



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:12 AM UTC

PDB ID : 5SXU / pdb_00005sxu
Title : X-ray structure of 2-bromoethanol bound to a pentameric ligand gated ion channel (ELIC) in a desensitized state
Authors : Chen, Q.; Kinde, M.; Cohen, A.; Xu, Y.; Tang, P.
Deposited on : 2016-08-10
Resolution : 3.10 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:

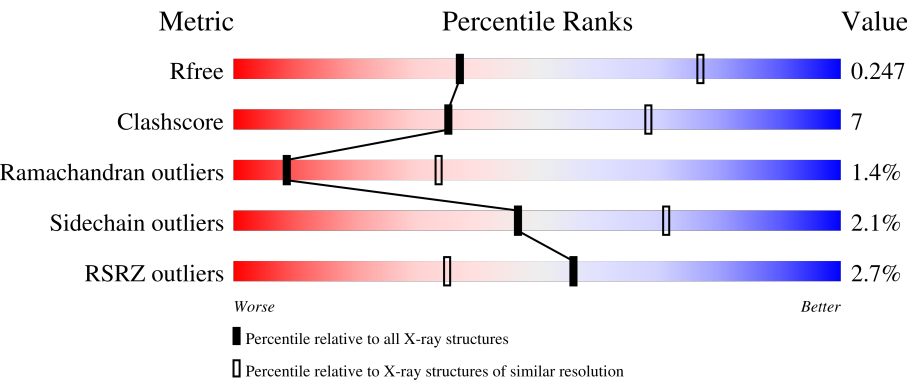
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	322	5% 82% 12% ..
1	B	322	% 74% 20% ..
1	C	322	2% 80% 14% ..
1	D	322	2% 75% 19% ..
1	E	322	3% 76% 19% ..

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Mol	Chain	Length	Quality of chain
1	F	322	
1	G	322	
1	H	322	
1	I	322	
1	J	322	

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	BRJ	A	401	-	-	X	-
2	BRJ	B	403	-	-	-	X
2	BRJ	C	401	-	-	X	-
2	BRJ	D	403	-	-	-	X
2	BRJ	F	401	-	-	X	-
2	BRJ	G	401	-	-	-	X
2	BRJ	H	401	-	-	X	X
2	BRJ	I	402	-	-	-	X
2	BRJ	I	403	-	-	X	-
2	BRJ	J	502	-	-	-	X
2	BRJ	J	503	-	-	-	X
3	3CN	H	404	-	-	-	X

2 Entry composition

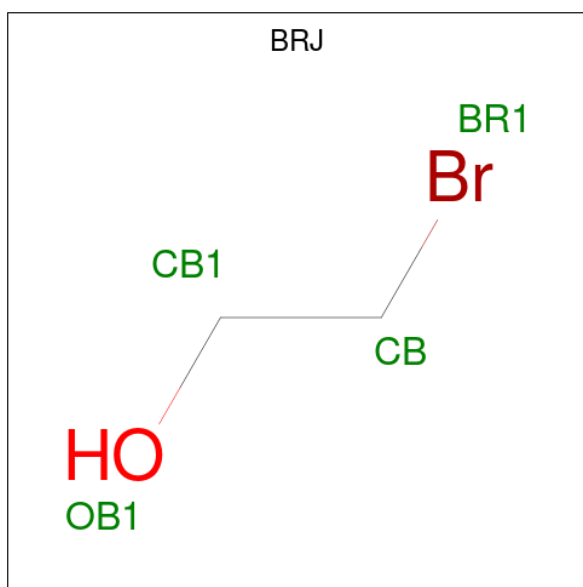
There are 6 unique types of molecules in this entry. The entry contains 25453 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Gamma-aminobutyric-acid receptor subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2516	1639	420	451	6			
1	B	308	Total	C	N	O	S	0	0	0
			2516	1639	420	451	6			
1	C	308	Total	C	N	O	S	0	0	0
			2516	1639	420	451	6			
1	D	308	Total	C	N	O	S	0	0	0
			2516	1639	420	451	6			
1	E	308	Total	C	N	O	S	0	0	0
			2516	1639	420	451	6			
1	F	308	Total	C	N	O	S	0	0	0
			2516	1639	420	451	6			
1	G	308	Total	C	N	O	S	0	0	0
			2516	1639	420	451	6			
1	H	308	Total	C	N	O	S	0	0	0
			2516	1639	420	451	6			
1	I	308	Total	C	N	O	S	0	0	0
			2516	1639	420	451	6			
1	J	308	Total	C	N	O	S	0	0	0
			2516	1639	420	451	6			

- Molecule 2 is 2-BROMOETHANOL (CCD ID: BRJ) (formula: C₂H₅BrO).



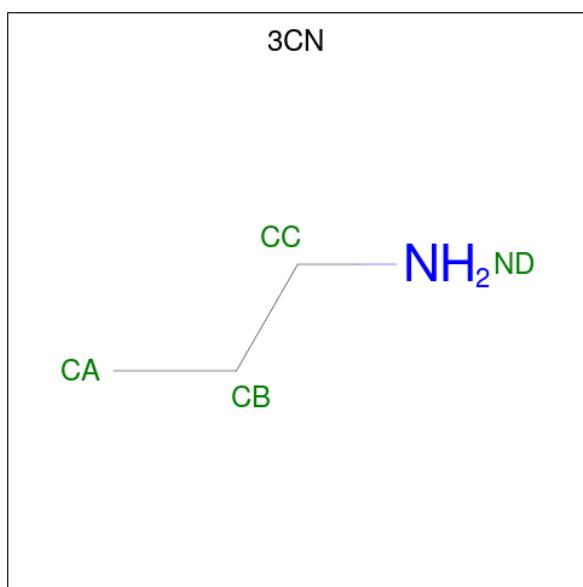
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	Br	C	O	0	0
			4	1	2	1		
2	A	1	Total	Br	C	O	0	0
			4	1	2	1		
2	A	1	Total	Br	C	O	0	0
			4	1	2	1		
2	A	1	Total	Br	C	O	0	0
			4	1	2	1		
2	B	1	Total	Br	C	O	0	0
			4	1	2	1		
2	B	1	Total	Br	C	O	0	0
			4	1	2	1		
2	B	1	Total	Br	C	O	0	0
			4	1	2	1		
2	C	1	Total	Br	C	O	0	0
			4	1	2	1		
2	C	1	Total	Br	C	O	0	0
			4	1	2	1		
2	C	1	Total	Br	C	O	0	0
			4	1	2	1		
2	D	1	Total	Br	C	O	0	0
			4	1	2	1		
2	D	1	Total	Br	C	O	0	0
			4	1	2	1		
2	D	1	Total	Br	C	O	0	0
			4	1	2	1		
2	E	1	Total	Br	C	O	0	0
			4	1	2	1		

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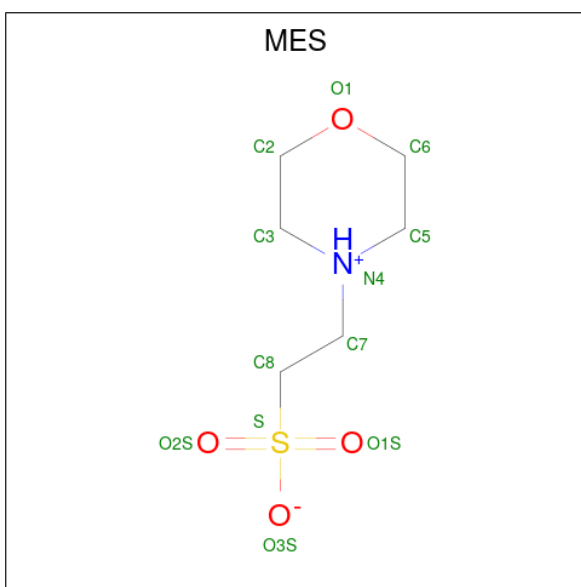
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total 4	Br 1	C 2	O 1	0	0
2	E	1	Total 4	Br 1	C 2	O 1	0	0
2	F	1	Total 4	Br 1	C 2	O 1	0	0
2	F	1	Total 4	Br 1	C 2	O 1	0	0
2	F	1	Total 4	Br 1	C 2	O 1	0	0
2	F	1	Total 4	Br 1	C 2	O 1	0	0
2	G	1	Total 4	Br 1	C 2	O 1	0	0
2	G	1	Total 4	Br 1	C 2	O 1	0	0
2	G	1	Total 4	Br 1	C 2	O 1	0	0
2	H	1	Total 4	Br 1	C 2	O 1	0	0
2	H	1	Total 4	Br 1	C 2	O 1	0	0
2	H	1	Total 4	Br 1	C 2	O 1	0	0
2	I	1	Total 4	Br 1	C 2	O 1	0	0
2	I	1	Total 4	Br 1	C 2	O 1	0	0
2	I	1	Total 4	Br 1	C 2	O 1	0	0
2	J	1	Total 4	Br 1	C 2	O 1	0	0
2	J	1	Total 4	Br 1	C 2	O 1	0	0
2	J	1	Total 4	Br 1	C 2	O 1	0	0

