



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:28 PM UTC

PDB ID : 5B3J / pdb_00005b3j
Title : Activation of NMDA receptors and the mechanism of inhibition by ifenprodil
Authors : Tajima, N.; Karakas, E.; Grant, T.; Simorowski, N.; Diaz-Avalos, R.; Grigorieff, N.; Furukawa, H.
Deposited on : 2016-03-01
Resolution : 2.90 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
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

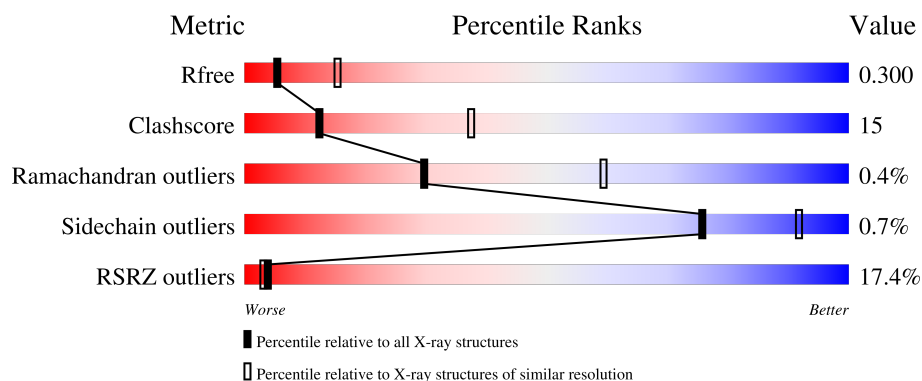
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	383	10% 64% 26% 9%
1	B	383	11% 64% 23% 12%
2	C	364	27% 62% 30% 8%
2	D	364	32% 65% 25% 10%
3	E	224	12% 73% 21% • •

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Mol	Chain	Length	Quality of chain
3	H	224	13% 71% 24%
4	F	213	5% 69% 31%
4	L	213	7% 76% 23%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15954 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 NMDA glutamate receptor subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	0
			2491	1595	422	464	10			
1	B	338	Total	C	N	O	S	0	0	0
			2370	1516	396	448	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	GLN	ASN	engineered mutation	UNP Q91977
A	371	GLN	ASN	engineered mutation	UNP Q91977
B	61	GLN	ASN	engineered mutation	UNP Q91977
B	371	GLN	ASN	engineered mutation	UNP Q91977

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	335	Total	C	N	O	S	0	2	0
			2390	1536	390	450	14			
2	D	329	Total	C	N	O	S	0	0	0
			2315	1477	386	439	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	348	ASP	ASN	engineered mutation	UNP Q00960
D	348	ASP	ASN	engineered mutation	UNP Q00960

- Molecule 3 is a protein called Fab, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	215	Total	C	N	O	S	0	0	0
			1536	976	252	300	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	216	Total	C	N	O	S	0	0	0
			1551	983	254	306	8			

- Molecule 4 is a protein called Fab, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	211	Total	C	N	O	S	0	0	0
			1595	1001	269	319	6			
4	L	212	Total	C	N	O	S	0	0	0
			1598	1007	267	318	6			

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Na	0	0
			1	1		

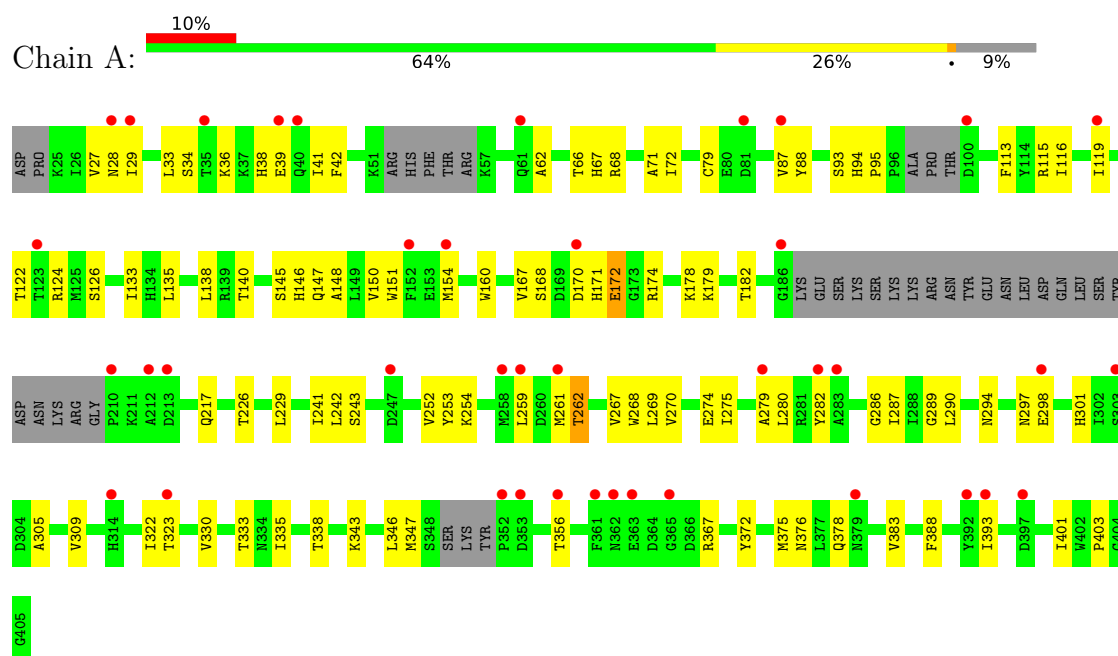
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	13	Total	O	0	0
			13	13		
6	B	8	Total	O	0	0
			8	8		
6	C	11	Total	O	0	0
			11	11		
6	E	10	Total	O	0	0
			10	10		
6	D	10	Total	O	0	0
			10	10		
6	F	16	Total	O	0	0
			16	16		
6	H	21	Total	O	0	0
			21	21		
6	L	18	Total	O	0	0
			18	18		

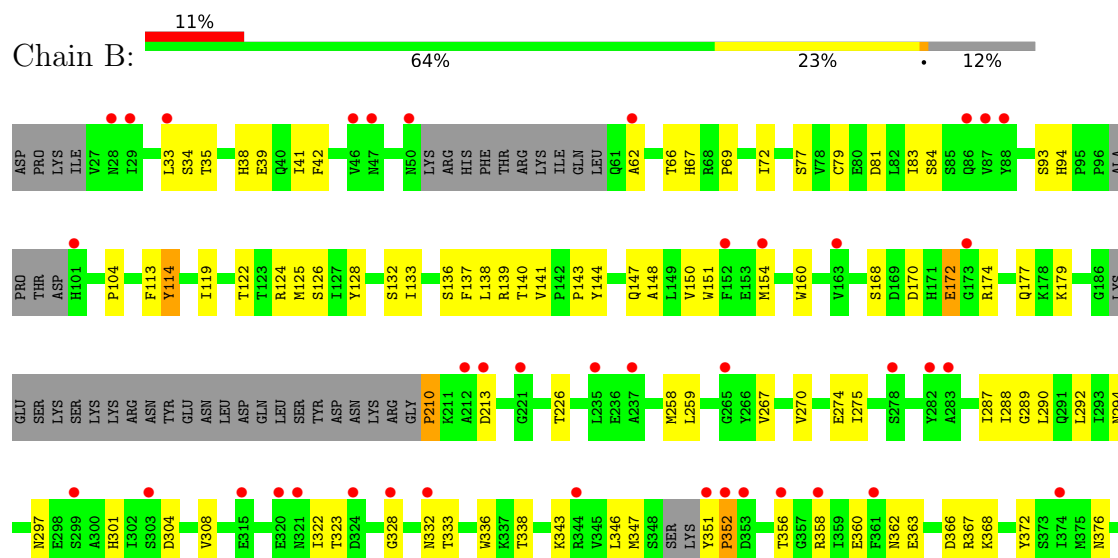
3 Residue-property plots [i](#)

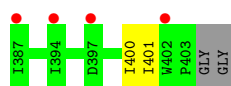
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: NMDA glutamate receptor subunit

