



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:53 PM UTC

PDB ID : 3UQR / pdb_00003uqr
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

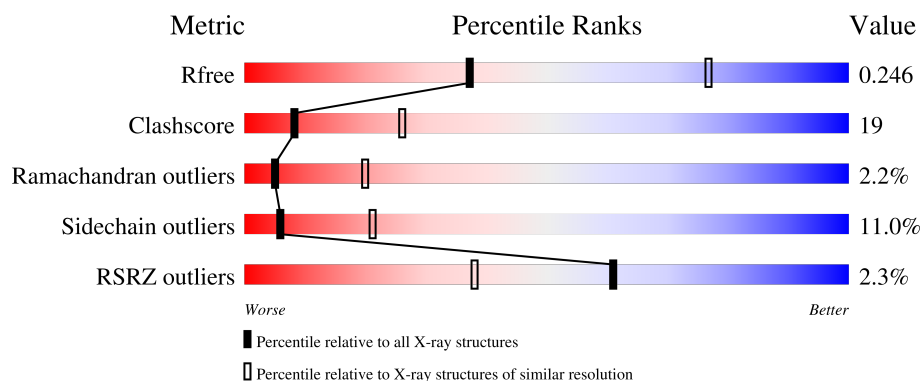
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.06 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}	180053	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (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	2% 57% 26% 13%
1	B	433	3% 56% 26% 5% 14%
1	C	433	2% 50% 31% 6% 13%
2	D	7	14% 43% 29% 14%
2	E	7	14% 43% 29% 14%

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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	E	3	-	X	-	-
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			

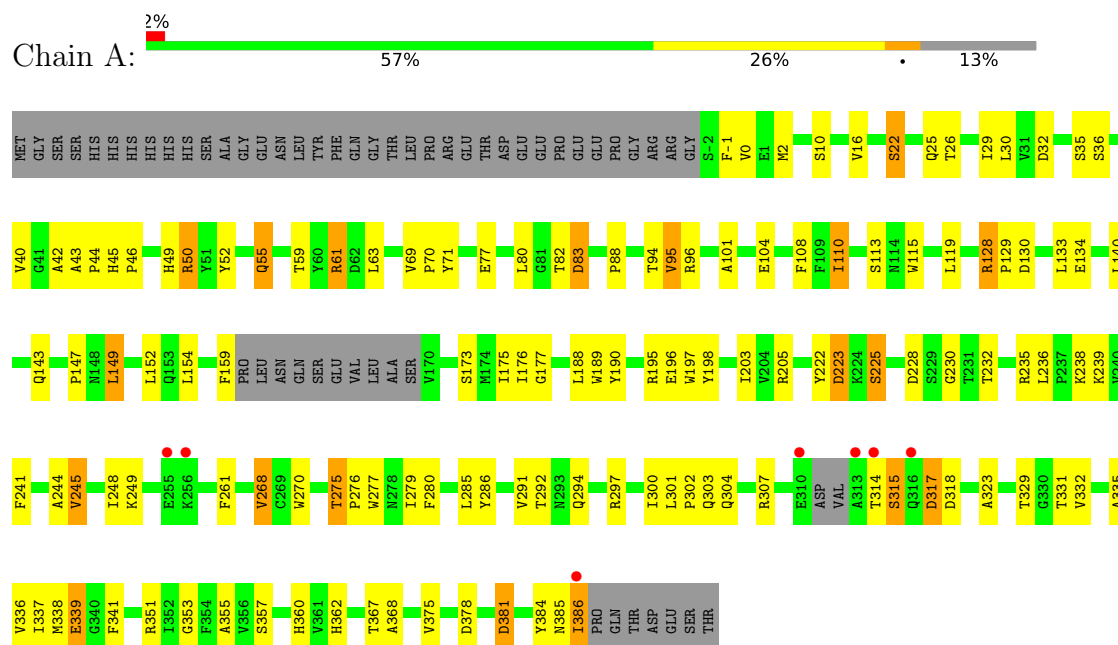
- Molecule 3 is water.