- Molecule 3 is 3-AMINOPROPANE (CCD ID: 3CN) (formula: C₃H₉N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			4	3	1		
3	B	1	Total	C	N	0	0
			4	3	1		
3	C	1	Total	C	N	0	0
			4	3	1		
3	D	1	Total	C	N	0	0
			4	3	1		
3	E	1	Total	C	N	0	0
			4	3	1		
3	F	1	Total	C	N	0	0
			4	3	1		
3	G	1	Total	C	N	0	0
			4	3	1		
3	H	1	Total	C	N	0	0
			4	3	1		
3	I	1	Total	C	N	0	0
			4	3	1		
3	J	1	Total	C	N	0	0
			4	3	1		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	I	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	J	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Cl	0	0
			1	1		
5	J	1	Total	Cl	0	0
			1	1		

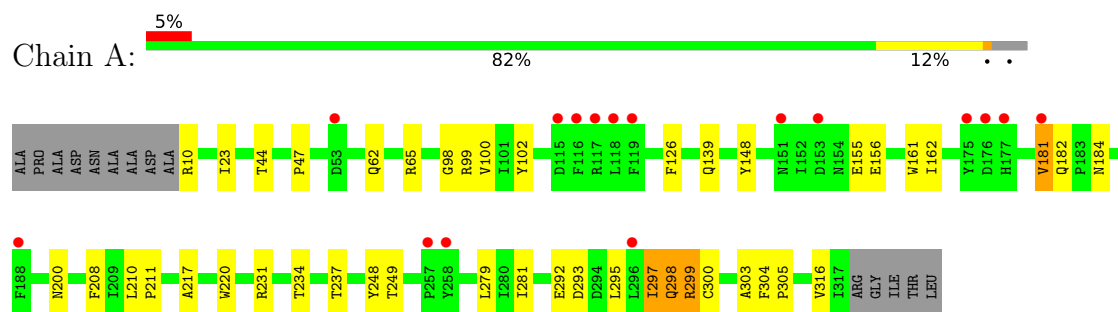
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total 1	O 1	0	0
6	I	1	Total 1	O 1	0	0
6	J	1	Total 1	O 1	0	0

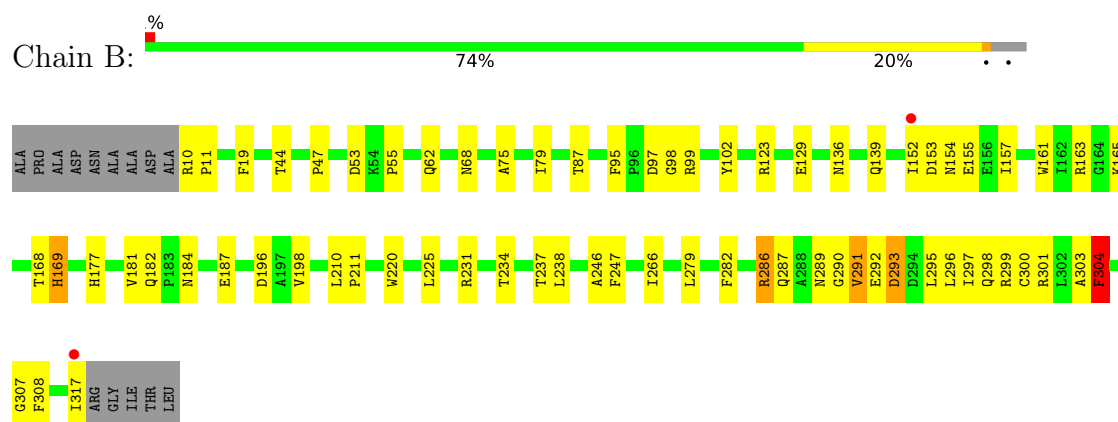
3 Residue-property plots [i](#)

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.

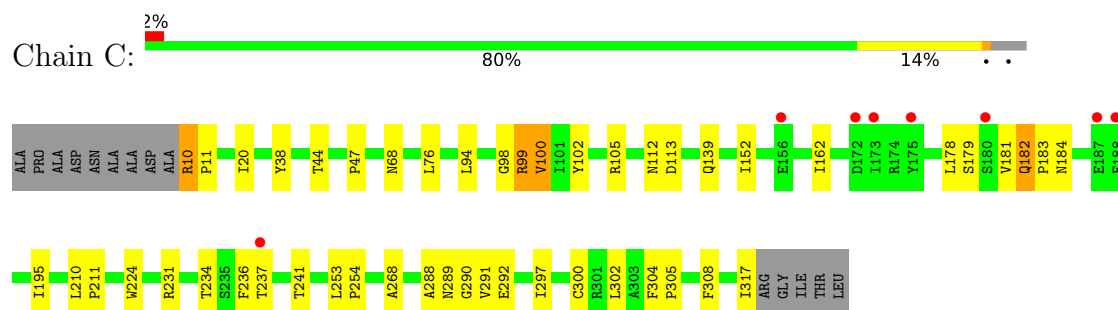
- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1



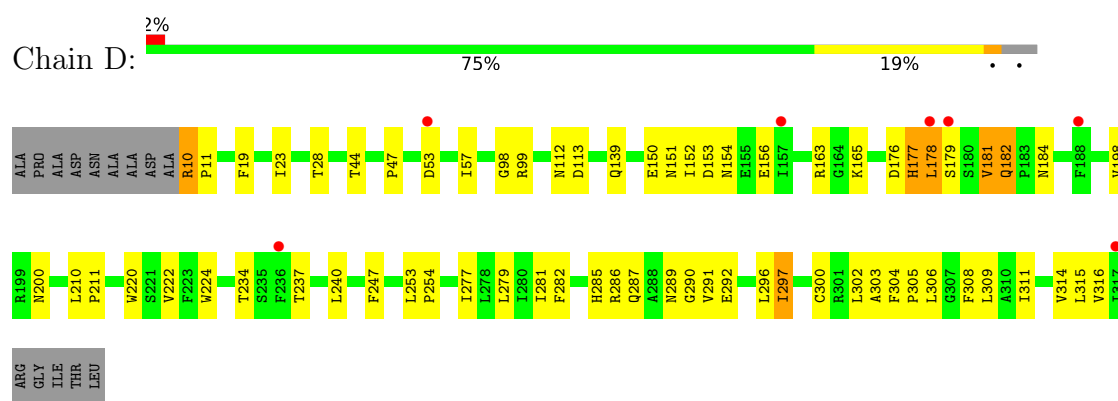
- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1



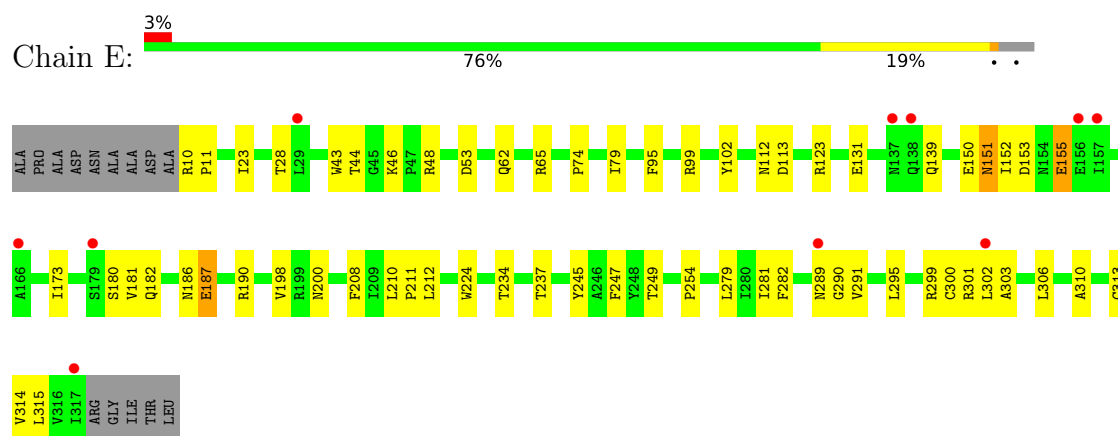
- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1



