TYR:N	2.81	0.49
1:C:143:GLN:O	1:C:144:THR:HG23	2.12	0.49
1:C:241:PHE:CZ	1:C:245:VAL:HG21	2.48	0.49
1:C:356:VAL:CG2	1:C:369:ALA:HA	2.43	0.49
1:B:205:ARG:HD3	1:B:286:TYR:CD1	2.47	0.49
1:A:16:VAL:HG13	1:A:16:VAL:O	2.13	0.48
1:A:30:LEU:HD13	1:A:115:TRP:CE2	2.48	0.48
1:A:301:LEU:HB3	1:A:302:PRO:HD2	1.95	0.48
1:A:42:ALA:CB	1:A:101:ALA:HB1	2.44	0.48
1:A:235:ARG:HB2	1:A:332:VAL:HB	1.95	0.48
1:C:71:TYR:HB3	2:F:3:PSA:HD1	1.95	0.48
1:A:159:PHE:CE2	1:A:318:ASP:HB3	2.49	0.48
1:C:-4:ARG:CG	1:C:-4:ARG:NH1	2.76	0.48
1:A:113:SER:HB2	1:A:115:TRP:NE1	2.27	0.48
1:B:8:GLY:HA3	1:B:170:VAL:CG1	2.43	0.48
1:C:193:ILE:CG1	1:C:352:ILE:HD12	2.43	0.48
1:C:300:ILE:HD13	1:C:337:ILE:HD13	1.96	0.48
1:B:57:SER:C	1:B:59:THR:H	2.18	0.47
1:C:45:HIS:ND1	1:C:46:PRO:HD2	2.29	0.47
1:C:45:HIS:HB3	1:C:48:LEU:HG	1.97	0.47
1:C:95:VAL:HG23	1:C:96:ARG:N	2.30	0.47
1:C:183:LEU:HD12	1:C:342:TYR:CE1	2.49	0.47
1:B:15:TYR:CD1	1:B:28:ASN:HB3	2.49	0.47
1:B:302:PRO:HA	1:B:305:TYR:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LEU:HD12	1:A:140:LEU:O	2.13	0.47
1:A:152:LEU:HD22	1:A:154:LEU:HD21	1.96	0.47
1:C:26:THR:HG22	1:C:50:ARG:HH12	1.80	0.47
1:B:103:THR:O	1:B:104:GLU:HG3	2.15	0.47
1:C:261:PHE:CE1	1:C:268:VAL:CG2	2.98	0.47
1:A:29:ILE:HG21	1:A:119:LEU:HB2	1.96	0.47
1:A:245:VAL:O	1:A:249:LYS:HB2	2.15	0.47
1:A:197:TRP:CG	1:A:198:TYR:N	2.83	0.46
1:A:205:ARG:HD3	1:A:286:TYR:CD1	2.50	0.46
1:B:246:LYS:H	1:B:246:LYS:CD	2.17	0.46
1:C:74:GLY:H	1:C:107:LYS:HE2	1.80	0.46
1:C:208:ILE:HG22	1:C:281:PRO:HB2	1.96	0.46
1:B:360:HIS:CE1	1:B:362:HIS:CD2	2.98	0.46
1:B:3:VAL:HG13	1:B:183:LEU:HD21	1.98	0.46
1:A:26:THR:HG22	1:A:50:ARG:HH21	1.81	0.46
1:B:243:ALA:CA	1:B:246:LYS:HD3	2.45	0.46
1:C:217:CYS:HB3	1:C:382:CYS:HA	1.96	0.46
1:C:277:TRP:HE3	1:C:302:PRO:HB2	1.81	0.46
1:A:304:GLN:HB3	1:A:336:VAL:O	2.16	0.46
2:F:3:PSA:CD1	2:F:3:PSA:N	2.78	0.45
1:B:40:VAL:HG23	1:B:41:GLY:O	2.16	0.45
1:B:276:PRO:HG2	1:B:279:ILE:HD11	1.98	0.45
1:C:153:GLN:HB2	1:C:342:TYR:HD1	1.82	0.45
1:B:47:PHE:CD1	1:B:111:ASN:HB2	2.51	0.45
1:C:124:ALA:HB2	1:C:135:PRO:CG	2.47	0.45
1:A:71:TYR:CE2	1:A:108:PHE:CE1	3.05	0.45
1:A:286:TYR:CD2	1:A:297:ARG:HB3	2.52	0.45
1:B:8:GLY:HA3	1:B:170:VAL:HG12	1.99	0.45
1:C:126:ILE:CG2	1:C:197:TRP:HB2	2.46	0.45
1:C:245:VAL:O	1:C:249:LYS:HB2	2.17	0.45
1:C:14:TYR:O	1:C:30:LEU:HD12	2.16	0.45