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		

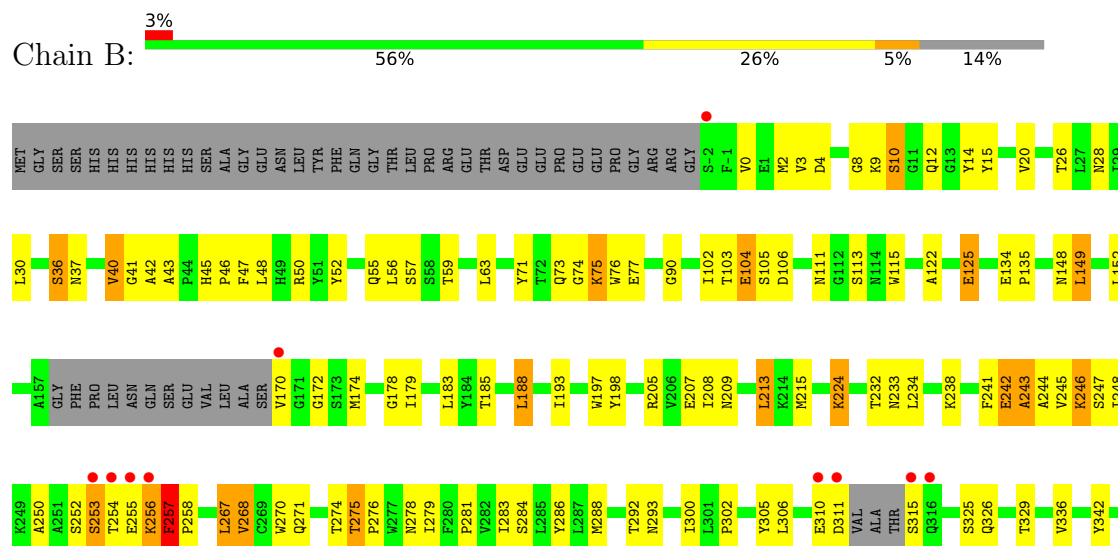
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Beta-secretase 1