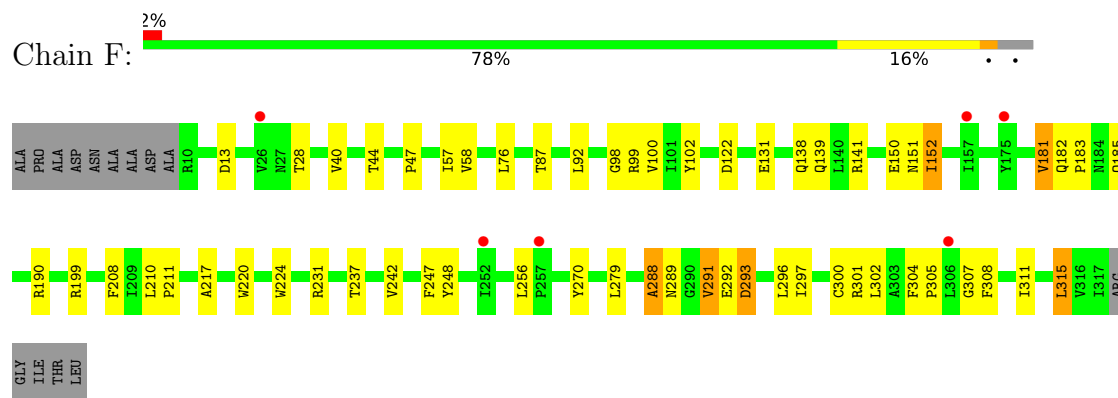
- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1



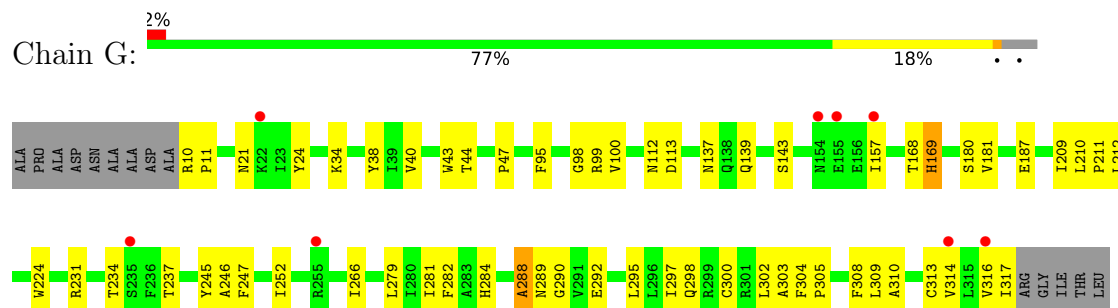
- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1



- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

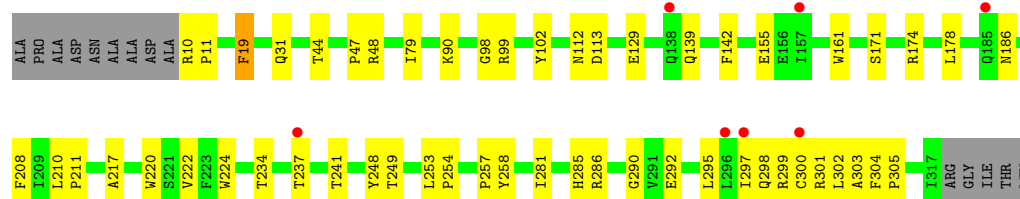


- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1



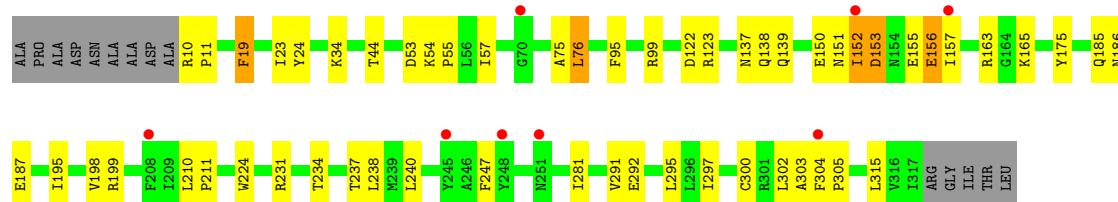
● Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

Chain H:  2% 78% 17%



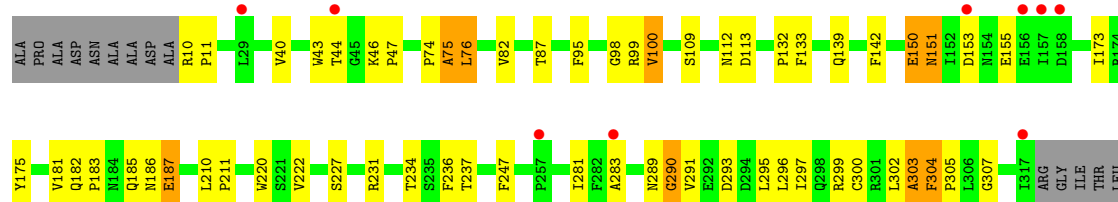
● Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

Chain I:  2% 78% 16%



● Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

Chain J:  3% 77% 16%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.90Å 266.79Å 111.11Å 90.00° 107.13° 90.00°	Depositor
Resolution (Å)	29.93 – 3.10 29.93 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.93-3.10) 99.8 (29.93-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.200 , 0.239 0.211 , 0.247	Depositor DCC
R_{free} test set	5202 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	108.7	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	25453	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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: MES, BRJ, CL, 3CN

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	0.39	0/2584	0.85	5/3522 (0.1%)
1	B	0.42	0/2584	0.90	7/3522 (0.2%)
1	C	0.43	0/2584	0.86	2/3522 (0.1%)
1	D	0.45	0/2584	0.91	7/3522 (0.2%)
1	E	0.40	0/2584	0.88	5/3522 (0.1%)
1	F	0.44	0/2584	0.88	2/3522 (0.1%)
1	G	0.41	0/2584	0.85	3/3522 (0.1%)
1	H	0.41	0/2584	0.84	5/3522 (0.1%)
1	I	0.40	0/2584	0.91	7/3522 (0.2%)
1	J	0.45	0/2584	0.91	6/3522 (0.2%)
All	All	0.42	0/25840	0.88	49/35220 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	53	ASP	N-CA-C	-9.62	101.75	112.72
1	E	155	GLU	N-CA-C	9.36	122.68	111.82
1	I	185	GLN	N-CA-C	-9.27	100.02	112.26
1	E	151	ASN	N-CA-C	-8.63	97.74	110.52
1	F	293	ASP	N-CA-C	-8.49	99.95	110.65
1	F	288	ALA	N-CA-C	-8.48	99.33	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	181	VAL	N-CA-C	-8.26	103.77	111.45
1	E	186	ASN	N-CA-C	-7.97	98.06	109.29
1	D	53	ASP	N-CA-C	-7.51	104.16	112.72
1	C	182	GLN	CA-C-N	7.50	129.21	119.84
1	C	182	GLN	C-N-CA	7.50	129.21	119.84
1	J	300	CYS	N-CA-C	7.49	121.66	112.23
1	J	304	PHE	CA-C-N	-7.15	112.27	119.56
1	J	304	PHE	C-N-CA	-7.15	112.27	119.56
1	A	297	ILE	N-CA-C	-7.15	99.34	109.63
1	B	153	ASP	N-CA-C	-7.10	103.24	112.68
1	H	299	ARG	N-CA-C	-6.96	103.70	111.71
1	B	291	VAL	N-CA-C	6.85	118.42	109.58
1	B	152	ILE	N-CA-C	6.70	117.51	107.80
1	I	54	LYS	N-CA-C	-6.63	101.70	109.93
1	I	295	LEU	N-CA-C	6.55	119.39	111.40
1	J	185	GLN	N-CA-C	-6.49	101.81	111.81
1	D	177	HIS	N-CA-C	6.44	119.40	108.90
1	A	10	ARG	CA-C-N	-6.39	113.39	119.85
1	A	10	ARG	C-N-CA	-6.39	113.39	119.85
1	J	303	ALA	N-CA-C	-6.35	104.28	111.07
1	A	299	ARG	N-CA-C	-6.21	104.51	111.28
1	I	150	GLU	N-CA-C	-5.91	102.91	110.53
1	J	151	ASN	N-CA-C	5.86	119.60	110.17
1	B	304	PHE	CA-C-N	-5.75	113.69	119.56
1	B	304	PHE	C-N-CA	-5.75	113.69	119.56
1	B	169	HIS	CB-CA-C	-5.70	104.36	111.43
1	D	10	ARG	CA-C-N	-5.61	114.18	119.85
1	D	10	ARG	C-N-CA	-5.61	114.18	119.85
1	D	287	GLN	N-CA-C	5.57	117.72	110.53
1	H	295	LEU	N-CA-C	-5.56	105.30	111.36
1	D	182	GLN	N-CA-C	-5.55	99.87	109.58
1	H	292	GLU	N-CA-C	-5.54	102.20	110.23
1	A	297	ILE	CA-C-O	-5.41	115.41	121.36
1	B	53	ASP	N-CA-C	-5.36	106.61	112.72
1	G	288	ALA	N-CA-C	-5.35	103.33	110.55
1	H	48	ARG	N-CA-C	5.32	117.34	108.99
1	H	286	ARG	N-CA-C	5.30	116.75	110.97
1	D	306	LEU	N-CA-C	-5.26	105.69	112.68
1	G	180	SER	N-CA-C	5.25	118.18	109.46
1	I	315	LEU	N-CA-C	-5.25	99.96	108.41
1	I	151	ASN	N-CA-C	5.22	118.44	110.36
1	E	53	ASP	N-CA-C	-5.09	106.91	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	169	HIS	CB-CA-C	-5.07	105.14	111.43