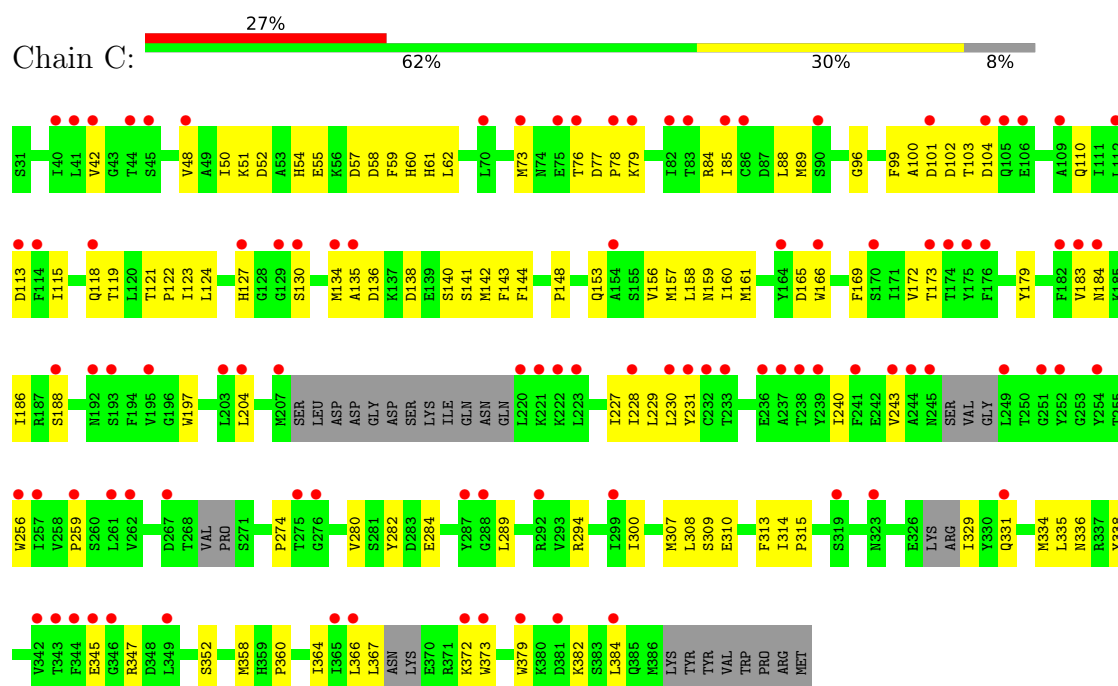


• Molecule 1: NMDA glutamate receptor subunit

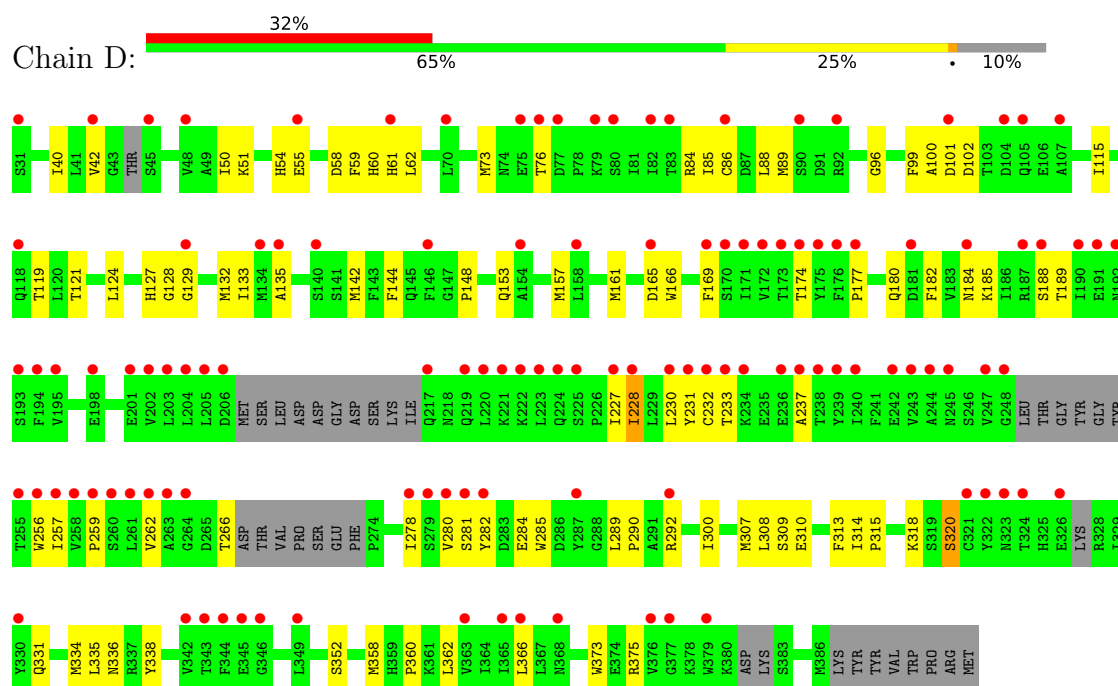




- Molecule 2: Glutamate receptor ionotropic, NMDA 2B

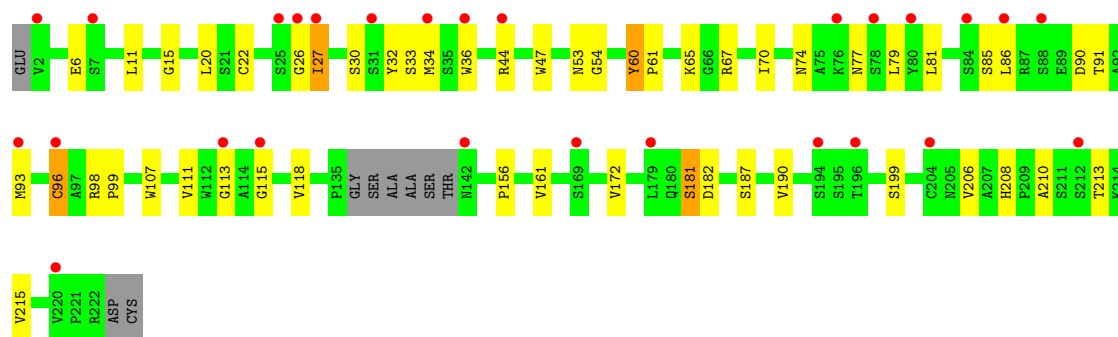


- Molecule 2: Glutamate receptor ionotropic, NMDA 2B

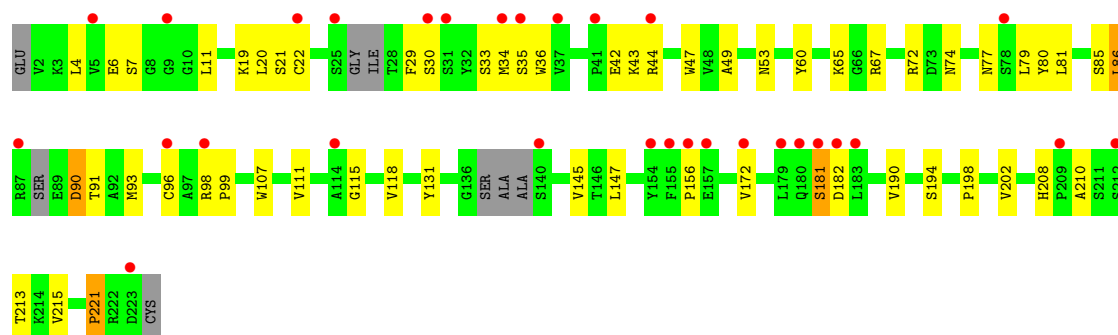


- Molecule 3: Fab, heavy chain

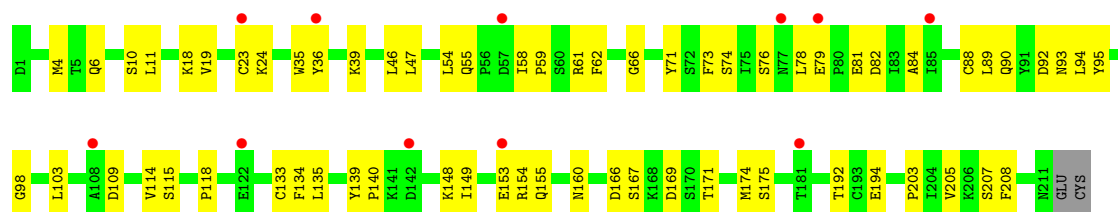




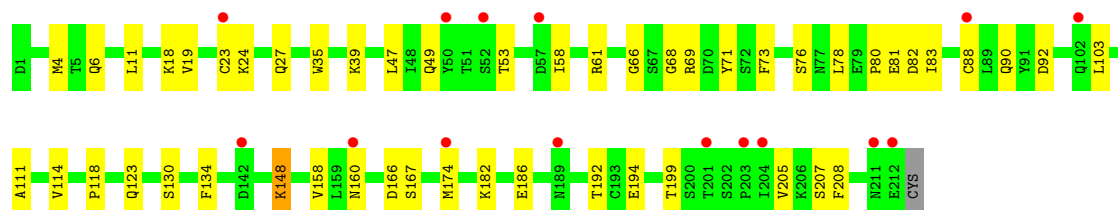
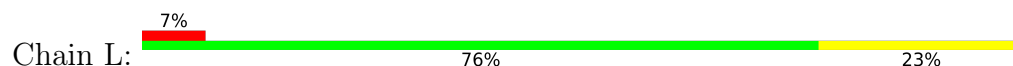
• Molecule 3: Fab, heavy chain



• Molecule 4: Fab, light chain



• Molecule 4: Fab, light chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	247.25Å 79.90Å 181.31Å 90.00° 127.09° 90.00°	Depositor
Resolution (Å)	29.93 – 2.90 29.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	84.1 (29.93-2.90) 80.8 (29.93-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.273 , 0.302 0.279 , 0.300	Depositor DCC
R_{free} test set	2944 reflections (4.13%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.9	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	0.85	EDS
Total number of atoms	15954	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.81 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.3336e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.29	0/2539	0.57	2/3470 (0.1%)
1	B	0.37	1/2417 (0.0%)	0.54	0/3317
2	C	0.32	0/2440	0.63	2/3340 (0.1%)
2	D	0.39	1/2361 (0.0%)	0.63	2/3228 (0.1%)
3	E	0.24	0/1580	0.57	0/2175
3	H	0.34	0/1593	0.66	1/2189 (0.0%)
4	F	0.38	0/1633	0.59	0/2225
4	L	0.29	0/1636	0.57	1/2230 (0.0%)
All	All	0.33	2/16199 (0.0%)	0.60	8/22174 (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
3	E	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	210	PRO	N-CD	-12.43	1.30	1.47
2	D	228	ILE	CG1-CD1	-10.24	1.11	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	228	ILE	CA-CB-CG1	-7.71	97.28	110.40
3	H	90	ASP	N-CA-C	-7.09	104.50	113.72
2	D	320	SER	CB-CA-C	-6.53	98.86	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	136	ASP	CA-C-N	-5.62	112.76	123.32
2	C	136	ASP	C-N-CA	-5.62	112.76	123.32
1	A	28	ASN	CA-C-N	5.60	130.93	122.98
1	A	28	ASN	C-N-CA	5.60	130.93	122.98
4	L	148	LYS	CD-CE-NZ	-5.50	94.30	111.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	26	GLY	Peptide
3	E	27	ILE	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	2491	0	2330	89	0
1	B	2370	0	2148	73	0
2	C	2390	0	2148	85	0
2	D	2315	0	2025	79	0
3	E	1536	0	1399	38	0
3	H	1551	0	1417	42	0
4	F	1595	0	1485	45	0
4	L	1598	0	1499	36	0
5	B	1	0	0	0	0
6	A	13	0	0	1	0
6	B	8	0	0	1	0
6	C	11	0	0	0	0
6	D	10	0	0	1	0
6	E	10	0	0	0	0
6	F	16	0	0	0	0
6	H	21	0	0	0	0
6	L	18	0	0	0	0
All	All	15954	0	14451	467	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 15.