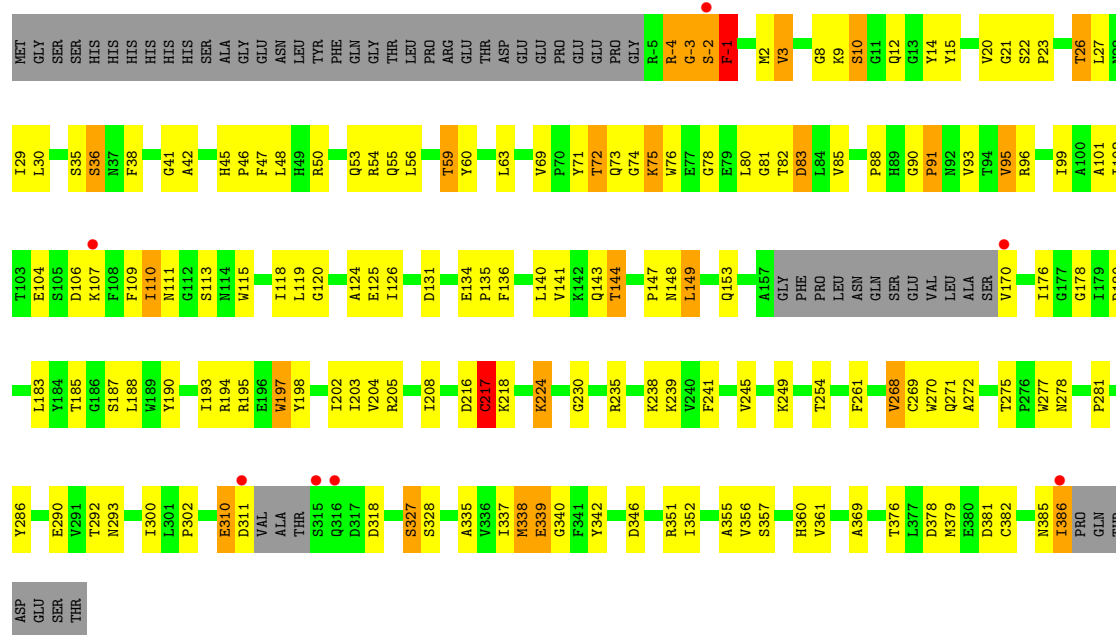


• Molecule 1: Beta-secretase 1

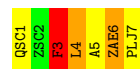




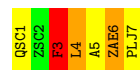
• Molecule 1: Beta-secretase 1



• Molecule 2: METHYL (2S)-1-[(2R,5S,8S,12S,13S)-2,13-DIBENZYL-12-HYDROXY-3,5-DIMETHYL-15-(3-[METHYL(METHYLSULFONYL)AMINO]-5-[[[(1R)-1-PHENYLETHYL]CARBAMOYL]PHENYL)-8-(2-METHYLPROPYL)-4,7,10,15-TETRAOXO-3,6,9,14-TETRAAZAPEN-1-TADECAN-1-OYL]PYRROLIDINE-2-CARBOXYLATE



• Molecule 2: METHYL (2S)-1-[(2R,5S,8S,12S,13S)-2,13-DIBENZYL-12-HYDROXY-3,5-DIMETHYL-15-(3-[METHYL(METHYLSULFONYL)AMINO]-5-[[[(1R)-1-PHENYLETHYL]CARBAMOYL]PHENYL)-8-(2-METHYLPROPYL)-4,7,10,15-TETRAOXO-3,6,9,14-TETRAAZAPEN-1-TADECAN-1-OYL]PYRROLIDINE-2-CARBOXYLATE



• Molecule 2: METHYL (2S)-1-[(2R,5S,8S,12S,13S)-2,13-DIBENZYL-12-HYDROXY-3,5-DIMETHYL-15-(3-[METHYL(METHYLSULFONYL)AMINO]-5-[[[(1R)-1-PHENYLETHYL]CARBAMOYL]PHENYL)-8-(2-METHYLPROPYL)-4,7,10,15-TETRAOXO-3,6,9,14-TETRAAZAPEN-1-TADECAN-1-OYL]PYRROLIDINE-2-CARBOXYLATE



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 66.06 – 3.06	Depositor EDS
% Data completeness (in resolution range)	91.7 (66.06-3.06) 96.4 (66.06-3.06)	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 0.192 , 0.246	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 , 49.7	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	0.55	0/2978	0.89	0/4059
1	B	0.52	0/2942	0.92	1/4013 (0.0%)
1	C	0.56	0/2975	0.91	3/4055 (0.1%)
2	D	2.16	1/12 (8.3%)	1.25	0/15
2	E	2.17	1/12 (8.3%)	2.04	0/15
2	F	2.29	1/12 (8.3%)	2.15	0/15
All	All	0.56	3/8931 (0.0%)	0.91	4/12172 (0.0%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	4	LEU	C-N	6.99	1.43	1.33
2	D	4	LEU	C-N	6.93	1.43	1.33
2	E	4	LEU	C-N	6.76	1.42	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	LEU	N-CA-C	-6.62	104.42	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	178	GLY	N-CA-C	6.12	120.24	111.12
1	C	134	GLU	CA-C-N	5.55	125.48	119.76
1	C	134	GLU	C-N-CA	5.55	125.48	119.76

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	3	PSA	Peptide,Mainchain
2	E	3	PSA	Peptide,Mainchain
2	F	3	PSA	Peptide,Mainchain

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	89	0
1	B	2868	0	2706	105	0
1	C	2901	0	2739	131	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	333	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 19.