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	304	PHE	Peptide

5.2 Too-close contacts [i](#)

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	2516	0	2490	30	0
1	B	2516	0	2490	49	0
1	C	2516	0	2490	34	0
1	D	2516	0	2490	53	0
1	E	2516	0	2490	38	0
1	F	2516	0	2490	41	0
1	G	2516	0	2490	37	0
1	H	2516	0	2490	38	0
1	I	2516	0	2490	47	0
1	J	2516	0	2490	44	0
2	A	16	0	12	3	0
2	B	12	0	9	1	0
2	C	12	0	9	3	0
2	D	12	0	9	1	0
2	E	12	0	9	2	0
2	F	16	0	12	2	0
2	G	12	0	9	1	0
2	H	12	0	9	2	0
2	I	12	0	9	4	0
2	J	12	0	9	1	0
3	A	4	0	9	0	0
3	B	4	0	9	0	0
3	C	4	0	9	0	0
3	D	4	0	9	0	0
3	E	4	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	4	0	9	0	0
3	G	4	0	9	0	0
3	H	4	0	9	1	0
3	I	4	0	9	0	0
3	J	4	0	9	0	0
4	A	12	0	13	0	0
4	B	12	0	13	0	0
4	C	12	0	13	0	0
4	D	12	0	12	0	0
4	E	12	0	13	0	0
4	F	12	0	12	0	0
4	G	12	0	13	0	0
4	H	12	0	13	0	0
4	I	12	0	13	0	0
4	J	12	0	13	0	0
5	C	1	0	0	0	0
5	J	1	0	0	0	0
6	C	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
All	All	25453	0	25214	377	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 7.