1:C:110:ILE:HB	1:C:113:SER:HB3	1.97	0.45
1:A:63:LEU:HB2	1:A:80:LEU:O	2.17	0.44
1:B:2:MET:CG	1:B:90:GLY:HA2	2.46	0.44
1:C:340:GLY:HA2	1:C:360:HIS:HB2	1.98	0.44
1:A:113:SER:HB2	1:A:115:TRP:CD1	2.52	0.44
1:B:197:TRP:CD1	1:B:198:TYR:N	2.85	0.44
1:C:93:VAL:HG12	1:C:144:THR:HG21	1.99	0.44
1:C:126:ILE:HG23	1:C:197:TRP:HB2	2.00	0.44
1:A:235:ARG:O	1:A:331:THR:HA	2.18	0.44
1:A:335:ALA:O	1:A:339:GLU:HB2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:ILE:HG21	1:C:119:LEU:HB2	1.98	0.44
1:A:385:ASN:C	1:A:386:ILE:HG23	2.38	0.44
1:B:42:ALA:O	1:B:43:ALA:HB2	2.17	0.44
1:B:71:TYR:CE1	2:E:3:PSA:HB2	2.52	0.44
1:B:233:ASN:HA	1:B:336:VAL:CG2	2.47	0.44
1:B:252:SER:O	1:B:253:SER:CB	2.65	0.44
1:B:242:GLU:HB2	1:B:243:ALA:H	1.67	0.44
2:F:5:ALA:HA	2:F:6:ZAE:H11	1.74	0.44
1:A:95:VAL:HG21	1:A:140:LEU:HA	1.98	0.44
1:B:300:ILE:O	1:B:300:ILE:HG13	2.16	0.44
1:C:95:VAL:CG2	1:C:96:ARG:N	2.79	0.44
1:A:197:TRP:CD1	1:A:198:TYR:N	2.85	0.44
1:B:4:ASP:HA	1:B:172:GLY:O	2.17	0.44
1:C:204:VAL:HG11	1:C:379:MET:HG2	2.00	0.44
1:A:95:VAL:HG12	1:A:96:ARG:N	2.33	0.43
1:B:134:GLU:HA	1:B:135:PRO:HD3	1.90	0.43
1:A:277:TRP:CE3	1:A:303:GLN:HG3	2.54	0.43
1:C:-3:GLY:O	1:C:-2:SER:HB3	2.19	0.43
1:B:76:TRP:CE3	1:B:102:ILE:HG12	2.53	0.43
1:B:208:ILE:CD1	1:B:283:ILE:HG12	2.48	0.43
1:C:75:LYS:HD2	1:C:106:ASP:HB3	2.00	0.43
1:A:378:ASP:O	1:A:381:ASP:HB2	2.19	0.43
1:C:69:VAL:HG11	1:C:71:TYR:CE1	2.53	0.43
1:B:45:HIS:CG	1:B:46:PRO:HD2	2.53	0.43
1:B:193:ILE:HG13	1:B:351:ARG:HA	2.01	0.43
1:C:26:THR:O	1:C:27:LEU:HD23	2.18	0.43
1:C:208:ILE:HG22	1:C:281:PRO:CB	2.48	0.43
1:C:124:ALA:HB2	1:C:135:PRO:CD	2.48	0.43
1:C:270:TRP:CE3	1:C:275:THR:HG23	2.54	0.43
1:A:276:PRO:O	1:A:279:ILE:HG12	2.19	0.43
1:A:61:ARG:NH2	1:C:3:VAL:HG13	2.32	0.43
1:A:341:PHE:C	1:A:357:SER:HB2	2.40	0.43
1:C:149:LEU:HD12	1:C:346:ASP:HA	2.01	0.43
1:A:95:VAL:HG13	1:A:143:GLN:CB	2.49	0.43
1:B:113:SER:HB2	1:B:115:TRP:NE1	2.34	0.43
1:C:41:GLY:HA2	1:C:102:ILE:HB	2.00	0.42
1:B:253:SER:N	1:B:254:THR:HA	2.33	0.42
1:C:22:SER:OG	1:C:59:THR:OG1	2.29	0.42
2:E:5:ALA:HA	2:E:6:ZAE:H11	1.76	0.42
1:B:232:THR:O	1:B:336:VAL:HG23	2.19	0.42
1:C:124:ALA:O	1:C:131:ASP:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:TYR:HB3	3:C:514:HOH:O	2.19	0.42
1:A:128:ARG:HD3	3:A:524:HOH:O	2.17	0.42
1:A:362:HIS:CD2	1:A:362:HIS:C	2.93	0.42
1:B:232:THR:OG1	2:E:1:QSC:CBE	2.68	0.42