All (333) 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	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:8:GLY:C	1:B:10:SER:H	1.89	0.80
1:C:194:ARG:HD2	1:C:202:ILE:HD11	1.66	0.78
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
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
2:F:4:LEU:CD1	2:F:4:LEU:C	2.66	0.69
1:C:82:THR:O	1:C:83:ASP:HB2	1.91	0.68
1:C:22:SER:HA	1:C:23:PRO:C	2.19	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:253:SER:CB	1:B:254:THR:C	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C	2:F:4:LEU:HD13	2.22	0.64
1:A:147:PRO:HG2	1:A:177:GLY:O	1.97	0.64
1:B:197:TRP:CG	1:B:198:TYR:H	2.15	0.64
1:B:360:HIS:O	1:B:361:VAL:C	2.41	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
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:74:GLY:C	1:B:75:LYS:HG3	2.25	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:C:190:TYR:CD2	1:C:351:ARG:HG3	2.37	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: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:C:74:GLY:C	1:C:75:LYS:HG3	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:197:TRP:CG	1:A:198:TYR:H	2.22	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: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:267:LEU:HD23	1:B:267:LEU:N	2.20	0.55
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:197:TRP:CD1	1:B:198:TYR:H	2.25	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: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:314:THR:O	1:A:315:SER:CB	2.54	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:A:228:ASP:C	1:A:228:ASP:OD1	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:57:SER:C	1:B:59:THR:H	2.18	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
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: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: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:A:197:TRP:CD1	1:A:198:TYR:H	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ASN:C	1:A:386:ILE:HG23	2.38	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:B:8:GLY:C	1:B:10:SER:N	2.59	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:A:341:PHE:C	1:A:357:SER:HB2	2.40	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
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:362:HIS:CD2	1:A:362:HIS:C	2.93	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:A:360:HIS:HE2	1:A:368:ALA:H	1.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:274:THR:O	1:B:275:THR:C	2.59	0.45
1:C:153:GLN:HB2	1:C:342:TYR:HD1	1.82	0.45
1:C:197:TRP:CG	1:C:198:TYR:H	2.34	0.45
1:A:133:LEU:O	1:A:134:GLU:C	2.58	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:338:MET:HE3	1:C:338:MET:HB3	1.77	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:A:238:LYS:O	1:A:239:LYS:C	2.60	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
1:C:29:ILE:HG21	1:C:119:LEU:HB2	1.98	0.44
1:A:55:GLN:H	1:A:55:GLN:CD	2.26	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:A:338:MET:HE2	1:A:338:MET:HB3	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-1:PHE:CD2	1:A:2:MET:HE3	2.53	0.44
1:C:55:GLN:C	1:C:56:LEU:HD23	2.42	0.44
1:C:136:PHE:CD2	1:C:136:PHE:C	2.95	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:22:SER:CA	1:C:23:PRO:C	2.91	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: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:B:215:MET:HE2	1:B:215:MET:HB3	1.86	0.42
1:B:288:MET:HE2	1:B:379:MET:HE3	2.01	0.42
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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:LEU:HD23	1:C:80:LEU:HA	1.82	0.42
1:C:216:ASP:O	1:C:217:CYS:C	2.62	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:C:271:GLN:O	1:C:272:ALA:C	2.62	0.41
1:C:385:ASN:O	1:C:386:ILE:C	2.63	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: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: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:C:63:LEU:HD13	1:C:81:GLY:C	2.45	0.41
1:C:180:ASP:OD2	1:C:180:ASP:C	2.64	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:238:LYS:O	1:C:239:LYS:C	2.64	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:A:149:LEU:HD23	1:A:149:LEU:C	2.46	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:244:ALA:O	1:A:248:ILE:HG13	2.22	0.40
1:C:310:GLU:O	1:C:311:ASP:C	2.63	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	372/433 (86%)	342 (92%)	24 (6%)	6 (2%)	7	26
1	B	368/433 (85%)	329 (89%)	31 (8%)	8 (2%)	5	20
1	C	371/433 (86%)	334 (90%)	27 (7%)	10 (3%)	4	16
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%)	5	21