All (467) 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:D:228:ILE:HD11	2:D:256:TRP:HA	1.47	0.93
1:B:210:PRO:HA	1:B:213:ASP:OD1	1.74	0.88
1:A:333:THR:HG1	2:C:76:THR:HG1	1.21	0.88
1:A:138:LEU:HD11	1:A:343:LYS:HG3	1.58	0.85
3:E:34:MET:HG2	3:E:98:ARG:HB2	1.59	0.84
3:H:60:TYR:HD2	3:H:65:LYS:HG3	1.44	0.83
2:D:51:LYS:O	2:D:55:GLU:HG3	1.79	0.82
2:C:113:ASP:OD2	2:C:143:PHE:HB3	1.79	0.82
1:A:174:ARG:NH2	1:A:217:GLN:OE1	2.13	0.81
3:H:147:LEU:HD13	3:H:202:VAL:HG21	1.60	0.81
3:E:98:ARG:HD3	3:E:111:VAL:HG21	1.63	0.81
4:F:18:LYS:NZ	4:F:74:SER:OG	2.15	0.79
1:A:38:HIS:HA	1:A:41:ILE:HD12	1.63	0.78
4:F:46:LEU:HD23	4:F:55:GLN:HG3	1.64	0.78
2:C:166:TRP:HB3	2:C:227:ILE:HG13	1.67	0.77
4:L:39:LYS:NZ	4:L:81:GLU:O	2.18	0.77
1:B:288:ILE:HD11	1:B:400:ILE:HD11	1.64	0.77
1:A:167:VAL:HG12	1:A:243:SER:HB3	1.65	0.77
3:H:67:ARG:NH2	3:H:90:ASP:OD2	2.17	0.76
2:D:352:SER:HB2	2:D:358:MET:HE3	1.68	0.76
4:F:61:ARG:NH1	4:F:79:GLU:OE1	2.19	0.75
1:B:38:HIS:HA	1:B:41:ILE:HD12	1.69	0.75
1:A:29:ILE:HD11	1:A:309:VAL:HG21	1.69	0.75
1:B:328:GLY:O	1:B:332:ASN:ND2	2.19	0.74
2:C:138:ASP:OD1	2:C:140:SER:OG	2.05	0.74
2:C:42:VAL:HG12	2:C:73:MET:HE2	1.70	0.73
2:C:159:ASN:HD22	2:C:379:TRP:HZ3	1.33	0.73
1:A:270:VAL:HG13	1:A:274:GLU:HB2	1.70	0.73
1:A:94:HIS:HB3	1:A:122:THR:OG1	1.89	0.72
4:F:148:LYS:NZ	4:F:194:GLU:OE1	2.21	0.72
2:C:101:ASP:OD1	2:C:102:ASP:N	2.23	0.72
4:L:61:ARG:NH2	4:L:82:ASP:OD1	2.23	0.72
2:D:101:ASP:OD1	2:D:102:ASP:N	2.24	0.71
3:H:22:CYS:HB3	3:H:79:LEU:HB3	1.72	0.70
2:C:51:LYS:O	2:C:55:GLU:HG3	1.90	0.70
2:D:40:ILE:HD11	2:D:73:MET:HE2	1.72	0.70
1:B:270:VAL:HG13	1:B:274:GLU:HB2	1.74	0.70
3:E:36:TRP:NE1	3:E:81:LEU:HB2	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:PHE:CE2	1:B:139:ARG:HG2	2.28	0.68
4:F:24:LYS:NZ	4:L:6:GLN:O	2.26	0.68
1:B:323:THR:HG22	1:B:338:THR:HG23	1.76	0.68
3:H:11:LEU:HB2	3:H:156:PRO:HG3	1.76	0.68
3:E:98:ARG:HD3	3:E:111:VAL:CG2	2.23	0.68
3:H:74:ASN:O	3:H:77:ASN:ND2	2.27	0.68
4:F:11:LEU:HD22	4:F:19:VAL:HB	1.75	0.67
2:C:153:GLN:NE2	2:C:259:PRO:HB3	2.09	0.67
4:F:47:LEU:HD23	4:F:58:ILE:HD12	1.77	0.67
1:A:146:HIS:HA	1:A:179:LYS:HE3	1.77	0.66
3:H:93:MET:HE3	3:H:115:GLY:HA3	1.77	0.66
1:A:42:PHE:CE2	1:A:62:ALA:HB1	2.30	0.66
2:D:180:GLN:O	2:D:184:ASN:ND2	2.28	0.66
1:B:351:TYR:N	1:B:352:PRO:HD3	2.11	0.66
1:A:113:PHE:CD2	2:C:78:PRO:HD3	2.31	0.66
2:C:160:ILE:HD11	2:C:364:ILE:HG12	1.78	0.65
2:C:85:ILE:O	2:C:89:MET:HG3	1.96	0.65
1:A:178:LYS:O	1:A:182:THR:HG23	1.97	0.65
1:A:170:ASP:OD1	1:A:171:HIS:N	2.30	0.65
3:E:74:ASN:O	3:E:77:ASN:ND2	2.30	0.65
2:D:42:VAL:CG2	2:D:101:ASP:HA	2.27	0.64
2:D:307:MET:HE3	2:D:315:PRO:HD3	1.78	0.64
1:B:148:ALA:HB3	1:B:179:LYS:HG2	1.79	0.64
4:L:182:LYS:O	4:L:186:GLU:HG3	1.97	0.64
1:B:226:THR:HG23	1:B:259:LEU:HD11	1.79	0.64
1:B:83:ILE:HD13	1:B:114:TYR:HE2	1.62	0.64
4:L:24:LYS:NZ	4:L:69:ARG:HH21	1.96	0.63
4:L:192:THR:HG23	4:L:207:SER:HB3	1.79	0.63
1:B:376:ASN:HD22	1:B:400:ILE:HG13	1.63	0.62
3:H:72:ARG:HE	3:H:74:ASN:ND2	1.97	0.62
1:B:356:THR:OG1	1:B:367:ARG:NH2	2.31	0.62
2:D:174:THR:HG23	2:D:232:CYS:HB3	1.80	0.62
1:A:71:ALA:HB3	2:C:118:GLN:OE1	1.99	0.62
4:F:194:GLU:HG2	4:F:203:PRO:HB3	1.81	0.62
1:B:94:HIS:HB3	1:B:122:THR:HB	1.82	0.62
2:C:307:MET:HE3	2:C:315:PRO:HD3	1.82	0.61
2:D:100:ALA:HB1	2:D:289:LEU:HD11	1.82	0.61
2:C:57:ASP:OD1	2:C:294:ARG:NH1	2.33	0.61
1:B:140:THR:O	1:B:367:ARG:NH1	2.29	0.61
1:A:226:THR:HG23	1:A:259:LEU:HD11	1.82	0.61
1:A:270:VAL:CG1	1:A:274:GLU:HB2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:HIS:O	1:B:122:THR:HG21	1.99	0.61
2:D:307:MET:HE1	2:D:335:LEU:HB2	1.80	0.61
4:L:194:GLU:HG3	4:L:205:VAL:HG23	1.83	0.61
1:A:67:HIS:NE2	1:A:93:SER:O	2.30	0.61
3:E:11:LEU:HD22	3:E:156:PRO:HG3	1.83	0.61
2:D:282:TYR:HE1	2:D:360:PRO:HB2	1.66	0.61
1:B:270:VAL:CG1	1:B:274:GLU:HB2	2.31	0.60
2:C:84:ARG:O	2:C:88:LEU:HG	2.01	0.60
2:C:184:ASN:O	2:C:188:SER:OG	2.14	0.60
3:H:4:LEU:HD21	3:H:96:CYS:HB3	1.83	0.60
1:A:113:PHE:HD2	2:C:78:PRO:HD3	1.66	0.60
1:A:305:ALA:O	1:A:309:VAL:HG22	2.01	0.60
1:B:137:PHE:HE2	1:B:139:ARG:HG2	1.66	0.60
2:D:42:VAL:HG22	2:D:100:ALA:O	2.00	0.60
2:D:318:LYS:NZ	2:D:320:SER:O	2.34	0.60
2:C:331:GLN:CD	2:C:331:GLN:H	2.09	0.60
2:D:84:ARG:O	2:D:88:LEU:HG	2.01	0.60
3:H:20:LEU:HD12	3:H:81:LEU:HD23	1.82	0.60
1:B:104:PRO:HG2	1:B:128:TYR:CE2	2.36	0.59
4:F:160:ASN:HB3	4:F:174:MET:HE3	1.84	0.59
2:C:307:MET:HE1	2:C:335:LEU:HB2	1.85	0.59
2:D:119:THR:HB	2:D:318:LYS:HE2	1.83	0.59
2:D:308:LEU:HB2	2:D:314:ILE:CG2	2.32	0.59
4:L:4:MET:HE3	4:L:23:CYS:SG	2.43	0.59
4:F:36:TYR:CZ	4:F:46:LEU:HD12	2.37	0.59
4:F:90:GLN:NE2	4:F:93:ASN:H	2.01	0.59
4:L:11:LEU:HD22	4:L:19:VAL:HB	1.85	0.59
4:L:123:GLN:HE22	4:L:130:SER:CB	2.15	0.59
3:E:67:ARG:NH2	3:E:90:ASP:OD2	2.36	0.59
4:L:80:PRO:O	4:L:83:ILE:HD12	2.03	0.59
1:B:270:VAL:HG21	1:B:287:ILE:HD11	1.84	0.59
4:F:18:LYS:HB2	4:F:76:SER:HA	1.85	0.59
1:A:274:GLU:H	1:A:274:GLU:CD	2.10	0.58
2:C:59:PHE:O	2:C:62:LEU:HB2	2.03	0.58
3:H:42:GLU:O	3:H:44:ARG:N	2.35	0.58
1:B:133:ILE:HD11	2:D:135:ALA:O	2.03	0.58
1:A:242:LEU:HD11	1:A:252:VAL:HG21	1.86	0.58
2:D:40:ILE:HG23	2:D:99:PHE:HA	1.86	0.58
1:B:323:THR:HG23	1:B:336:TRP:HE1	1.68	0.57
2:D:119:THR:OG1	2:D:121:THR:OG1	2.21	0.57