1:A:386:ILE:HG12	1:A:386:ILE:O	2.20	0.42
1:C:45:HIS:CE1	1:C:46:PRO:HD2	2.55	0.42
1:C:294:GLN:O	1:C:379:MET:HE1	2.19	0.42
2:F:6:ZAE:O	2:F:7:PLJ:C	2.67	0.42
1:C:15:TYR:HB2	1:C:29:ILE:O	2.20	0.42
1:C:48:LEU:HD21	1:C:109:PHE:CD2	2.55	0.42
1:C:80:LEU:HD23	1:C:80:LEU:HA	1.82	0.42
1:A:43:ALA:HB1	1:A:44:PRO:HD2	2.00	0.41
1:C:-4:ARG:O	1:C:-3:GLY:O	2.38	0.41
1:A:222:TYR:O	1:A:223:ASP:CB	2.68	0.41
1:A:280:PHE:HB2	1:A:302:PRO:CG	2.50	0.41
1:A:294:GLN:O	1:A:379:MET:HE1	2.19	0.41
1:A:304:GLN:O	1:A:336:VAL:HG13	2.20	0.41
1:B:205:ARG:HD3	1:B:286:TYR:CE1	2.56	0.41
1:C:10:SER:HB2	1:C:170:VAL:HG21	2.03	0.41
1:A:95:VAL:CG1	1:A:143:GLN:CB	2.99	0.41
1:A:384:TYR:CG	1:A:385:ASN:N	2.88	0.41
1:B:288:MET:HE3	1:B:379:MET:HB3	2.01	0.41
1:B:305:TYR:O	1:B:306:LEU:HD23	2.19	0.41
1:C:47:PHE:CE2	1:C:111:ASN:HB2	2.56	0.41
1:A:95:VAL:HG12	1:A:96:ARG:H	1.86	0.41
1:B:207:GLU:HB2	1:B:284:SER:HB2	2.02	0.41
1:B:213:LEU:HD12	1:B:213:LEU:HA	1.87	0.41
1:B:257:PHE:HB3	1:B:258:PRO:HD3	2.01	0.41
1:A:22:SER:OG	1:A:59:THR:CB	2.69	0.41
1:C:35:SER:O	1:C:120:GLY:CA	2.69	0.41
1:C:72:THR:HB	2:F:2:ZSC:OAK	2.21	0.41
1:A:307[B]:ARG:CG	1:A:323:ALA:HB2	2.38	0.41
1:B:242:GLU:O	1:B:245:VAL:N	2.53	0.41
1:C:63:LEU:HD11	1:C:82:THR:HG23	2.03	0.41
1:C:76:TRP:CD2	1:C:102:ILE:HD12	2.56	0.41
1:C:269:CYS:HA	1:C:318:ASP:O	2.20	0.41
1:C:386:ILE:O	1:C:386:ILE:CG1	2.68	0.41
2:D:5:ALA:HA	2:D:6:ZAE:H11	1.94	0.41
1:A:129:PRO:O	1:A:130:ASP:HB3	2.21	0.41
1:B:271:GLN:O	1:B:274:THR:HG23	2.21	0.41
1:C:235:ARG:CZ	1:C:327:SER:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:THR:O	1:B:275:THR:C	2.59	0.40
1:C:54:ARG:HB3	1:C:60:TYR:CD1	2.56	0.40
1:C:71:TYR:CB	2:F:3:PSA:HD1	2.50	0.40
1:A:52:TYR:OH	1:A:83:ASP:OD2	2.25	0.40
1:A:203:ILE:HD13	1:A:285:LEU:HD13	2.03	0.40
1:A:317:ASP:OD1	1:A:317:ASP:N	2.53	0.40
1:B:378:ASP:O	1:B:381:ASP:HB2	2.22	0.40
1:C:147:PRO:O	1:C:149:LEU:N	2.52	0.40
1:A:133:LEU:O	1:A:134:GLU:C	2.58	0.40
1:A:244:ALA:O	1:A:248:ILE:HG13	2.22	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	372/433 (86%)	342 (92%)	24 (6%)	6 (2%)	9	33
1	B	368/433 (85%)	329 (89%)	31 (8%)	8 (2%)	6	25
1	C	371/433 (86%)	334 (90%)	27 (7%)	10 (3%)	5	21
2	D	2/7 (29%)	2 (100%)	0	0	100	100
2	E	2/7 (29%)	2 (100%)	0	0	100	100
2	F	2/7 (29%)	2 (100%)	0	0	100	100
All	All	1117/1320 (85%)	1011 (90%)	82 (7%)	24 (2%)	6	26