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	ASP
1	A	315	SER
1	B	253	SER
1	B	256	LYS
1	B	361	VAL
1	C	-2	SER
1	C	-1	PHE
1	C	10	SER

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Mol	Chain	Res	Type
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%)	271 (90%)	31 (10%)	7	24
1	B	299/370 (81%)	269 (90%)	30 (10%)	7	25
1	C	304/370 (82%)	267 (88%)	37 (12%)	5	17
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%)	808 (89%)	100 (11%)	6	21

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	VAL
1	A	22	SER

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Mol	Chain	Res	Type
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	110	ILE
1	A	128	ARG
1	A	149	LEU
1	A	173	SER
1	A	176	ILE
1	A	195	ARG
1	A	196	GLU
1	A	225	SER
1	A	232	THR
1	A	245	VAL
1	A	268	VAL
1	A	275	THR
1	A	292	THR
1	A	317	ASP
1	A	329	THR
1	A	339	GLU
1	A	367	THR
1	A	375	VAL
1	A	381	ASP
1	A	386	ILE
1	B	0	VAL
1	B	12	GLN
1	B	20	VAL
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	104	GLU
1	B	105	SER
1	B	125	GLU
1	B	149	LEU

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Mol	Chain	Res	Type
1	B	185	THR
1	B	188	LEU
1	B	213	LEU
1	B	224	LYS
1	B	234	LEU
1	B	246	LYS
1	B	247	SER
1	B	256	LYS
1	B	257	PHE
1	B	267	LEU
1	B	268	VAL
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	3	VAL
1	C	26	THR
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	104	GLU
1	C	110	ILE
1	C	118	ILE
1	C	125	GLU
1	C	141	VAL
1	C	144	THR
1	C	149	LEU
1	C	176	ILE
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

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Mol	Chain	Res	Type
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	338	MET
1	C	339	GLU
1	C	361	VAL
1	C	376	THR
1	C	378	ASP
1	C	386	ILE
2	E	4	LEU
2	F	4	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	114	ASN
1	B	114	ASN
1	B	233	ASN
1	B	293	ASN
1	B	362	HIS
1	C	73	GLN
1	C	293	ASN
1	C	385	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	PSA	F	3	2	14,14,15	3.88	6 (42%)	15,17,19	2.52	8 (53%)
2	PSA	D	3	2	14,14,15	4.18	7 (50%)	15,17,19	1.27	1 (6%)
2	ZAE	E	6	2	11,12,13	4.34	6 (54%)	13,14,16	1.31	3 (23%)
2	PLJ	E	7	2	9,9,9	1.37	2 (22%)	11,11,11	1.50	4 (36%)
2	ZAE	D	6	2	11,12,13	4.57	6 (54%)	13,14,16	1.05	1 (7%)
2	PSA	E	3	2	14,14,15	3.93	8 (57%)	15,17,19	1.95	4 (26%)
2	PLJ	D	7	2	9,9,9	1.41	2 (22%)	11,11,11	1.55	4 (36%)
2	ZAE	F	6	2	11,12,13	4.33	6 (54%)	13,14,16	2.66	8 (61%)
2	PLJ	F	7	2	9,9,9	1.32	1 (11%)	11,11,11	1.49	2 (18%)