2:C:274:PRO:O	2:C:367:LEU:HD23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:307:MET:SD	2:C:334:MET:HE3	2.43	0.57
1:A:270:VAL:HG21	1:A:287:ILE:HD11	1.87	0.57
1:B:69:PRO:HB3	4:F:153:GLU:OE2	2.04	0.57
2:C:352:SER:HB2	2:C:358:MET:HE3	1.87	0.57
3:E:93:MET:HE3	3:E:115:GLY:HA3	1.87	0.57
1:B:35:THR:O	1:B:39:GLU:HG3	2.04	0.57
1:B:72:ILE:HD11	2:D:115:ILE:HD11	1.87	0.57
2:D:50:ILE:HD11	2:D:289:LEU:HD23	1.86	0.56
2:D:282:TYR:CE1	2:D:360:PRO:HB2	2.39	0.56
1:A:275:ILE:HD13	1:A:289:GLY:HA3	1.87	0.56
2:C:366:LEU:O	2:C:373:TRP:HA	2.05	0.56
2:D:308:LEU:HB2	2:D:314:ILE:HG23	1.88	0.56
3:H:98:ARG:HD2	3:H:111:VAL:CG2	2.35	0.56
2:C:228:ILE:HG12	2:C:256:TRP:CD2	2.41	0.56
1:A:34:SER:OG	1:A:298:GLU:OE2	2.15	0.56
3:E:60:TYR:HD2	3:E:65:LYS:HG3	1.70	0.56
2:C:50:ILE:HD11	2:C:289:LEU:HD23	1.86	0.56
2:C:100:ALA:HB1	2:C:289:LEU:HD11	1.87	0.56
2:D:101:ASP:OD2	2:D:129:GLY:N	2.36	0.56
2:D:310:GLU:OE1	2:D:338:TYR:OH	2.19	0.56
1:A:33:LEU:HD12	1:A:39:GLU:HA	1.88	0.56
1:A:378:GLN:HG2	1:A:401:ILE:HD12	1.88	0.56
1:B:79:CYS:O	1:B:84:SER:OG	2.24	0.55
3:E:22:CYS:HB3	3:E:79:LEU:HB3	1.86	0.55
3:E:30:SER:O	3:E:53:ASN:HB2	2.06	0.55
4:F:4:MET:HE3	4:F:23:CYS:SG	2.46	0.55
4:F:194:GLU:HG3	4:F:205:VAL:HG23	1.87	0.55
1:B:323:THR:HG23	1:B:336:TRP:NE1	2.22	0.55
1:A:388:PHE:CD1	1:A:393:ILE:HG22	2.42	0.55
2:D:185:LYS:O	2:D:189:THR:HG23	2.06	0.55
1:A:330:VAL:HG23	2:C:79:LYS:HD3	1.89	0.55
2:C:42:VAL:HG22	2:C:100:ALA:O	2.07	0.55
1:A:229:LEU:HB3	1:A:261:MET:SD	2.47	0.55
2:C:282:TYR:O	2:C:284:GLU:HG2	2.06	0.55
2:D:228:ILE:HD11	2:D:256:TRP:CA	2.27	0.55
2:D:230:LEU:HD11	2:D:232:CYS:SG	2.47	0.55
2:C:345:GLU:C	2:C:347:ARG:H	2.15	0.55
2:D:313:PHE:CZ	2:D:334:MET:HE1	2.42	0.55
3:H:34:MET:HE2	3:H:98:ARG:HG3	1.89	0.55
1:A:378:GLN:CD	1:A:383:VAL:HG21	2.31	0.54
2:D:228:ILE:HD12	2:D:256:TRP:CE3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:LEU:HD22	1:B:372:TYR:CB	2.38	0.54
2:D:101:ASP:HB3	2:D:127:HIS:O	2.08	0.54
3:H:36:TRP:CH2	3:H:96:CYS:SG	3.01	0.54
1:A:115:ARG:CD	1:A:335:ILE:HD11	2.37	0.54
2:D:157:MET:HE1	2:D:259:PRO:HG3	1.90	0.54
1:B:126:SER:N	1:B:172:GLU:OE1	2.39	0.54
2:C:313:PHE:CZ	2:C:334:MET:HE1	2.42	0.53
3:E:172:VAL:HG12	3:E:190:VAL:HG23	1.90	0.53
4:L:35:TRP:CE2	4:L:73:PHE:HB2	2.43	0.53
2:D:228:ILE:CD1	2:D:256:TRP:HA	2.29	0.53
2:D:230:LEU:HD12	2:D:262:VAL:HG21	1.90	0.53
4:L:160:ASN:HD22	4:L:174:MET:CE	2.21	0.53
1:A:343:LYS:HA	1:A:346:LEU:HD12	1.90	0.53
1:B:376:ASN:ND2	1:B:400:ILE:HG13	2.22	0.53
1:B:124:ARG:HB2	1:B:144:TYR:CZ	2.44	0.53
1:B:333:THR:OG1	2:D:76:THR:HG23	2.09	0.53
2:D:86:CYS:HA	2:D:89:MET:HG3	1.91	0.53
4:F:78:LEU:HD22	4:F:103:LEU:HD21	1.90	0.53
2:C:119:THR:OG1	2:C:121:THR:OG1	2.14	0.53
2:C:172:VAL:HG13	2:C:230:LEU:HD13	1.91	0.53
1:A:27:VAL:HG13	1:A:88:TYR:CD1	2.44	0.53
2:C:58:ASP:HB2	3:E:53:ASN:OD1	2.08	0.53
3:E:36:TRP:CG	3:E:81:LEU:HD22	2.45	0.53
2:D:281:SER:HB3	6:D:408:HOH:O	2.08	0.52
1:A:147:GLN:HG2	1:A:372:TYR:HE2	1.75	0.52
1:B:150:VAL:O	1:B:154:MET:HG2	2.09	0.52
1:B:322:ILE:HA	1:B:338:THR:HG21	1.91	0.52
2:C:331:GLN:OE1	2:C:331:GLN:N	2.38	0.52
3:E:15:GLY:HA2	3:E:85:SER:HA	1.92	0.52
1:B:258:MET:O	1:B:258:MET:HG2	2.10	0.52
2:C:153:GLN:HB3	2:C:280:VAL:HG11	1.91	0.52
2:D:60:HIS:O	2:D:61:HIS:HB2	2.09	0.52
2:D:166:TRP:HB3	2:D:227:ILE:HG13	1.92	0.52
2:C:54:HIS:HA	2:C:57:ASP:OD2	2.10	0.52
3:E:6:GLU:OE2	3:E:113:GLY:HA3	2.10	0.52
3:E:99:PRO:HB2	3:E:107:TRP:HB2	1.91	0.52
1:B:119:ILE:HD13	1:B:138:LEU:HB2	1.91	0.52
3:H:198:PRO:HG3	3:H:221:PRO:HG3	1.91	0.52
2:C:60:HIS:O	2:C:61:HIS:HB2	2.10	0.52
2:C:96:GLY:HA3	2:C:300:ILE:HD13	1.91	0.51
3:H:60:TYR:CD2	3:H:65:LYS:HG3	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:110:GLN:HG2	2:C:134[A]:MET:HE3	1.91	0.51
2:C:310:GLU:OE1	2:C:338:TYR:OH	2.26	0.51
1:A:68:ARG:HH21	4:L:194:GLU:CD	2.18	0.51
1:B:362:ASN:CG	1:B:363:GLU:N	2.68	0.51
3:E:98:ARG:HH11	3:E:111:VAL:HG22	1.75	0.51
1:A:274:GLU:CD	1:A:274:GLU:N	2.68	0.51
1:B:147:GLN:NE2	6:B:601:HOH:O	2.32	0.51
3:E:33:SER:O	3:E:34:MET:HG3	2.10	0.51
4:L:68:GLY:O	4:L:71:TYR:OH	2.25	0.51
1:A:151:TRP:HA	1:A:154:MET:HG2	1.93	0.51
2:C:161:MET:O	2:C:165:ASP:N	2.43	0.51
1:B:362:ASN:OD1	1:B:363:GLU:N	2.44	0.51
4:F:6:GLN:HE21	4:F:98:GLY:HA3	1.75	0.51
3:H:85:SER:C	3:H:86:LEU:O	2.45	0.51
1:B:362:ASN:CG	1:B:363:GLU:H	2.19	0.51
4:L:123:GLN:HE22	4:L:130:SER:HB2	1.76	0.50
4:F:39:LYS:HG2	4:F:84:ALA:HB2	1.93	0.50
2:D:59:PHE:O	2:D:62:LEU:HB2	2.12	0.50
2:C:77:ASP:HB2	2:C:78:PRO:HD2	1.92	0.50
4:F:192:THR:HG23	4:F:207:SER:HB3	1.93	0.50
3:H:42:GLU:CD	3:H:42:GLU:H	2.19	0.50
3:H:72:ARG:HE	3:H:74:ASN:HD21	1.59	0.50
1:A:376:ASN:ND2	1:A:401:ILE:H	2.09	0.50
1:B:83:ILE:HD13	1:B:114:TYR:CE2	2.45	0.50
1:A:119:ILE:HD13	1:A:138:LEU:HB2	1.94	0.50
1:B:124:ARG:HD2	1:B:141:VAL:HG12	1.93	0.50
1:B:139:ARG:HH12	1:B:143:PRO:HB3	1.77	0.50
1:B:351:TYR:CB	1:B:360:GLU:HG2	2.42	0.50
3:E:27:ILE:HG21	3:E:77:ASN:OD1	2.12	0.50
1:B:275:ILE:HD13	1:B:289:GLY:HA3	1.94	0.49
4:F:35:TRP:CE2	4:F:73:PHE:HB2	2.47	0.49
2:C:308:LEU:HB2	2:C:314:ILE:CG2	2.42	0.49
4:F:89:LEU:HD11	4:F:95:TYR:HB3	1.93	0.49
2:C:127:HIS:O	2:C:130:SER:OG	2.30	0.49
4:L:47:LEU:HD23	4:L:58:ILE:HD12	1.94	0.49
1:A:356:THR:OG1	1:A:367:ARG:NH2	2.43	0.49
2:C:99:PHE:HD2	2:C:130:SER:HB3	1.77	0.49