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	ASP
1	A	315	SER

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Mol	Chain	Res	Type
1	B	253	SER
1	B	256	LYS
1	B	361	VAL
1	C	-2	SER
1	C	-1	PHE
1	C	10	SER
1	B	242	GLU
1	C	-3	GLY
1	C	83	ASP
1	C	91	PRO
1	C	310	GLU
1	A	10	SER
1	C	148	ASN
1	A	83	ASP
1	B	9	LYS
1	B	10	SER
1	C	88	PRO
1	C	217	CYS
1	B	243	ALA
1	A	70	PRO
1	B	257	PHE
1	A	88	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	302/370 (82%)	280 (93%)	22 (7%)	14	40
1	B	299/370 (81%)	271 (91%)	28 (9%)	8	28
1	C	304/370 (82%)	271 (89%)	33 (11%)	6	22
2	D	1/1 (100%)	1 (100%)	0	100	100
2	E	1/1 (100%)	0	1 (100%)	0	0
2	F	1/1 (100%)	0	1 (100%)	0	0
All	All	908/1113 (82%)	823 (91%)	85 (9%)	8	28

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	SER
1	A	25	GLN
1	A	36	SER
1	A	40	VAL
1	A	49	HIS
1	A	50	ARG
1	A	55	GLN
1	A	61	ARG
1	A	94	THR
1	A	95	VAL
1	A	173	SER
1	A	196	GLU
1	A	197	TRP
1	A	225	SER
1	A	232	THR
1	A	268	VAL
1	A	275	THR
1	A	317	ASP
1	A	329	THR
1	A	367	THR
1	A	381	ASP
1	A	386	ILE
1	B	12	GLN
1	B	36	SER
1	B	37	ASN
1	B	40	VAL
1	B	73	GLN
1	B	75	LYS
1	B	77	GLU
1	B	105	SER
1	B	125	GLU
1	B	149	LEU
1	B	185	THR
1	B	188	LEU
1	B	195	ARG
1	B	197	TRP
1	B	213	LEU
1	B	224	LYS
1	B	234	LEU
1	B	246	LYS
1	B	247	SER
1	B	256	LYS