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

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	PSA	CE2-CD2	7.42	1.51	1.38
2	D	6	ZAE	CE1-CD1	7.15	1.51	1.38
2	D	3	PSA	CE1-CD1	7.12	1.51	1.38
2	F	3	PSA	CD2-CG	6.80	1.52	1.38
2	F	6	ZAE	CE1-CD1	6.74	1.50	1.38
2	F	3	PSA	CE2-CD2	6.53	1.50	1.38
2	E	3	PSA	CE1-CD1	6.46	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	6	ZAE	CD2-CG	6.44	1.51	1.38
2	E	3	PSA	CE2-CD2	6.36	1.49	1.38
2	D	6	ZAE	CZ-CE1	6.33	1.52	1.38
2	E	6	ZAE	CE1-CD1	6.33	1.49	1.38
2	D	6	ZAE	CE2-CD2	6.32	1.49	1.38
2	F	6	ZAE	CZ-CE1	6.31	1.52	1.38
2	D	3	PSA	CD2-CG	6.28	1.51	1.38
2	E	6	ZAE	CD2-CG	6.15	1.51	1.38
2	E	6	ZAE	CE2-CD2	6.13	1.49	1.38
2	E	6	ZAE	CZ-CE1	6.10	1.51	1.38
2	E	3	PSA	CD2-CG	5.99	1.50	1.38
2	F	6	ZAE	CD1-CG	5.89	1.50	1.38
2	D	3	PSA	CD1-CG	5.78	1.50	1.38
2	F	3	PSA	CE1-CD1	5.77	1.48	1.38
2	F	3	PSA	CZ-CE1	5.44	1.50	1.38
2	F	6	ZAE	CD2-CG	5.39	1.49	1.38
2	E	3	PSA	CD1-CG	5.37	1.49	1.38
2	D	3	PSA	CZ-CE1	5.33	1.50	1.38
2	E	6	ZAE	CD1-CG	5.32	1.49	1.38
2	F	6	ZAE	CE2-CD2	5.30	1.48	1.38
2	D	6	ZAE	CZ-CE2	5.29	1.49	1.38
2	D	6	ZAE	CD1-CG	5.28	1.49	1.38
2	F	3	PSA	CD1-CG	5.24	1.49	1.38
2	E	3	PSA	CZ-CE2	5.17	1.49	1.38
2	F	6	ZAE	CZ-CE2	5.11	1.49	1.38
2	E	3	PSA	CZ-CE1	5.09	1.49	1.38
2	E	6	ZAE	CZ-CE2	5.03	1.49	1.38
2	D	3	PSA	CZ-CE2	4.94	1.49	1.38
2	F	3	PSA	CZ-CE2	4.46	1.48	1.38
2	D	7	PLJ	OXT-C	2.75	1.40	1.33
2	E	7	PLJ	OXT-CM	-2.68	1.39	1.45
2	E	3	PSA	OH-CH	-2.68	1.37	1.43
2	D	3	PSA	OH-CH	-2.62	1.37	1.43
2	F	7	PLJ	OXT-C	2.56	1.39	1.33
2	D	7	PLJ	OXT-CM	-2.44	1.39	1.45
2	E	7	PLJ	OXT-C	2.41	1.39	1.33
2	E	3	PSA	CM-C	2.40	1.56	1.50