2:D:119:THR:CB	2:D:318:LYS:HE2	2.42	0.49
2:D:282:TYR:HD1	2:D:362:LEU:HD23	1.78	0.49
3:H:19:LYS:HE2	3:H:80:TYR:CD1	2.47	0.49
1:B:160:TRP:CH2	1:B:267:VAL:HG11	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:98:ARG:HD2	3:H:111:VAL:HG21	1.94	0.49
2:C:367:LEU:HD12	2:C:372:LYS:H	1.78	0.49
4:F:18:LYS:HE2	4:F:76:SER:HB3	1.94	0.49
1:B:304:ASP:O	1:B:308:VAL:HG23	2.12	0.49
3:E:77:ASN:N	3:E:77:ASN:HD22	2.10	0.49
2:D:228:ILE:CD1	2:D:256:TRP:CD2	2.96	0.49
4:F:61:ARG:NH2	4:F:82:ASP:OD1	2.46	0.49
3:H:35:SER:HB2	3:H:49:ALA:O	2.12	0.49
1:B:124:ARG:HB2	1:B:144:TYR:CE2	2.48	0.48
3:E:60:TYR:CD2	3:E:65:LYS:HG3	2.48	0.48
3:H:145:VAL:HG13	3:H:194:SER:OG	2.13	0.48
1:B:113:PHE:HD1	1:B:114:TYR:CD1	2.31	0.48
2:D:180:GLN:HB3	2:D:184:ASN:HD21	1.77	0.48
3:E:20:LEU:HD12	3:E:81:LEU:HD23	1.95	0.48
3:E:32:TYR:HB2	3:E:34:MET:HE3	1.95	0.48
1:A:115:ARG:NH2	1:A:135:LEU:HD13	2.28	0.48
1:B:290:LEU:HD22	1:B:372:TYR:HB2	1.95	0.48
2:C:169:PHE:HE2	2:C:197:TRP:CE3	2.32	0.48
1:B:67:HIS:NE2	1:B:93:SER:O	2.34	0.48
4:F:59:PRO:HB2	4:F:61:ARG:HG2	1.96	0.48
1:A:133:ILE:HD11	2:C:135:ALA:O	2.14	0.48
1:B:125:MET:O	1:B:139:ARG:NH2	2.46	0.48
1:B:323:THR:HG22	1:B:338:THR:CG2	2.44	0.48
1:A:115:ARG:HD3	1:A:335:ILE:HD11	1.95	0.48
2:C:89:MET:HE1	2:C:119:THR:HB	1.96	0.48
3:H:208:HIS:CE1	3:H:210:ALA:HB3	2.49	0.48
2:C:282:TYR:HB3	2:C:284:GLU:OE2	2.13	0.47
2:C:379:TRP:HE3	2:C:384:LEU:CD2	2.26	0.47
1:A:322:ILE:HA	1:A:338:THR:HG21	1.95	0.47
2:D:228:ILE:H	2:D:228:ILE:HG12	1.49	0.47
1:A:36:LYS:HE3	1:A:36:LYS:HB2	1.66	0.47
3:H:91:THR:HA	3:H:118:VAL:O	2.13	0.47
2:C:157:MET:SD	2:C:229:LEU:HD22	2.54	0.47
2:C:315:PRO:HG2	2:C:335:LEU:HD22	1.97	0.47
3:H:47:TRP:NE1	3:H:49:ALA:O	2.47	0.47
1:A:174:ARG:HH22	1:A:217:GLN:CD	2.22	0.47
4:F:169:ASP:HB3	4:F:171:THR:HG23	1.95	0.47
2:C:42:VAL:CG1	2:C:73:MET:HE2	2.41	0.47
3:E:44:ARG:HE	3:E:44:ARG:HB3	1.54	0.47
3:H:98:ARG:HD2	3:H:111:VAL:HG22	1.97	0.47
2:C:153:GLN:HE21	2:C:259:PRO:HB3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:6:GLU:HG2	3:H:96:CYS:SG	2.55	0.47
1:A:148:ALA:HB3	1:A:179:LYS:HG2	1.97	0.46
1:A:148:ALA:HA	1:A:151:TRP:CE3	2.50	0.46
1:A:274:GLU:N	1:A:274:GLU:OE1	2.35	0.46
3:E:53:ASN:OD1	3:E:54:GLY:N	2.45	0.46
4:F:134:PHE:CE1	4:F:175:SER:HB2	2.50	0.46
4:L:66:GLY:HA3	4:L:71:TYR:HA	1.96	0.46
4:F:90:GLN:HE21	4:F:93:ASN:H	1.63	0.46
2:D:54:HIS:NE2	2:D:55:GLU:HG2	2.30	0.46
2:D:230:LEU:HD13	2:D:231:TYR:N	2.30	0.46
3:H:29:PHE:CD2	3:H:74:ASN:HA	2.51	0.46
4:L:27:GLN:C	4:L:69:ARG:HG2	2.40	0.46
4:L:78:LEU:HD22	4:L:103:LEU:HD21	1.96	0.46
1:A:147:GLN:HG2	1:A:372:TYR:CE2	2.49	0.46
1:A:150:VAL:O	1:A:154:MET:HG2	2.15	0.46
3:E:33:SER:O	3:E:99:PRO:HD2	2.16	0.46
4:L:49:GLN:NE2	4:L:53:THR:OG1	2.48	0.46
1:A:124:ARG:NH2	6:A:502:HOH:O	2.48	0.46
2:D:285:TRP:HB3	2:D:375:ARG:NH2	2.30	0.46
2:C:379:TRP:CH2	2:C:382:LYS:HA	2.50	0.46
3:H:72:ARG:NE	3:H:74:ASN:HD21	2.13	0.46
3:H:99:PRO:HB2	3:H:107:TRP:HB2	1.97	0.46
2:C:148:PRO:HB3	2:C:360:PRO:HG3	1.98	0.46
2:D:307:MET:SD	2:D:334:MET:HE3	2.55	0.46
4:F:61:ARG:HG2	4:F:61:ARG:H	1.51	0.46
2:C:42:VAL:HG23	2:C:101:ASP:HA	1.97	0.46
2:C:179:TYR:O	2:C:183:VAL:HG23	2.16	0.46
3:H:213:THR:HG22	3:H:215:VAL:HG23	1.98	0.46
2:C:142:MET:HG2	2:C:336:ASN:HD21	1.81	0.46
2:C:173:THR:O	2:C:204:LEU:HA	2.17	0.46
2:D:233:THR:O	2:D:237:ALA:N	2.43	0.46
2:D:157:MET:HE2	2:D:257:ILE:HG22	1.98	0.45
2:D:161:MET:O	2:D:165:ASP:N	2.49	0.45
4:F:66:GLY:HA3	4:F:71:TYR:HA	1.98	0.45
4:L:19:VAL:HG13	4:L:78:LEU:HD11	1.98	0.45
1:B:174:ARG:HA	1:B:177:GLN:HB3	1.99	0.45
4:L:90:GLN:HG2	4:L:92:ASP:H	1.82	0.45
3:E:181:SER:HA	3:E:182:ASP:HA	1.62	0.45
2:D:96:GLY:HA3	2:D:300:ILE:HD13	1.97	0.45
4:F:90:GLN:HE21	4:F:92:ASP:N	2.15	0.45
2:D:58:ASP:OD1	2:D:60:HIS:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:SER:O	1:A:170:ASP:N	2.49	0.45
1:B:33:LEU:HA	1:B:93:SER:OG	2.16	0.45
1:B:294:ASN:O	1:B:301:HIS:NE2	2.48	0.45
1:B:297:ASN:O	1:B:301:HIS:HD2	2.00	0.45
4:F:166:ASP:OD1	4:F:167:SER:N	2.50	0.45
1:A:148:ALA:HA	1:A:151:TRP:CD2	2.52	0.45
4:F:149:ILE:HD12	4:F:154:ARG:HG3	1.98	0.45
1:A:280:LEU:HD12	1:A:280:LEU:HA	1.37	0.45
1:B:77:SER:OG	1:B:81:ASP:OD2	2.25	0.45
1:B:367:ARG:HG2	1:B:368:LYS:N	2.32	0.45
2:D:315:PRO:HB3	2:D:331:GLN:NE2	2.31	0.45
1:B:148:ALA:HA	1:B:151:TRP:CE3	2.52	0.45
2:D:42:VAL:O	2:D:42:VAL:HG23	2.17	0.45
4:L:114:VAL:HA	4:L:134:PHE:O	2.17	0.45
1:A:87:VAL:HG13	1:A:116:ILE:HG21	1.99	0.45
1:A:297:ASN:O	1:A:301:HIS:HD2	2.00	0.45
1:A:343:LYS:O	1:A:347:MET:HG3	2.16	0.45
2:C:113:ASP:OD2	2:C:141:SER:OG	2.30	0.45
2:C:142:MET:HG2	2:C:336:ASN:ND2	2.32	0.45
3:H:33:SER:O	3:H:99:PRO:HD2	2.16	0.45
1:B:141:VAL:HG13	1:B:292:LEU:HD21	2.00	0.44
1:B:290:LEU:HD22	1:B:372:TYR:HB3	1.99	0.44
2:C:122:PRO:HG3	2:C:142:MET:HE2	1.99	0.44
2:C:42:VAL:CG2	2:C:101:ASP:HA	2.47	0.44
3:E:67:ARG:HH22	3:E:90:ASP:CG	2.26	0.44
2:D:285:TRP:HB3	2:D:375:ARG:HH22	1.82	0.44
4:F:194:GLU:HG3	4:F:205:VAL:CG2	2.47	0.44
2:D:153:GLN:HB3	2:D:280:VAL:HG11	2.00	0.44
3:H:147:LEU:CD1	3:H:202:VAL:HG21	2.39	0.44
2:C:158:LEU:HD11	2:C:186:ILE:HG23	1.99	0.44
1:B:33:LEU:HD12	1:B:39:GLU:HA	1.99	0.44
3:H:131:TYR:CE2	4:L:123:GLN:HG3	2.53	0.44
2:C:329:ILE:N	2:C:331:GLN:NE2	2.65	0.44
1:A:323:THR:H	1:A:338:THR:HG21	1.83	0.44