All (377) 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:C:231:ARG:NH2	1:C:292:GLU:OE2	2.12	0.82
1:B:168:THR:C	1:B:169:HIS:HD1	1.88	0.80
1:F:138:GLN:OE1	1:F:185:GLN:NE2	2.15	0.80
1:B:168:THR:O	1:B:169:HIS:ND1	2.15	0.78
1:D:112:ASN:OD1	1:D:113:ASP:N	2.20	0.74
1:C:178:LEU:HD11	1:C:181:VAL:HG22	1.71	0.73
1:J:112:ASN:OD1	1:J:113:ASP:N	2.23	0.72
1:G:112:ASN:OD1	1:G:113:ASP:N	2.24	0.70
1:I:195:ILE:HD13	2:I:403:BRJ:BR1	2.48	0.68
1:F:13:ASP:OD1	1:F:141:ARG:NH1	2.27	0.68
1:C:112:ASN:OD1	1:C:113:ASP:N	2.27	0.67
1:D:304:PHE:HB2	1:D:305:PRO:HD3	1.76	0.66
1:H:224:TRP:CG	1:I:281:ILE:HD11	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:112:ASN:OD1	1:H:113:ASP:N	2.28	0.66
1:D:289:ASN:OD1	1:D:291:VAL:HB	1.96	0.65
1:D:304:PHE:CB	1:D:305:PRO:HD3	2.27	0.64
1:D:182:GLN:O	1:D:184:ASN:N	2.32	0.61
1:C:99:ARG:O	1:C:100:VAL:HB	2.00	0.61
1:D:304:PHE:O	1:D:308:PHE:N	2.31	0.61
1:E:112:ASN:OD1	1:E:113:ASP:N	2.33	0.61
1:B:182:GLN:O	1:B:184:ASN:N	2.31	0.61
1:G:168:THR:C	1:G:169:HIS:ND1	2.59	0.61
1:A:281:ILE:HD11	1:E:224:TRP:CG	2.36	0.60
1:F:288:ALA:O	1:F:289:ASN:CG	2.44	0.60
1:G:168:THR:O	1:G:169:HIS:ND1	2.35	0.60
1:D:302:LEU:HD23	1:D:305:PRO:HG2	1.82	0.60
1:F:302:LEU:HA	1:F:305:PRO:HD2	1.84	0.59
1:A:156:GLU:OE1	1:A:200:ASN:ND2	2.37	0.58
1:C:224:TRP:CD2	1:D:281:ILE:HD11	2.38	0.58
1:F:289:ASN:OD1	1:F:291:VAL:N	2.24	0.58
1:G:231:ARG:NH2	1:G:292:GLU:OE2	2.37	0.58
1:G:284:HIS:ND1	1:G:292:GLU:OE1	2.32	0.58
1:B:304:PHE:HA	1:B:307:GLY:H	1.69	0.58
1:D:156:GLU:OE1	1:D:200:ASN:ND2	2.35	0.58
1:G:224:TRP:CG	1:H:281:ILE:HD11	2.39	0.58
1:E:152:ILE:HD11	1:E:155:GLU:HG2	1.85	0.57
1:J:186:ASN:OD1	1:J:187:GLU:N	2.33	0.57
2:A:401:BRJ:BR1	2:A:402:BRJ:HB11	2.60	0.57
1:I:137:ASN:HD22	1:I:187:GLU:HB3	1.69	0.56
1:J:76:LEU:HD12	2:J:502:BRJ:BR1	2.59	0.56
1:J:44:THR:HA	1:J:99:ARG:HA	1.88	0.56
1:E:306:LEU:O	1:E:310:ALA:N	2.38	0.56
1:I:186:ASN:O	1:I:186:ASN:OD1	2.23	0.56
1:F:224:TRP:CG	1:G:281:ILE:HD11	2.41	0.55
1:I:76:LEU:HD12	2:I:401:BRJ:BR1	2.62	0.55
1:D:289:ASN:O	1:D:291:VAL:N	2.40	0.55
1:D:286:ARG:HH11	1:D:296:LEU:HD21	1.72	0.55
1:H:224:TRP:CE2	1:H:301:ARG:HD3	2.43	0.54
1:B:300:CYS:HA	1:B:303:ALA:HB3	1.90	0.54
1:A:297:ILE:O	1:A:298:GLN:CB	2.56	0.54
1:I:302:LEU:HD23	1:I:305:PRO:HG2	1.89	0.54
1:A:297:ILE:O	1:A:298:GLN:HB3	2.07	0.54
1:B:296:LEU:HA	1:B:299:ARG:HH11	1.71	0.54
1:F:182:GLN:N	1:F:183:PRO:HD3	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:304:PHE:O	1:F:308:PHE:N	2.33	0.54
1:D:47:PRO:HA	1:D:98:GLY:HA2	1.89	0.53
1:G:297:ILE:O	1:G:298:GLN:HB3	2.07	0.53
1:J:173:ILE:O	1:J:187:GLU:HA	2.08	0.53
1:G:10:ARG:N	1:G:11:PRO:CD	2.72	0.53
1:B:62:GLN:NE2	1:C:68:ASN:OD1	2.36	0.53
1:J:283:ALA:CA	1:J:296:LEU:HD23	2.39	0.53
1:D:285:HIS:O	1:D:285:HIS:ND1	2.42	0.52
1:H:302:LEU:HD12	1:H:305:PRO:HB2	1.90	0.52
1:J:231:ARG:CZ	1:J:297:ILE:HD11	2.40	0.52
1:D:44:THR:HA	1:D:99:ARG:HA	1.90	0.52
1:D:279:LEU:O	1:D:282:PHE:N	2.43	0.52
1:D:314:VAL:HG23	1:D:315:LEU:N	2.23	0.52
1:A:208:PHE:CD1	1:A:249:THR:HG22	2.45	0.52
1:C:289:ASN:OD1	1:C:291:VAL:HB	2.10	0.52
1:E:152:ILE:HD11	1:E:155:GLU:CG	2.39	0.52
1:F:307:GLY:O	1:F:311:ILE:HG12	2.10	0.52
1:B:279:LEU:O	1:B:282:PHE:N	2.40	0.52
1:E:295:LEU:HB3	1:E:299:ARG:HH12	1.74	0.52
1:C:288:ALA:O	1:C:289:ASN:CG	2.53	0.52
1:E:10:ARG:N	1:E:11:PRO:CD	2.72	0.52
1:E:10:ARG:N	1:E:11:PRO:HD2	2.25	0.52
1:B:238:LEU:HD21	1:C:236:PHE:CD1	2.45	0.51
1:B:293:ASP:C	1:B:295:LEU:H	2.18	0.51
1:A:300:CYS:HA	1:A:303:ALA:HB3	1.93	0.51
1:F:150:GLU:HG3	1:F:151:ASN:H	1.76	0.51
1:H:297:ILE:HG22	1:H:298:GLN:N	2.26	0.51
1:F:231:ARG:NH2	1:F:292:GLU:OE2	2.44	0.50
1:B:47:PRO:HA	1:B:98:GLY:HA2	1.92	0.50
1:H:19:PHE:N	1:H:19:PHE:CD1	2.79	0.50
1:H:300:CYS:HA	1:H:303:ALA:HB3	1.92	0.50
1:D:304:PHE:CB	1:D:305:PRO:CD	2.89	0.50
1:G:304:PHE:HB2	1:G:305:PRO:HD3	1.92	0.50
1:I:10:ARG:N	1:I:11:PRO:HD2	2.25	0.50
1:B:304:PHE:CD1	1:B:304:PHE:C	2.90	0.50
1:C:182:GLN:O	1:C:184:ASN:N	2.45	0.50
1:J:43:TRP:CH2	1:J:74:PRO:HD2	2.47	0.50
1:G:309:LEU:O	1:G:313:CYS:HB2	2.12	0.50
1:G:288:ALA:O	1:G:289:ASN:CG	2.55	0.49
1:I:195:ILE:CD1	2:I:403:BRJ:BR1	3.15	0.49
1:D:210:LEU:HB3	1:D:211:PRO:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:ILE:O	1:D:300:CYS:N	2.44	0.49
1:H:224:TRP:CD2	1:I:281:ILE:HD11	2.46	0.49
1:C:224:TRP:CG	1:D:281:ILE:HD11	2.48	0.49
1:E:46:LYS:HE3	1:E:48:ARG:HH21	1.77	0.49
1:I:137:ASN:OD1	1:I:138:GLN:HG3	2.13	0.49
1:A:281:ILE:HD11	1:E:224:TRP:CD2	2.46	0.49
1:B:286:ARG:HD2	1:B:296:LEU:HD11	1.94	0.49
1:I:210:LEU:HB3	1:I:211:PRO:HD3	1.94	0.49
1:J:75:ALA:CB	1:J:133:PHE:HB3	2.43	0.49
1:F:152:ILE:O	1:F:152:ILE:HG13	2.13	0.49
1:H:102:TYR:CE1	2:H:401:BRJ:BR1	3.21	0.49
1:F:288:ALA:O	1:F:289:ASN:ND2	2.45	0.49
1:B:289:ASN:OD1	1:B:291:VAL:HB	2.13	0.49
1:B:304:PHE:C	1:B:304:PHE:HD1	2.20	0.48
1:G:44:THR:HA	1:G:99:ARG:HA	1.94	0.48
1:G:302:LEU:HD23	1:G:305:PRO:HG2	1.95	0.48
1:D:178:LEU:HG	1:D:179:SER:N	2.28	0.48
1:J:283:ALA:HA	1:J:296:LEU:HD23	1.95	0.48
1:B:210:LEU:HB3	1:B:211:PRO:HD3	1.94	0.48
1:F:224:TRP:CE2	1:F:301:ARG:HD3	2.49	0.48
1:G:137:ASN:ND2	1:G:187:GLU:HB3	2.28	0.48
1:D:23:ILE:HD12	2:D:403:BRJ:BR1	2.69	0.48
1:B:44:THR:HG22	1:B:99:ARG:HB3	1.95	0.48
1:I:175:TYR:N	1:I:186:ASN:OD1	2.46	0.48
1:D:224:TRP:CB	1:E:281:ILE:HD11	2.43	0.48
1:E:313:CYS:C	1:E:315:LEU:H	2.22	0.48
1:H:10:ARG:N	1:H:11:PRO:HD2	2.28	0.48
1:A:47:PRO:HA	1:A:98:GLY:HA2	1.96	0.48
1:D:10:ARG:N	1:D:11:PRO:HD2	2.29	0.48
2:G:401:BRJ:BR1	2:G:402:BRJ:HB11	2.68	0.48
1:A:248:TYR:CD1	1:B:247:PHE:HA	2.48	0.48
1:C:10:ARG:N	1:C:11:PRO:CD	2.77	0.48
1:A:279:LEU:HD23	1:A:300:CYS:SG	2.54	0.47
1:B:55:PRO:HB3	1:B:95:PHE:CD1	2.49	0.47
1:B:304:PHE:HA	1:B:307:GLY:N	2.28	0.47
1:C:241:THR:HA	1:D:240:LEU:HD12	1.96	0.47
1:D:224:TRP:CG	1:E:281:ILE:HD11	2.49	0.47
1:H:298:GLN:HG2	1:H:301:ARG:CZ	2.44	0.47
1:I:137:ASN:HD22	1:I:187:GLU:CB	2.27	0.47
1:J:153:ASP:O	1:J:155:GLU:HG3	2.14	0.47
1:B:168:THR:C	1:B:169:HIS:ND1	2.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:VAL:O	1:B:293:ASP:N	2.45	0.47
1:E:62:GLN:OE1	1:E:65:ARG:NH1	2.44	0.47
1:A:210:LEU:HB3	1:A:211:PRO:HD3	1.96	0.47
1:C:253:LEU:HB3	1:C:254:PRO:HD2	1.95	0.47
1:B:298:GLN:HG2	1:B:301:ARG:CZ	2.45	0.47
1:H:224:TRP:CD2	1:H:301:ARG:HD3	2.50	0.47
1:C:210:LEU:HB3	1:C:211:PRO:HD3	1.95	0.47
1:E:95:PHE:HB2	1:E:99:ARG:HG2	1.95	0.47
1:F:210:LEU:HB3	1:F:211:PRO:HD3	1.96	0.47
1:H:210:LEU:HB3	1:H:211:PRO:HD3	1.96	0.47
1:H:217:ALA:HA	1:H:220:TRP:CE3	2.50	0.47
1:I:300:CYS:HA	1:I:303:ALA:HB3	1.95	0.47
1:J:210:LEU:HB3	1:J:211:PRO:HD3	1.97	0.47
1:A:295:LEU:O	1:A:299:ARG:HG3	2.14	0.47
1:C:10:ARG:N	1:C:11:PRO:HD2	2.29	0.47
1:C:94:LEU:CD2	1:C:100:VAL:HG22	2.45	0.47
1:C:302:LEU:HD23	1:C:305:PRO:HG2	1.97	0.47
1:H:47:PRO:HA	1:H:98:GLY:HA2	1.97	0.47
1:I:224:TRP:CB	1:J:281:ILE:HD11	2.45	0.47
1:C:47:PRO:HA	1:C:98:GLY:HA2	1.97	0.47
1:F:220:TRP:CE3	1:F:305:PRO:HG3	2.50	0.47
1:H:304:PHE:CB	1:H:305:PRO:HD3	2.45	0.47
1:I:304:PHE:HB2	1:I:305:PRO:HD3	1.97	0.47
1:B:10:ARG:N	1:B:11:PRO:CD	2.78	0.46
1:A:65:ARG:HH12	1:B:68:ASN:HA	1.80	0.46
1:B:97:ASP:OD1	1:B:99:ARG:HG2	2.16	0.46
1:F:304:PHE:HB2	1:F:305:PRO:HD3	1.98	0.46
1:I:11:PRO:HB3	1:I:138:GLN:C	2.40	0.46
1:I:304:PHE:CB	1:I:305:PRO:HD3	2.46	0.46
1:D:300:CYS:HA	1:D:303:ALA:HB3	1.97	0.46
1:J:231:ARG:CZ	1:J:297:ILE:CD1	2.94	0.46
1:B:308:PHE:C	1:B:308:PHE:CD1	2.93	0.46
1:F:44:THR:HA	1:F:99:ARG:HA	1.96	0.46
1:G:300:CYS:HA	1:G:303:ALA:HB3	1.98	0.46
1:C:44:THR:HA	1:C:99:ARG:HA	1.96	0.46
1:I:44:THR:HG22	1:I:99:ARG:HB3	1.97	0.46
1:J:132:PRO:HD3	1:J:142:PHE:CE2	2.51	0.46
1:I:291:VAL:HG22	1:I:292:GLU:N	2.30	0.46
1:G:224:TRP:CD2	1:H:281:ILE:HD11	2.51	0.46
1:A:62:GLN:OE1	1:A:65:ARG:NH1	2.48	0.46
1:D:153:ASP:OD1	1:D:154:ASN:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:231:ARG:CZ	1:F:297:ILE:CD1	2.94	0.46
1:G:297:ILE:O	1:G:298:GLN:CB	2.63	0.46
1:I:137:ASN:OD1	1:I:137:ASN:C	2.58	0.46
1:A:23:ILE:HG21	1:A:126:PHE:CD2	2.51	0.45
1:H:102:TYR:CD1	2:H:401:BRJ:HB11	2.52	0.45
1:I:44:THR:HA	1:I:99:ARG:HA	1.97	0.45
1:J:304:PHE:HB2	1:J:305:PRO:HD3	1.98	0.45
1:A:208:PHE:CE1	1:A:248:TYR:CE2	3.05	0.45
1:B:79:ILE:HB	1:B:129:GLU:HB2	1.98	0.45
1:C:76:LEU:HD12	2:C:401:BRJ:BR1	2.72	0.45
1:F:304:PHE:CB	1:F:305:PRO:HD3	2.47	0.45
1:G:210:LEU:HB3	1:G:211:PRO:HD3	1.98	0.45
1:A:181:VAL:HG12	1:A:182:GLN:H	1.82	0.45
1:B:44:THR:HA	1:B:99:ARG:HA	1.97	0.45
1:F:231:ARG:CZ	1:F:297:ILE:HD13	2.47	0.45
1:C:178:LEU:CD1	1:C:181:VAL:HG22	2.43	0.45
1:C:304:PHE:HB2	1:C:305:PRO:HD3	1.98	0.45