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Mol	Chain	Res	Type
1	B	257	PHE
1	B	267	LEU
1	B	275	THR
1	B	278	ASN
1	B	315	SER
1	B	325	SER
1	B	329	THR
1	B	385	ASN
1	C	-4	ARG
1	C	-1	PHE
1	C	36	SER
1	C	53	GLN
1	C	59	THR
1	C	72	THR
1	C	75	LYS
1	C	95	VAL
1	C	96	ARG
1	C	104	GLU
1	C	125	GLU
1	C	128	ARG
1	C	141	VAL
1	C	144	THR
1	C	149	LEU
1	C	181	HIS
1	C	185	THR
1	C	187	SER
1	C	195	ARG
1	C	197	TRP
1	C	203	ILE
1	C	217	CYS
1	C	224	LYS
1	C	254	THR
1	C	268	VAL
1	C	278	ASN
1	C	290	GLU
1	C	327	SER
1	C	328	SER
1	C	339	GLU
1	C	376	THR
1	C	378	ASP
1	C	386	ILE
2	E	4	LEU

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Mol	Chain	Res	Type
2	F	4	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	293	ASN
1	B	362	HIS
1	C	293	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

9 non-standard protein/DNA/RNA residues 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	ZAE	D	6	2	11,12,13	3.91	6 (54%)	13,14,16	1.00	1 (7%)
2	PLJ	D	7	2	9,9,9	1.39	2 (22%)	11,11,11	1.54	4 (36%)
2	ZAE	F	6	2	11,12,13	3.72	6 (54%)	13,14,16	2.46	7 (53%)
2	ZAE	E	6	2	11,12,13	3.73	6 (54%)	13,14,16	1.27	3 (23%)
2	PLJ	F	7	2	9,9,9	1.30	1 (11%)	11,11,11	1.49	2 (18%)
2	PSA	F	3	2	14,14,15	3.38	6 (42%)	15,17,19	2.43	7 (46%)
2	PSA	D	3	2	14,14,15	3.61	7 (50%)	15,17,19	1.32	2 (13%)
2	PLJ	E	7	2	9,9,9	1.34	2 (22%)	11,11,11	1.50	4 (36%)
2	PSA	E	3	2	14,14,15	3.43	8 (57%)	15,17,19	2.01	3 (20%)

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	ZAE	D	6	2	-	0/5/8/10	0/1/1/1
2	PLJ	D	7	2	-	1/6/13/13	0/1/1/1
2	ZAE	F	6	2	-	1/5/8/10	0/1/1/1
2	ZAE	E	6	2	-	2/5/8/10	0/1/1/1
2	PLJ	F	7	2	-	4/6/13/13	0/1/1/1
2	PSA	F	3	2	-	7/11/11/12	0/1/1/1
2	PSA	D	3	2	-	6/11/11/12	0/1/1/1
2	PLJ	E	7	2	-	3/6/13/13	0/1/1/1
2	PSA	E	3	2	-	6/11/11/12	0/1/1/1