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	3	PSA	CM-CH-CA	5.01	120.67	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	6	ZAE	CB-CG-CD2	-4.92	111.76	120.90
2	F	3	PSA	OH-CH-CM	4.68	120.00	109.24
2	E	3	PSA	OH-CH-CM	4.66	119.97	109.24
2	F	3	PSA	CZ-CE2-CD2	-3.42	116.02	120.24
2	F	6	ZAE	CZ-CE2-CD2	-3.35	116.10	120.24
2	F	6	ZAE	CB-CA-N	-3.33	105.57	110.48
2	F	7	PLJ	OXT-C-CA	3.27	119.80	111.49
2	E	3	PSA	OH-CH-CA	3.15	115.47	109.48
2	D	3	PSA	OH-CH-CA	3.06	115.31	109.48
2	F	6	ZAE	CD2-CG-CD1	2.95	122.62	118.23
2	D	7	PLJ	OXT-C-CA	2.91	118.88	111.49
2	E	3	PSA	CG-CB-CA	-2.85	107.43	113.48
2	F	6	ZAE	CE1-CD1-CG	-2.78	116.71	120.61
2	F	6	ZAE	CE2-CZ-CE1	2.75	123.64	119.87
2	F	3	PSA	CB-CG-CD1	-2.70	115.88	120.90
2	D	6	ZAE	C10-N-CA	2.55	121.33	113.70
2	F	3	PSA	CE2-CZ-CE1	2.54	123.34	119.87
2	F	6	ZAE	CB-CG-CD1	2.54	125.63	120.90
2	F	3	PSA	CE1-CD1-CG	-2.52	117.07	120.61
2	E	7	PLJ	C-CA-N	2.52	115.74	111.00
2	E	7	PLJ	OXT-C-O	-2.43	119.11	123.85
2	F	6	ZAE	CB-CA-C	2.40	116.58	111.81
2	F	7	PLJ	OXT-C-O	-2.37	119.24	123.85
2	D	7	PLJ	OXT-C-O	-2.35	119.27	123.85
2	D	7	PLJ	CM-OXT-C	2.28	121.09	115.92
2	E	7	PLJ	OXT-C-CA	2.25	117.21	111.49
2	D	7	PLJ	O-C-CA	-2.23	117.33	123.94
2	F	3	PSA	CD2-CG-CD1	2.21	121.52	118.23
2	E	6	ZAE	CG-CB-CA	-2.12	110.49	113.51
2	E	7	PLJ	CM-OXT-C	2.09	120.65	115.92
2	E	6	ZAE	C10-N-CA	2.07	119.88	113.70
2	F	3	PSA	CH-CM-C	-2.06	109.51	113.02
2	E	3	PSA	CD2-CG-CD1	2.05	121.28	118.23
2	E	6	ZAE	CB-CA-N	-2.01	107.52	110.48

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

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

There are no ring outliers.

7 monomers are involved in 13 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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%)	-0.26	7 (1%) 66 43	30, 52, 79, 132	1 (0%)
1	B	374/433 (86%)	-0.11	12 (3%) 50 28	43, 59, 83, 121	0
1	C	377/433 (87%)	-0.20	7 (1%) 66 43	40, 55, 72, 101	0
2	D	2/7 (28%)	-0.54	0 100 100	41, 41, 41, 46	0
2	E	2/7 (28%)	-0.02	0 100 100	49, 49, 49, 50	0
2	F	2/7 (28%)	-0.03	0 100 100	51, 51, 51, 53	0
All	All	1134/1320 (85%)	-0.19	26 (2%) 61 38	30, 55, 79, 132	1 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	311	ASP	6.3
1	C	311	ASP	5.3
1	A	313	ALA	4.9
1	C	386	ILE	4.4
1	C	107	LYS	4.1
1	B	361	VAL	3.8
1	A	255	GLU	3.5
1	A	310	GLU	3.4
1	C	170	VAL	3.4
1	B	315	SER	3.3
1	C	315	SER	3.3
1	B	386	ILE	3.2
1	A	386	ILE	3.2
1	B	170	VAL	3.1
1	B	254	THR	2.8
1	C	-2	SER	2.8
1	A	316	GLN	2.7
1	B	316	GLN	2.7
1	B	255	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	310	GLU	2.5
1	C	316	GLN	2.4
1	B	256	LYS	2.3
1	B	253	SER	2.3
1	B	-2	SER	2.2
1	A	314	THR	2.1
1	A	256	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	PLJ	D	7	9/9	0.93	0.14	46,49,60,61	0
2	ZAE	E	6	12/13	0.93	0.14	49,53,57,61	0
2	PLJ	F	7	9/9	0.95	0.12	52,56,58,65	0
2	PLJ	E	7	9/9	0.96	0.14	51,52,58,61	0
2	ZAE	D	6	12/13	0.96	0.09	41,44,50,53	0
2	PSA	F	3	14/15	0.96	0.10	42,45,50,50	0
2	ZAE	F	6	12/13	0.96	0.12	49,57,64,65	0
2	PSA	D	3	14/15	0.97	0.10	37,43,50,51	0
2	PSA	E	3	14/15	0.97	0.09	46,47,51,53	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.