1:D:151:ASN:OD1	1:D:165:LYS:NZ	2.44	0.45
1:B:246:ALA:HA	1:B:266:ILE:HD13	1.98	0.45
1:C:297:ILE:O	1:C:300:CYS:N	2.50	0.45
1:H:220:TRP:CE3	1:H:305:PRO:HG3	2.52	0.45
1:I:175:TYR:O	1:I:186:ASN:OD1	2.34	0.45
1:J:289:ASN:O	1:J:291:VAL:N	2.49	0.45
1:B:161:TRP:HB2	1:B:198:VAL:CG2	2.46	0.45
1:D:152:ILE:HD12	1:D:152:ILE:C	2.42	0.45
1:J:150:GLU:HG3	1:J:151:ASN:H	1.82	0.45
1:I:95:PHE:CD2	1:I:99:ARG:HG3	2.51	0.45
1:I:224:TRP:CG	1:J:281:ILE:HD11	2.51	0.45
1:J:95:PHE:HB2	1:J:99:ARG:HG2	1.99	0.45
1:A:182:GLN:O	1:A:184:ASN:N	2.46	0.44
1:E:150:GLU:HG3	1:E:151:ASN:O	2.17	0.44
1:I:155:GLU:HG3	1:I:156:GLU:N	2.31	0.44
1:J:302:LEU:HA	1:J:305:PRO:HD2	1.98	0.44
1:F:181:VAL:O	1:F:182:GLN:C	2.60	0.44
1:F:293:ASP:O	1:F:296:LEU:N	2.50	0.44
1:I:155:GLU:HG3	1:I:157:ILE:H	1.82	0.44
1:A:102:TYR:CD2	2:A:401:BRJ:HB11	2.52	0.44
1:G:95:PHE:CD2	1:G:99:ARG:HG3	2.52	0.44
1:J:296:LEU:HA	1:J:299:ARG:NE	2.33	0.44
1:G:246:ALA:HA	1:G:266:ILE:HD13	1.98	0.44
1:I:10:ARG:N	1:I:11:PRO:CD	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ASN:HB2	1:B:187:GLU:O	2.17	0.44
1:B:196:ASP:CG	1:I:165:LYS:HZ1	2.26	0.44
1:I:238:LEU:HD21	1:J:236:PHE:CD1	2.53	0.44
1:J:295:LEU:O	1:J:299:ARG:HG3	2.17	0.44
1:J:295:LEU:CG	1:J:299:ARG:HH21	2.31	0.44
1:G:224:TRP:CB	1:H:281:ILE:HD11	2.48	0.43
1:D:277:ILE:O	1:D:281:ILE:HG22	2.17	0.43
1:F:58:VAL:HB	1:F:92:LEU:HB2	2.00	0.43
1:J:10:ARG:N	1:J:11:PRO:CD	2.82	0.43
1:B:231:ARG:CZ	1:B:297:ILE:CD1	2.96	0.43
1:D:150:GLU:CG	1:D:152:ILE:HG23	2.49	0.43
1:F:102:TYR:CD1	2:F:401:BRJ:BR1	3.27	0.43
1:F:289:ASN:OD1	1:F:289:ASN:C	2.61	0.43
1:I:224:TRP:HB2	1:J:281:ILE:HD11	1.99	0.43
1:A:65:ARG:NH1	1:B:68:ASN:HA	2.34	0.43
1:D:163:ARG:HD2	1:D:198:VAL:HG13	2.00	0.43
1:H:285:HIS:O	1:H:285:HIS:ND1	2.52	0.43
1:D:220:TRP:CE3	1:D:305:PRO:HG3	2.54	0.43
1:D:285:HIS:O	1:D:285:HIS:CG	2.71	0.43
1:E:173:ILE:O	1:E:187:GLU:HA	2.18	0.43
1:H:19:PHE:CD2	3:H:404:3CN:HA2	2.54	0.43
1:H:241:THR:HA	1:I:240:LEU:HD12	2.01	0.43
1:I:152:ILE:O	1:I:153:ASP:CB	2.66	0.43
1:A:155:GLU:HG2	1:A:161:TRP:CD1	2.53	0.43
1:B:154:ASN:HB3	1:B:157:ILE:HD12	2.01	0.43
1:E:79:ILE:HD11	1:E:131:GLU:HB3	2.00	0.43
1:F:76:LEU:HD12	2:F:401:BRJ:BR1	2.74	0.43
1:J:220:TRP:C	1:J:222:VAL:H	2.27	0.43
1:C:38:TYR:CE1	1:C:105:ARG:HD2	2.54	0.43
1:D:177:HIS:O	1:D:178:LEU:HB2	2.18	0.43
1:E:313:CYS:O	1:E:315:LEU:N	2.52	0.43
1:J:44:THR:HG22	1:J:99:ARG:HB3	1.99	0.43
1:J:175:TYR:O	1:J:186:ASN:ND2	2.52	0.43
1:G:10:ARG:N	1:G:11:PRO:HD2	2.33	0.43
1:C:224:TRP:CE3	1:D:281:ILE:HD11	2.54	0.43
1:D:150:GLU:HG3	1:D:152:ILE:HG23	2.01	0.43
1:E:224:TRP:CD2	1:E:301:ARG:HD3	2.54	0.43
1:I:19:PHE:CD1	1:I:19:PHE:N	2.87	0.43
1:A:44:THR:HG22	1:A:99:ARG:CB	2.49	0.42
1:B:123:ARG:HG2	1:B:198:VAL:HG12	2.01	0.42
1:E:180:SER:OG	1:E:182:GLN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:VAL:HG22	1:D:292:GLU:O	2.18	0.42
1:D:304:PHE:HB2	1:D:305:PRO:CD	2.48	0.42
1:I:123:ARG:HG2	1:I:198:VAL:HG12	2.00	0.42
1:D:44:THR:HG22	1:D:99:ARG:HB3	2.01	0.42
1:A:231:ARG:NH2	1:A:292:GLU:OE2	2.52	0.42
1:B:220:TRP:HZ2	1:B:308:PHE:CD1	2.37	0.42
1:D:247:PHE:CD2	1:E:247:PHE:HE2	2.38	0.42
1:E:43:TRP:CH2	1:E:74:PRO:HD2	2.55	0.42
1:E:279:LEU:O	1:E:282:PHE:N	2.47	0.42
1:F:247:PHE:CD2	1:G:247:PHE:HE2	2.38	0.42
1:A:162:ILE:HG13	2:A:403:BRJ:BR1	2.74	0.42
1:D:220:TRP:C	1:D:222:VAL:H	2.27	0.42
1:E:152:ILE:CD1	1:E:155:GLU:HG2	2.49	0.42
1:I:175:TYR:O	1:I:186:ASN:ND2	2.52	0.42
1:C:102:TYR:CG	2:C:401:BRJ:HB11	2.54	0.42
1:C:181:VAL:O	1:C:182:GLN:C	2.61	0.42
1:D:10:ARG:N	1:D:11:PRO:CD	2.82	0.42
1:H:44:THR:HA	1:H:99:ARG:HA	2.01	0.42
1:B:196:ASP:CG	1:I:165:LYS:NZ	2.78	0.42
1:D:311:ILE:O	1:D:314:VAL:HG22	2.19	0.42
1:F:28:THR:HB	1:F:256:LEU:HD21	2.02	0.42
1:F:242:VAL:HG12	1:F:270:TYR:CZ	2.54	0.42
1:G:21:ASN:HD21	1:G:38:TYR:HE1	1.66	0.42
1:I:137:ASN:ND2	1:I:187:GLU:CB	2.83	0.42
1:D:28:THR:HG21	1:D:254:PRO:HB2	2.02	0.42
1:D:253:LEU:HB3	1:D:254:PRO:HD2	2.01	0.42
1:F:131:GLU:OE1	1:F:190:ARG:NE	2.48	0.42
1:H:90:LYS:HE3	1:H:102:TYR:OH	2.19	0.42
1:A:304:PHE:HB2	1:A:305:PRO:HD3	2.02	0.42
1:D:176:ASP:C	1:D:177:HIS:CD2	2.97	0.42
1:D:224:TRP:CD2	1:E:281:ILE:HD11	2.55	0.42
1:E:102:TYR:CG	2:E:502:BRJ:HB11	2.55	0.42
1:E:210:LEU:HB3	1:E:211:PRO:HD3	2.01	0.42
1:G:157:ILE:HG22	1:H:31:GLN:HE22	1.85	0.42
1:I:23:ILE:HD12	2:I:403:BRJ:BR1	2.75	0.42
1:J:283:ALA:HB2	1:J:296:LEU:HD23	2.01	0.42
1:A:293:ASP:C	1:A:295:LEU:N	2.78	0.42
1:D:305:PRO:O	1:D:309:LEU:HB3	2.20	0.42
1:G:212:LEU:HD13	1:G:245:TYR:CD2	2.55	0.42
1:H:248:TYR:CD1	1:I:247:PHE:HA	2.55	0.42
1:D:150:GLU:HG3	1:D:152:ILE:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:10:ARG:N	1:H:11:PRO:CD	2.83	0.41
1:I:24:TYR:CE2	1:I:34:LYS:HD2	2.55	0.41
1:E:208:PHE:CD1	1:E:249:THR:HG22	2.55	0.41
1:A:44:THR:HA	1:A:99:ARG:HA	2.03	0.41
1:B:299:ARG:O	1:B:303:ALA:HB2	2.20	0.41
1:E:212:LEU:HD13	1:E:245:TYR:CD2	2.55	0.41
1:F:47:PRO:HA	1:F:98:GLY:HA2	2.02	0.41
1:F:122:ASP:OD2	1:F:199:ARG:NH1	2.53	0.41
1:G:44:THR:HG22	1:G:99:ARG:HB3	2.02	0.41
1:J:10:ARG:N	1:J:11:PRO:HD2	2.35	0.41
1:C:268:ALA:HB1	1:C:308:PHE:CZ	2.55	0.41
1:E:44:THR:HG22	1:E:99:ARG:HB3	2.03	0.41
1:F:247:PHE:CZ	1:J:247:PHE:CD1	3.08	0.41
1:I:155:GLU:HG2	1:I:157:ILE:HB	2.02	0.41
1:A:217:ALA:HA	1:A:220:TRP:CE3	2.56	0.41
1:F:208:PHE:HE1	1:F:248:TYR:CZ	2.38	0.41
1:F:301:ARG:C	1:F:302:LEU:HD12	2.46	0.41
1:F:307:GLY:O	1:F:311:ILE:HG23	2.21	0.41
1:G:279:LEU:O	1:G:282:PHE:N	2.52	0.41
1:H:155:GLU:HG2	1:H:161:TRP:CD1	2.55	0.41
1:H:174:ARG:NH1	1:H:186:ASN:OD1	2.53	0.41
1:J:75:ALA:HB3	1:J:133:PHE:H	1.85	0.41
1:D:181:VAL:HG12	1:D:182:GLN:H	1.86	0.41
1:D:314:VAL:O	1:D:316:VAL:HG23	2.20	0.41
1:G:314:VAL:O	1:G:314:VAL:HG23	2.20	0.41
1:I:231:ARG:CZ	1:I:297:ILE:HD13	2.50	0.41
1:J:47:PRO:HA	1:J:98:GLY:HA2	2.02	0.41
1:J:227:SER:O	1:J:231:ARG:NH1	2.53	0.41
1:J:303:ALA:O	1:J:307:GLY:N	2.53	0.41
1:E:23:ILE:HG13	2:E:504:BRJ:BR1	2.76	0.41
1:F:315:LEU:N	1:F:315:LEU:HD23	2.36	0.41
1:G:43:TRP:CZ2	1:G:100:VAL:HG11	2.56	0.41
1:B:295:LEU:HG	1:B:299:ARG:NH1	2.36	0.41
1:F:279:LEU:HD23	1:F:300:CYS:SG	2.61	0.41
1:B:165:LYS:HE2	1:I:163:ARG:HE	1.85	0.41
1:C:20:ILE:HD12	1:C:195:ILE:HD11	2.03	0.41
1:C:162:ILE:HG13	2:C:403:BRJ:BR1	2.75	0.41
1:E:300:CYS:HA	1:E:303:ALA:HB3	2.02	0.41
1:F:217:ALA:HA	1:F:220:TRP:CE3	2.55	0.41
1:G:47:PRO:HA	1:G:98:GLY:HA2	2.01	0.41
1:H:208:PHE:CE1	1:H:248:TYR:CE2	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:43:TRP:CE2	1:J:100:VAL:HG11	2.56	0.41
1:J:220:TRP:CE2	1:J:304:PHE:HB3	2.56	0.41
1:J:289:ASN:O	1:J:290:GLY:C	2.64	0.41
1:E:301:ARG:O	1:E:302:LEU:HD12	2.21	0.41
1:J:293:ASP:C	1:J:295:LEU:N	2.77	0.41
1:E:173:ILE:CD1	1:E:190:ARG:HB3	2.51	0.40
1:E:289:ASN:O	1:E:291:VAL:N	2.54	0.40
1:H:208:PHE:CD1	1:H:249:THR:HG22	2.56	0.40
1:C:289:ASN:O	1:C:291:VAL:N	2.55	0.40
1:F:224:TRP:CB	1:G:281:ILE:HD11	2.51	0.40
1:G:295:LEU:HD12	1:G:295:LEU:N	2.35	0.40
1:H:79:ILE:HB	1:H:129:GLU:HB2	2.02	0.40
1:J:181:VAL:O	1:J:182:GLN:HB3	2.21	0.40
1:B:155:GLU:OE2	1:B:163:ARG:NH1	2.53	0.40
1:B:161:TRP:HB2	1:B:198:VAL:HG23	2.02	0.40
1:G:308:PHE:C	1:G:310:ALA:N	2.79	0.40
1:H:142:PHE:CD2	1:H:191:ILE:HG13	2.57	0.40
1:A:148:TYR:CE1	1:B:177:HIS:ND1	2.89	0.40
1:A:293:ASP:C	1:A:295:LEU:H	2.29	0.40
1:C:152:ILE:O	1:C:152:ILE:HG13	2.22	0.40
1:E:28:THR:HG21	1:E:254:PRO:HB2	2.03	0.40
1:E:123:ARG:HG2	1:E:198:VAL:HG12	2.02	0.40
1:G:289:ASN:OD1	1:G:289:ASN:C	2.64	0.40
1:H:253:LEU:HB3	1:H:254:PRO:HD2	2.02	0.40
1:H:257:PRO:HG2	1:H:258:TYR:CD2	2.56	0.40
1:I:55:PRO:HB3	1:I:95:PHE:CD1	2.56	0.40
1:B:102:TYR:CG	2:B:401:BRJ:HB11	2.56	0.40
1:B:165:LYS:CE	1:I:163:ARG:HE	2.35	0.40
1:B:225:LEU:HB2	1:B:231:ARG:HG2	2.03	0.40
1:B:293:ASP:C	1:B:295:LEU:N	2.78	0.40
1:C:304:PHE:CB	1:C:305:PRO:HD3	2.50	0.40
1:G:24:TYR:CE2	1:G:34:LYS:HD2	2.56	0.40
1:H:220:TRP:C	1:H:222:VAL:H	2.29	0.40
1:I:122:ASP:OD1	1:I:199:ARG:NH1	2.54	0.40
1:J:82:VAL:N	1:J:109:SER:O	2.52	0.40
1:J:296:LEU:HA	1:J:299:ARG:CD	2.52	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	306/322 (95%)	278 (91%)	25 (8%)	3 (1%)	12	41
1	B	306/322 (95%)	270 (88%)	28 (9%)	8 (3%)	4	21
1	C	306/322 (95%)	274 (90%)	27 (9%)	5 (2%)	7	30
1	D	306/322 (95%)	274 (90%)	28 (9%)	4 (1%)	9	35
1	E	306/322 (95%)	275 (90%)	26 (8%)	5 (2%)	7	30
1	F	306/322 (95%)	278 (91%)	26 (8%)	2 (1%)	18	49
1	G	306/322 (95%)	273 (89%)	30 (10%)	3 (1%)	12	41
1	H	306/322 (95%)	273 (89%)	30 (10%)	3 (1%)	12	41
1	I	306/322 (95%)	274 (90%)	28 (9%)	4 (1%)	9	35
1	J	306/322 (95%)	273 (89%)	27 (9%)	6 (2%)	6	25
All	All	3060/3220 (95%)	2742 (90%)	275 (9%)	43 (1%)	9	34