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	3	PSA	CD2-CG	6.25	1.52	1.38
2	D	3	PSA	CE2-CD2	6.02	1.51	1.38
2	D	6	ZAE	CD2-CG	5.92	1.51	1.38
2	D	6	ZAE	CE1-CD1	5.80	1.51	1.38
2	D	3	PSA	CD2-CG	5.78	1.51	1.38
2	D	3	PSA	CE1-CD1	5.77	1.51	1.38
2	E	6	ZAE	CD2-CG	5.66	1.51	1.38
2	E	3	PSA	CD2-CG	5.51	1.50	1.38
2	F	6	ZAE	CE1-CD1	5.47	1.50	1.38
2	F	6	ZAE	CD1-CG	5.42	1.50	1.38
2	D	6	ZAE	CZ-CE1	5.33	1.52	1.38
2	F	6	ZAE	CZ-CE1	5.32	1.52	1.38
2	D	3	PSA	CD1-CG	5.32	1.50	1.38
2	F	3	PSA	CE2-CD2	5.29	1.50	1.38
2	E	3	PSA	CE1-CD1	5.24	1.50	1.38
2	E	3	PSA	CE2-CD2	5.16	1.49	1.38
2	E	6	ZAE	CZ-CE1	5.15	1.51	1.38
2	E	6	ZAE	CE1-CD1	5.13	1.49	1.38
2	D	6	ZAE	CE2-CD2	5.12	1.49	1.38
2	F	6	ZAE	CD2-CG	4.97	1.49	1.38
2	E	6	ZAE	CE2-CD2	4.97	1.49	1.38
2	E	3	PSA	CD1-CG	4.94	1.49	1.38
2	E	6	ZAE	CD1-CG	4.90	1.49	1.38
2	D	6	ZAE	CD1-CG	4.86	1.49	1.38
2	F	3	PSA	CD1-CG	4.83	1.49	1.38
2	F	3	PSA	CE1-CD1	4.68	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	3	PSA	CZ-CE1	4.59	1.50	1.38
2	D	3	PSA	CZ-CE1	4.51	1.50	1.38
2	D	6	ZAE	CZ-CE2	4.47	1.49	1.38
2	E	3	PSA	CZ-CE2	4.37	1.49	1.38
2	F	6	ZAE	CZ-CE2	4.32	1.49	1.38
2	E	3	PSA	CZ-CE1	4.31	1.49	1.38
2	F	6	ZAE	CE2-CD2	4.30	1.48	1.38
2	E	6	ZAE	CZ-CE2	4.26	1.49	1.38
2	D	3	PSA	CZ-CE2	4.18	1.49	1.38
2	F	3	PSA	CZ-CE2	3.79	1.48	1.38
2	D	7	PLJ	OXT-C	2.78	1.40	1.33
2	E	3	PSA	OH-CH	-2.66	1.37	1.43
2	D	3	PSA	OH-CH	-2.59	1.37	1.43
2	F	7	PLJ	OXT-C	2.59	1.39	1.33
2	E	7	PLJ	OXT-CM	-2.55	1.39	1.45
2	E	3	PSA	CM-C	2.50	1.56	1.49
2	E	7	PLJ	OXT-C	2.44	1.39	1.33
2	D	7	PLJ	OXT-CM	-2.32	1.39	1.45

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	3	PSA	OH-CH-CM	5.09	120.00	109.08
2	E	3	PSA	OH-CH-CM	5.08	119.97	109.08
2	F	3	PSA	CM-CH-CA	4.92	120.67	112.94
2	F	6	ZAE	CB-CG-CD2	-4.61	111.76	120.91
2	E	3	PSA	OH-CH-CA	3.36	115.47	109.40
2	F	6	ZAE	CB-CA-N	-3.28	105.57	110.65
2	D	3	PSA	OH-CH-CA	3.27	115.31	109.40
2	F	7	PLJ	OXT-C-CA	3.24	119.80	111.52
2	D	7	PLJ	OXT-C-CA	2.88	118.88	111.52
2	E	3	PSA	CG-CB-CA	-2.84	107.43	113.46
2	F	6	ZAE	CD2-CG-CD1	2.83	122.62	118.17
2	F	3	PSA	CZ-CE2-CD2	-2.74	116.02	120.19
2	F	6	ZAE	CZ-CE2-CD2	-2.68	116.10	120.19
2	F	6	ZAE	CB-CA-C	2.60	116.58	111.65
2	E	7	PLJ	C-CA-N	2.56	115.74	111.08
2	F	6	ZAE	CE1-CD1-CG	-2.56	116.71	120.63
2	F	3	PSA	CB-CG-CD1	-2.53	115.88	120.91
2	D	6	ZAE	C10-N-CA	2.47	121.33	113.64
2	E	7	PLJ	OXT-C-O	-2.42	119.11	123.84
2	F	6	ZAE	CB-CG-CD1	2.38	125.63	120.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	7	PLJ	OXT-C-O	-2.35	119.24	123.84
2	D	7	PLJ	OXT-C-O	-2.34	119.27	123.84
2	F	3	PSA	CE1-CD1-CG	-2.32	117.07	120.63
2	D	7	PLJ	CM-OXT-C	2.28	121.09	115.94
2	E	7	PLJ	OXT-C-CA	2.22	117.21	111.52
2	D	3	PSA	OH-CH-CM	2.22	113.83	109.08
2	D	7	PLJ	O-C-CA	-2.21	117.33	123.92
2	E	6	ZAE	CG-CB-CA	-2.19	110.49	113.63
2	F	3	PSA	CD2-CG-CD1	2.13	121.52	118.17
2	E	7	PLJ	CM-OXT-C	2.08	120.65	115.94
2	F	3	PSA	CH-CM-C	-2.05	109.51	113.11
2	E	6	ZAE	CB-CA-N	-2.02	107.52	110.65
2	E	6	ZAE	C10-N-CA	2.01	119.88	113.64