2:C:103:THR:HG22	2:C:104:ASP:H	1.83	0.44
3:E:161:VAL:HG22	3:E:206:VAL:HG22	1.99	0.44
1:A:148:ALA:HB3	1:A:179:LYS:CG	2.48	0.43
2:D:85:ILE:O	2:D:89:MET:HG3	2.18	0.43
3:H:181:SER:HA	3:H:182:ASP:HA	1.65	0.43
1:A:133:ILE:HD13	2:C:134[A]:MET:HE2	2.00	0.43
1:A:113:PHE:CE2	2:C:77:ASP:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:139:TYR:CD1	4:F:140:PRO:HA	2.53	0.43
4:F:153:GLU:OE1	4:F:155:GLN:NE2	2.51	0.43
1:A:113:PHE:CD1	1:A:113:PHE:C	2.96	0.43
1:B:124:ARG:HD2	1:B:141:VAL:CG1	2.48	0.43
4:F:47:LEU:CD2	4:F:58:ILE:HD12	2.45	0.43
2:C:231:TYR:CD1	2:C:231:TYR:C	2.97	0.43
2:D:284:GLU:HG2	2:D:292:ARG:HH12	1.84	0.43
3:H:72:ARG:NE	3:H:74:ASN:ND2	2.66	0.43
4:F:118:PRO:HB3	4:F:208:PHE:CE2	2.54	0.43
1:A:393:ILE:HD13	1:A:393:ILE:HG21	1.70	0.43
2:C:367:LEU:CD1	2:C:372:LYS:H	2.32	0.43
2:C:169:PHE:HA	2:C:227:ILE:O	2.19	0.43
2:D:129:GLY:HA2	2:D:132:MET:HG3	2.01	0.43
4:L:24:LYS:HZ1	4:L:69:ARG:HH21	1.66	0.43
4:L:166:ASP:OD1	4:L:167:SER:N	2.52	0.43
1:A:146:HIS:HA	1:A:179:LYS:CE	2.45	0.42
1:A:254:LYS:NZ	1:A:282:TYR:CD2	2.87	0.42
1:B:34:SER:O	1:B:66:THR:HG23	2.18	0.42
2:D:228:ILE:CD1	2:D:256:TRP:CG	3.01	0.42
4:F:39:LYS:NZ	4:F:81:GLU:O	2.28	0.42
4:L:18:LYS:HB2	4:L:76:SER:HA	2.01	0.42
1:B:168:SER:O	1:B:170:ASP:N	2.53	0.42
4:F:61:ARG:NH2	4:F:82:ASP:OD2	2.52	0.42
4:F:114:VAL:HG22	4:F:135:LEU:HD23	2.01	0.42
1:A:151:TRP:HA	1:A:154:MET:CG	2.48	0.42
1:A:376:ASN:O	1:A:383:VAL:HG22	2.19	0.42
1:A:94:HIS:HB3	1:A:122:THR:HG1	1.79	0.42
1:A:286:GLY:O	1:A:403:PRO:HD3	2.19	0.42
1:A:294:ASN:O	1:A:301:HIS:NE2	2.49	0.42
2:C:115:ILE:HG22	2:C:123:ILE:HD11	2.00	0.42
1:A:160:TRP:CH2	1:A:267:VAL:HG11	2.54	0.42
3:E:34:MET:HE2	3:E:98:ARG:HD2	2.01	0.42
1:B:139:ARG:HD2	1:B:366:ASP:OD1	2.19	0.42
2:C:294:ARG:HH11	2:C:294:ARG:HD2	1.73	0.42
3:E:208:HIS:CE1	3:E:210:ALA:HB3	2.54	0.42
1:A:126:SER:OG	1:A:172:GLU:OE1	2.26	0.42
1:A:262:THR:HA	1:A:268:TRP:HE1	1.84	0.42
2:D:42:VAL:HG23	2:D:101:ASP:HA	1.99	0.42
1:A:145:SER:O	1:A:179:LYS:HD2	2.20	0.42
3:E:91:THR:HA	3:E:118:VAL:O	2.20	0.42
1:A:119:ILE:HD13	1:A:138:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:213:THR:HG22	3:E:215:VAL:HG23	2.02	0.42
4:F:109:ASP:OD2	4:F:140:PRO:HD3	2.19	0.42
1:B:119:ILE:HD11	1:B:346:LEU:HD13	2.02	0.42
2:C:48:VAL:O	2:C:52:ASP:OD1	2.38	0.42
2:D:257:ILE:HA	2:D:278:ILE:O	2.19	0.42
3:H:172:VAL:HG22	3:H:190:VAL:HG23	2.00	0.42
1:A:253:TYR:HE2	1:A:279:ALA:HB1	1.85	0.41
1:B:376:ASN:ND2	1:B:401:ILE:H	2.18	0.41
3:E:60:TYR:HE1	3:E:70:ILE:HG22	1.85	0.41
2:D:289:LEU:N	2:D:290:PRO:HD2	2.35	0.41
4:F:94:LEU:HD23	4:F:94:LEU:HA	1.89	0.41
4:L:111:ALA:HA	4:L:199:THR:HG21	2.00	0.41
2:C:124:LEU:HA	2:C:144:PHE:O	2.20	0.41
2:C:156:VAL:HG22	2:C:379:TRP:CD2	2.55	0.41
1:A:343:LYS:HE3	1:A:343:LYS:HB3	1.83	0.41
2:D:182:PHE:CG	2:D:231:TYR:CD2	3.08	0.41
2:D:266:THR:HB	2:D:373:TRP:CD1	2.55	0.41
3:H:7:SER:HB2	3:H:21:SER:HB2	2.01	0.41
3:H:86:LEU:HD23	3:H:86:LEU:HA	1.92	0.41
1:A:113:PHE:C	1:A:113:PHE:HD1	2.28	0.41
2:C:240:ILE:O	2:C:243:VAL:HG22	2.21	0.41
3:E:79:LEU:HD23	3:E:96:CYS:SG	2.60	0.41
4:L:6:GLN:HE22	4:L:88:CYS:H	1.67	0.41
1:A:126:SER:N	1:A:172:GLU:OE1	2.43	0.41
2:D:133:ILE:HG13	2:D:148:PRO:O	2.20	0.41
2:D:142:MET:HG2	2:D:336:ASN:ND2	2.36	0.41
4:F:35:TRP:CH2	4:F:88:CYS:HB3	2.56	0.41
1:A:375:MET:HA	1:A:383:VAL:O	2.21	0.41
1:A:378:GLN:OE1	1:A:383:VAL:HG11	2.19	0.41
4:F:54:LEU:HD21	4:F:62:PHE:O	2.21	0.41
4:L:194:GLU:HG3	4:L:205:VAL:CG2	2.50	0.41
1:B:290:LEU:HD23	1:B:290:LEU:HA	1.80	0.41
1:B:343:LYS:O	1:B:347:MET:HG3	2.20	0.41
2:D:315:PRO:HA	2:D:331:GLN:OE1	2.19	0.41
3:E:47:TRP:O	3:E:61:PRO:HG3	2.21	0.41
2:D:169:PHE:HA	2:D:227:ILE:O	2.21	0.41
3:H:30:SER:O	3:H:53:ASN:HB2	2.21	0.41
4:L:118:PRO:HB3	4:L:208:PHE:CE2	2.56	0.41
1:A:66:THR:CG2	4:L:148:LYS:NZ	2.84	0.41
1:A:79:CYS:SG	2:C:79:LYS:HB2	2.61	0.40
1:A:140:THR:O	1:A:367:ARG:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:LEU:HD22	1:A:372:TYR:CB	2.51	0.40
2:C:228:ILE:HD11	2:C:256:TRP:HB3	2.04	0.40
2:D:142:MET:HG2	2:D:336:ASN:HD21	1.86	0.40
3:H:77:ASN:N	3:H:77:ASN:HD22	2.18	0.40
2:C:228:ILE:HD12	2:C:228:ILE:C	2.46	0.40
2:D:40:ILE:HD11	2:D:73:MET:CE	2.46	0.40
2:D:124:LEU:HA	2:D:144:PHE:O	2.21	0.40
2:D:278:ILE:HG12	2:D:366:LEU:HD13	2.02	0.40
4:L:24:LYS:HA	4:L:69:ARG:O	2.22	0.40
1:A:66:THR:CG2	4:L:148:LYS:HZ1	2.34	0.40
1:B:132:SER:N	2:D:177:PRO:HG2	2.37	0.40
2:D:184:ASN:O	2:D:188:SER:OG	2.22	0.40
1:A:94:HIS:HA	1:A:95:PRO:HD3	1.83	0.40
1:A:241:ILE:HA	1:A:269:LEU:O	2.21	0.40
1:B:42:PHE:CE2	1:B:62:ALA:HB1	2.56	0.40
4:F:115:SER:O	4:F:133:CYS:HA	2.21	0.40
4:L:158:VAL:HG12	4:L:160:ASN:OD1	2.21	0.40
3:E:86:LEU:HD22	3:E:86:LEU:H	1.87	0.40
2:D:101:ASP:HB3	2:D:128:GLY:HA3	2.04	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	337/383 (88%)	312 (93%)	25 (7%)	0	100	100
1	B	328/383 (86%)	307 (94%)	18 (6%)	3 (1%)	14	41
2	C	325/364 (89%)	294 (90%)	31 (10%)	0	100	100
2	D	315/364 (86%)	291 (92%)	24 (8%)	0	100	100
3	E	211/224 (94%)	194 (92%)	15 (7%)	2 (1%)	14	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	208/224 (93%)	192 (92%)	12 (6%)	4 (2%)	6	23
4	F	209/213 (98%)	198 (95%)	11 (5%)	0	100	100
4	L	210/213 (99%)	198 (94%)	12 (6%)	0	100	100
All	All	2143/2368 (90%)	1986 (93%)	148 (7%)	9 (0%)	30	59