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	181	VAL
1	B	181	VAL
1	B	286	ARG
1	B	292	GLU
1	C	99	ARG
1	C	183	PRO
1	D	178	LEU
1	D	181	VAL
1	D	290	GLY
1	F	152	ILE
1	F	181	VAL
1	G	181	VAL
1	G	316	VAL
1	H	178	LEU

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Mol	Chain	Res	Type
1	I	152	ILE
1	A	298	GLN
1	B	290	GLY
1	B	293	ASP
1	C	100	VAL
1	C	290	GLY
1	E	187	GLU
1	E	290	GLY
1	E	314	VAL
1	H	290	GLY
1	I	153	ASP
1	J	75	ALA
1	J	187	GLU
1	J	290	GLY
1	E	153	ASP
1	I	75	ALA
1	B	75	ALA
1	C	179	SER
1	G	290	GLY
1	J	76	LEU
1	B	287	GLN
1	I	76	LEU
1	J	150	GLU
1	A	316	VAL
1	E	200	ASN
1	B	304	PHE
1	H	200	ASN
1	D	297	ILE
1	J	183	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	276/284 (97%)	272 (99%)	4 (1%)	59	76
1	B	276/284 (97%)	269 (98%)	7 (2%)	42	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	276/284 (97%)	271 (98%)	5 (2%)	51	73
1	D	276/284 (97%)	271 (98%)	5 (2%)	51	73
1	E	276/284 (97%)	273 (99%)	3 (1%)	65	78
1	F	276/284 (97%)	268 (97%)	8 (3%)	37	66
1	G	276/284 (97%)	268 (97%)	8 (3%)	37	66
1	H	276/284 (97%)	271 (98%)	5 (2%)	51	73
1	I	276/284 (97%)	270 (98%)	6 (2%)	45	71
1	J	276/284 (97%)	269 (98%)	7 (2%)	42	69
All	All	2760/2840 (97%)	2702 (98%)	58 (2%)	47	71