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3	PSA	CH-CA-CB-CG
2	D	3	PSA	N-CA-CH-CM
2	D	3	PSA	CB-CA-CH-CM
2	D	3	PSA	O-C-CM-CH
2	E	3	PSA	OH-CH-CM-C
2	E	3	PSA	O-C-CM-CH
2	F	3	PSA	CH-CA-CB-CG
2	F	3	PSA	N-CA-CH-CM
2	F	3	PSA	CB-CA-CH-CM
2	F	3	PSA	CA-CH-CM-C
2	F	3	PSA	OH-CH-CM-C
2	F	7	PLJ	OXT-C-CA-CB
2	F	7	PLJ	OXT-C-CA-N
2	F	6	ZAE	C-CA-CB-CG
2	E	7	PLJ	CA-C-OXT-CM
2	E	7	PLJ	O-C-OXT-CM
2	D	3	PSA	N-CA-CB-CG
2	F	7	PLJ	O-C-CA-CB
2	D	3	PSA	CB-CA-CH-OH
2	E	3	PSA	N-CA-CB-CG
2	F	3	PSA	N-CA-CB-CG
2	F	7	PLJ	O-C-CA-N
2	E	3	PSA	CA-CB-CG-CD2
2	E	3	PSA	CH-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	E	6	ZAE	CA-CB-CG-CD2
2	E	3	PSA	CA-CB-CG-CD1
2	E	6	ZAE	CA-CB-CG-CD1
2	F	3	PSA	O-C-CM-CH
2	D	7	PLJ	OXT-C-CA-CB
2	E	7	PLJ	OXT-C-CA-CB

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	6	ZAE	1	0
2	F	6	ZAE	2	0
2	E	6	ZAE	1	0
2	F	7	PLJ	2	0
2	F	3	PSA	4	0
2	D	3	PSA	1	0
2	E	3	PSA	3	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	377/433 (87%)	-0.11	6 (1%) 72 49	38, 52, 79, 132	0
1	B	374/433 (86%)	-0.12	3 (0%) 86 70	43, 59, 83, 121	0
1	C	377/433 (87%)	-0.22	0 100 100	40, 55, 72, 101	0
2	D	2/7 (28%)	-0.24	0 100 100	41, 41, 41, 46	0
2	E	2/7 (28%)	-0.06	0 100 100	49, 49, 49, 50	0
2	F	2/7 (28%)	-0.05	0 100 100	51, 51, 51, 53	0
All	All	1134/1320 (85%)	-0.15	9 (0%) 86 70	38, 55, 79, 132	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	314	THR	3.4
1	A	158	GLY	2.9
1	A	159	PHE	2.8
1	A	317	ASP	2.3
1	B	21	GLY	2.3
1	B	253	SER	2.3
1	B	23	PRO	2.2
1	A	319	CYS	2.2
1	A	313	ALA	2.2

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

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	PSA	D	3	14/15	0.96	0.28	37,43,50,51	0
2	PLJ	E	7	9/9	0.96	0.31	51,52,58,61	0
2	PLJ	F	7	9/9	0.96	0.27	52,56,58,65	0
2	ZAE	F	6	12/13	0.96	0.27	49,57,64,65	0
2	PSA	F	3	14/15	0.97	0.22	42,45,50,50	0
2	PSA	E	3	14/15	0.97	0.24	46,47,51,53	0
2	ZAE	E	6	12/13	0.97	0.27	49,53,57,61	0
2	PLJ	D	7	9/9	0.97	0.26	46,49,60,61	0
2	ZAE	D	6	12/13	0.98	0.19	41,44,50,53	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.