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	114	TYR
3	H	43	LYS
3	E	181	SER
3	H	181	SER
3	H	221	PRO
3	E	199	SER
1	B	358	ARG
3	H	86	LEU
1	B	352	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	238/329 (72%)	235 (99%)	3 (1%)	61	86
1	B	219/329 (67%)	217 (99%)	2 (1%)	70	90
2	C	227/327 (69%)	226 (100%)	1 (0%)	84	94
2	D	213/327 (65%)	212 (100%)	1 (0%)	81	93
3	E	159/191 (83%)	156 (98%)	3 (2%)	50	79
3	H	163/191 (85%)	163 (100%)	0	100	100
4	F	171/190 (90%)	170 (99%)	1 (1%)	78	93
4	L	172/190 (90%)	172 (100%)	0	100	100
All	All	1562/2074 (75%)	1551 (99%)	11 (1%)	76	92

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ILE
1	A	172	GLU
1	A	262	THR
1	B	136	SER
1	B	172	GLU
2	C	309	SER
3	E	60	TYR
3	E	96	CYS
3	E	187	SER
2	D	309	SER
4	F	10	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	A	94	HIS
1	B	94	HIS
1	B	294	ASN
1	B	311	GLN
2	C	95	GLN
2	C	153	GLN
3	E	142	ASN
2	D	95	GLN
2	D	184	ASN
2	D	336	ASN
4	F	6	GLN
4	F	37	GLN
4	F	90	GLN
4	F	155	GLN
3	H	74	ASN
3	H	77	ASN
4	L	6	GLN
4	L	49	GLN
4	L	123	GLN
4	L	136	ASN
4	L	189	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	347/383 (90%)	1.08	40 (11%) 9 8	36, 48, 68, 88	0
1	B	338/383 (88%)	1.14	44 (13%) 7 6	38, 53, 72, 86	0
2	C	335/364 (92%)	1.49	98 (29%) 1 1	26, 48, 79, 123	2 (0%)
2	D	329/364 (90%)	1.73	118 (35%) 1 0	28, 53, 92, 140	0
3	E	215/224 (95%)	0.99	27 (12%) 8 6	27, 42, 58, 69	0
3	H	216/224 (96%)	1.03	30 (13%) 6 5	28, 40, 52, 66	0
4	F	211/213 (99%)	0.74	11 (5%) 33 26	23, 32, 50, 67	0
4	L	212/213 (99%)	0.80	15 (7%) 22 17	24, 32, 47, 82	0
All	All	2203/2368 (93%)	1.17	383 (17%) 4 3	23, 45, 74, 140	2 (0%)

All (383) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	346	GLY	6.8
2	D	239	TYR	6.7
2	C	245	ASN	5.3
2	D	236	GLU	5.2
2	C	267	ASP	5.0
2	C	220	LEU	4.8
1	B	397	ASP	4.8
2	D	342	VAL	4.7
2	C	239	TYR	4.6
3	E	88	SER	4.6
1	B	332	ASN	4.6
2	D	184	ASN	4.6
2	D	368	ASN	4.6
1	A	397	ASP	4.5
2	D	256	TRP	4.5
2	D	287	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
2	D	82	ILE	4.4
2	C	243	VAL	4.3
2	D	195	VAL	4.2
2	D	230	LEU	4.2
2	C	76	THR	4.1
1	A	352	PRO	4.1
2	C	78	PRO	4.1
2	D	244	ALA	4.1
2	C	112	LEU	4.1
2	D	232	CYS	4.1
2	D	259	PRO	4.0
2	D	323	ASN	4.0
2	C	207	MET	4.0
1	B	87	VAL	4.0
2	D	365	ILE	3.9
2	D	76	THR	3.8
2	D	83	THR	3.8
4	L	57	ASP	3.8
2	C	231	TYR	3.8
2	D	170	SER	3.7
2	D	172	VAL	3.7
2	C	105[A]	GLN	3.7
2	D	261	LEU	3.7
2	D	173	THR	3.7
2	D	193	SER	3.7
2	C	381	ASP	3.7
2	D	206	ASP	3.6
2	C	287	TYR	3.6
2	D	330	TYR	3.6
2	D	255	THR	3.6
1	B	86	GLN	3.6
2	C	344	PHE	3.6
2	D	104	ASP	3.6
2	C	192	ASN	3.6
2	D	220	LEU	3.6
3	H	96	CYS	3.5
1	B	321	ASN	3.5
2	D	238	THR	3.5
2	D	140	SER	3.5
1	A	356	THR	3.5
2	D	192	ASN	3.5
2	D	240	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	202	VAL	3.4
2	D	175	TYR	3.4
2	C	373	TRP	3.4
1	B	265	GLY	3.4
3	H	183	LEU	3.4
2	C	101	ASP	3.4
2	C	204	LEU	3.3
3	H	157	GLU	3.3
3	H	87	ARG	3.3
3	E	96	CYS	3.3
3	E	179	LEU	3.2
2	C	113	ASP	3.2
1	A	361	PHE	3.2
2	D	282	TYR	3.2
2	D	79	LYS	3.2
2	D	203	LEU	3.1
2	D	75	GLU	3.1
2	C	70	LEU	3.1
2	D	187	ARG	3.1
2	D	263	ALA	3.1
2	D	243	VAL	3.1
2	D	245	ASN	3.1
2	D	228	ILE	3.1
2	D	324	THR	3.1
3	E	86	LEU	3.1
2	D	237	ALA	3.1
2	D	231	TYR	3.1
2	C	346	GLY	3.1
2	D	224	GLN	3.1
2	C	349	LEU	3.1
2	D	343	THR	3.1
2	D	225	SER	3.0
2	C	228	ILE	3.0
2	C	221	LYS	3.0
2	C	223	LEU	3.0
4	F	108	ALA	3.0
1	B	152	PHE	3.0
3	E	31	SER	3.0
3	E	78	SER	3.0
4	F	181	THR	3.0
1	A	81	ASP	3.0
2	C	276	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
2	C	230	LEU	3.0
3	H	140	SER	3.0
4	F	142	ASP	3.0
2	C	342	VAL	3.0
2	C	331	GLN	3.0
3	H	25	SER	3.0
3	E	142	ASN	2.9
1	B	356	THR	2.9
2	D	223	LEU	2.9
2	C	175	TYR	2.9
3	H	212	SER	2.9
2	C	222	LYS	2.9
2	D	344	PHE	2.9
2	D	349	LEU	2.9
4	L	203	PRO	2.9
2	C	170	SER	2.9
2	D	247	VAL	2.9
1	A	35	THR	2.9
1	A	39	GLU	2.9
4	F	77	ASN	2.9
2	D	279	SER	2.9
4	L	201	THR	2.9
1	A	29	ILE	2.9
2	D	278	ILE	2.9
3	H	179	LEU	2.9
4	L	23	CYS	2.9
2	C	372	LYS	2.8
2	C	193	SER	2.8
2	D	219	GLN	2.8
2	C	256	TRP	2.8
4	L	212	GLU	2.8
2	D	176	PHE	2.8
1	B	47	ASN	2.8
2	C	323	ASN	2.8
2	D	221	LYS	2.8
2	D	345	GLU	2.8
1	A	213	ASP	2.8
3	E	76	LYS	2.8
2	C	195	VAL	2.8
2	C	249	LEU	2.8
2	C	257	ILE	2.8
2	C	82	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
4	L	204	ILE	2.7
1	A	100	ASP	2.7
2	C	83	THR	2.7
2	C	174	THR	2.7
3	E	196	THR	2.7
1	A	393	ILE	2.7
2	C	384	LEU	2.7
1	B	324	ASP	2.7
2	C	288	GLY	2.7
2	D	281	SER	2.7
1	B	62	ALA	2.7
2	D	379	TRP	2.7
3	H	22	CYS	2.7
2	C	44	THR	2.7
4	L	211	ASN	2.7
1	B	320	GLU	2.7
2	C	188	SER	2.7
2	D	198	GLU	2.7
2	D	260	SER	2.7
3	E	25	SER	2.7
1	A	362	ASN	2.7
2	C	104	ASP	2.7
2	D	171	ILE	2.6
1	A	279	ALA	2.6
1	B	88	TYR	2.6
2	D	86	CYS	2.6
2	C	236	GLU	2.6
2	D	165	ASP	2.6
3	E	220	VAL	2.6
1	B	237	ALA	2.6
1	B	344	ARG	2.6
2	C	232	CYS	2.6
4	F	23	CYS	2.6
1	B	29	ILE	2.6
1	B	353	ASP	2.6
2	D	194	PHE	2.6
2	C	254	TYR	2.6
2	D	77	ASP	2.6
3	E	36	TRP	2.6
1	B	328	GLY	2.6
2	D	366	LEU	2.6
2	D	258	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	28	ASN	2.6
1	B	212	ALA	2.6
1	A	314	HIS	2.5
2	C	90	SER	2.5
3	H	31	SER	2.5
2	D	248	GLY	2.5
3	H	37	VAL	2.5
2	C	275	THR	2.5
4	F	79	GLU	2.5
2	C	86	CYS	2.5
2	D	321	CYS	2.5
1	B	101	HIS	2.5
2	D	234	LYS	2.5
2	D	158	LEU	2.5
2	D	190	ILE	2.5
2	C	241	PHE	2.5
1	A	170	ASP	2.5
2	D	101	ASP	2.5
2	C	130	SER	2.5
2	D	217	GLN	2.5
2	C	127	HIS	2.5
2	C	319	SER	2.5
3	H	209	PRO	2.5
2	D	264	GLY	2.5
1	B	163	VAL	2.5
3	E	2	VAL	2.5
2	C	379	TRP	2.5
2	C	75	GLU	2.5
2	D	242	GLU	2.5
2	C	73	MET	2.4
2	C	42	VAL	2.4
2	C	45	SER	2.4
2	D	201	GLU	2.4
2	D	222	LYS	2.4
2	C	261	LEU	2.4
1	B	394	ILE	2.4
2	D	257	ILE	2.4
1	B	173	GLY	2.4
2	D	363	VAL	2.4
1	B	299	SER	2.4
1	A	61	GLN	2.4
2	D	280	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
3	H	172	VAL	2.4
1	B	361	PHE	2.4
2	D	90	SER	2.4
2	C	244	ALA	2.4
1	B	282	TYR	2.4
1	A	365	GLY	2.4
2	C	251	GLY	2.4
2	C	262	VAL	2.4
2	D	262	VAL	2.4
2	C	79	LYS	2.4
1	A	152	PHE	2.4
1	B	402	TRP	2.4
2	C	118	GLN	2.4
2	D	188	SER	2.4
2	C	109	ALA	2.3
2	C	237	ALA	2.3
3	E	84	SER	2.3
1	B	33	LEU	2.3
1	B	235	LEU	2.3
2	C	233	THR	2.3
2	D	70	LEU	2.3
1	B	352	PRO	2.3
2	C	259	PRO	2.3
2	D	129	GLY	2.3
2	D	181	ASP	2.3
2	D	326	GLU	2.3
2	D	118	GLN	2.3
3	H	34	MET	2.3
2	D	205	LEU	2.3
1	A	282	TYR	2.3
2	C	164	TYR	2.3
2	D	174	THR	2.3
3	E	27	ILE	2.3
2	D	177	PRO	2.3
1	A	212	ALA	2.3
1	A	298	GLU	2.3
2	D	135	ALA	2.3
3	H	114	ALA	2.3
1	A	258	MET	2.3
1	A	261	MET	2.3
2	C	134[A]	MET	2.3
3	H	182	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	105	GLN	2.3
2	D	31	SER	2.3
3	E	194	SER	2.3
3	H	98	ARG	2.3
2	D	376	VAL	2.3
2	C	184	ASN	2.3
3	H	155	PHE	2.3
1	A	363	GLU	2.3
2	D	80	SER	2.3
2	D	233	THR	2.3
2	D	292	ARG	2.3
2	D	322	TYR	2.3
1	B	46	VAL	2.3
1	B	221	GLY	2.3
2	C	135	ALA	2.2
2	C	154	ALA	2.2
4	F	122	GLU	2.2
2	D	204	LEU	2.2
1	A	353	ASP	2.2
4	L	142	ASP	2.2
1	A	392	TYR	2.2
4	L	50	TYR	2.2
4	L	174	MET	2.2
1	A	283	ALA	2.2
1	B	283	ALA	2.2
2	C	203	LEU	2.2
2	C	365	ILE	2.2
4	L	102	GLN	2.2
1	A	323	THR	2.2
3	E	26	GLY	2.2
2	D	134	MET	2.2
3	E	93	MET	2.2
1	A	259	LEU	2.2
2	C	345	GLU	2.2
4	F	153	GLU	2.2
1	B	374	ILE	2.2
1	B	387	ILE	2.2
4	F	85	ILE	2.2
3	H	156	PRO	2.2
4	L	88	CYS	2.2
3	H	78	SER	2.2
2	C	176	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	146	PHE	2.2
2	D	169	PHE	2.2
2	C	366	LEU	2.2
2	C	106	GLU	2.2
2	D	92	ARG	2.2
3	H	223	ASP	2.2
4	F	57	ASP	2.2
2	C	114	PHE	2.2
3	H	35	SER	2.2
2	C	292	ARG	2.1
3	E	44	ARG	2.1
1	A	40	GLN	2.1
1	A	28	ASN	2.1
2	D	61	HIS	2.1
1	A	210	PRO	2.1
2	C	183	VAL	2.1
1	A	154	MET	2.1
1	B	213	ASP	2.1
1	A	186	GLY	2.1
2	C	166	TRP	2.1
2	C	41	LEU	2.1
2	C	252	TYR	2.1
1	B	303	SER	2.1
2	D	154	ALA	2.1
3	H	181	SER	2.1
4	L	52	SER	2.1
2	C	40	ILE	2.1
1	A	379	ASN	2.1
2	D	377	GLY	2.1
1	B	358	ARG	2.1
1	B	278	SER	2.1
3	E	7	SER	2.1
3	E	204	CYS	2.1
2	C	343	THR	2.1
3	H	44	ARG	2.1
2	C	299	ILE	2.1
2	D	227	ILE	2.1
1	A	303	SER	2.1
3	E	169	SER	2.1
3	H	30	SER	2.1
3	E	34	MET	2.1
3	H	41	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	50	ASN	2.1
4	L	189	ASN	2.1
2	C	182	PHE	2.1
1	A	123	THR	2.1
2	C	173	THR	2.1
2	C	238	THR	2.1
3	E	80	TYR	2.1
3	H	154	TYR	2.1
3	E	212	SER	2.0
2	D	48	VAL	2.0
4	L	160	ASN	2.0
2	C	129	GLY	2.0
3	H	9	GLY	2.0
2	D	107	ALA	2.0
2	D	55	GLU	2.0
1	B	154	MET	2.0
2	D	45	SER	2.0
3	H	180	GLN	2.0
3	E	113	GLY	2.0
3	E	115	GLY	2.0
1	A	119	ILE	2.0
2	C	85	ILE	2.0
1	A	247	ASP	2.0
1	B	315	GLU	2.0
2	D	191	GLU	2.0
1	B	351	TYR	2.0
4	F	36	TYR	2.0
1	A	87	VAL	2.0
2	C	48	VAL	2.0
2	D	42	VAL	2.0
3	H	5	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
5	NA	B	501	1/1	0.87	0.20	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.