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	VAL
1	A	139	GLN
1	A	234	THR
1	A	237	THR
1	B	19	PHE
1	B	87	THR
1	B	139	GLN
1	B	234	THR
1	B	237	THR
1	B	304	PHE
1	B	317	ILE
1	C	10	ARG
1	C	139	GLN
1	C	234	THR
1	C	237	THR
1	C	317	ILE
1	D	19	PHE
1	D	57	ILE
1	D	139	GLN
1	D	234	THR
1	D	237	THR
1	E	139	GLN
1	E	234	THR
1	E	237	THR
1	F	40	VAL
1	F	57	ILE

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Mol	Chain	Res	Type
1	F	87	THR
1	F	100	VAL
1	F	139	GLN
1	F	237	THR
1	F	291	VAL
1	F	315	LEU
1	G	40	VAL
1	G	139	GLN
1	G	143	SER
1	G	209	ILE
1	G	234	THR
1	G	237	THR
1	G	252	ILE
1	G	317	ILE
1	H	19	PHE
1	H	139	GLN
1	H	171	SER
1	H	234	THR
1	H	237	THR
1	I	19	PHE
1	I	57	ILE
1	I	139	GLN
1	I	156	GLU
1	I	234	THR
1	I	237	THR
1	J	40	VAL
1	J	46	LYS
1	J	87	THR
1	J	100	VAL
1	J	139	GLN
1	J	234	THR
1	J	237	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	139	GLN
1	A	146	GLN
1	A	177	HIS
1	B	139	GLN
1	B	185	GLN

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Mol	Chain	Res	Type
1	B	298	GLN
1	C	139	GLN
1	C	251	ASN
1	D	62	GLN
1	D	139	GLN
1	D	146	GLN
1	D	251	ASN
1	D	264	GLN
1	E	139	GLN
1	E	146	GLN
1	E	169	HIS
1	E	233	GLN
1	F	139	GLN
1	F	146	GLN
1	F	185	GLN
1	G	177	HIS
1	H	103	ASN
1	H	169	HIS
1	I	103	ASN
1	I	139	GLN
1	I	177	HIS
1	J	62	GLN
1	J	139	GLN
1	J	169	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 54 ligands modelled in this entry, 2 are monoatomic - leaving 52 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	3CN	B	404	-	3,3,3	0.69	0	2,2,2	0.23	0
4	MES	D	405	-	12,12,12	2.27	1 (8%)	15,16,16	1.41	3 (20%)
3	3CN	J	501	-	3,3,3	0.83	0	2,2,2	0.12	0
2	BRJ	A	404	-	3,3,3	0.30	0	2,2,2	0.40	0
2	BRJ	D	401	-	3,3,3	0.30	0	2,2,2	0.30	0
2	BRJ	F	403	-	3,3,3	0.30	0	2,2,2	0.54	0
2	BRJ	D	403	-	3,3,3	0.32	0	2,2,2	0.24	0
4	MES	B	405	-	12,12,12	2.27	1 (8%)	15,16,16	1.36	2 (13%)
2	BRJ	J	502	-	3,3,3	0.27	0	2,2,2	0.59	0
3	3CN	I	404	-	3,3,3	0.74	0	2,2,2	0.16	0
3	3CN	C	404	-	3,3,3	0.71	0	2,2,2	0.18	0
2	BRJ	I	401	-	3,3,3	0.31	0	2,2,2	0.29	0
2	BRJ	A	402	-	3,3,3	0.29	0	2,2,2	1.18	0
2	BRJ	F	404	-	3,3,3	0.29	0	2,2,2	0.54	0
2	BRJ	F	401	-	3,3,3	0.27	0	2,2,2	0.34	0
3	3CN	E	501	-	3,3,3	0.70	0	2,2,2	0.16	0
3	3CN	H	404	-	3,3,3	0.84	0	2,2,2	0.10	0
2	BRJ	I	403	-	3,3,3	0.30	0	2,2,2	0.44	0
4	MES	H	405	-	12,12,12	2.27	1 (8%)	15,16,16	1.37	3 (20%)
2	BRJ	C	403	-	3,3,3	0.29	0	2,2,2	0.43	0
2	BRJ	D	402	-	3,3,3	0.27	0	2,2,2	0.44	0
4	MES	F	406	-	12,12,12	2.23	1 (8%)	15,16,16	1.44	3 (20%)
2	BRJ	E	502	-	3,3,3	0.31	0	2,2,2	0.35	0
2	BRJ	J	504	-	3,3,3	0.29	0	2,2,2	1.28	0
3	3CN	A	405	-	3,3,3	0.76	0	2,2,2	0.25	0
2	BRJ	C	401	-	3,3,3	0.31	0	2,2,2	0.28	0
4	MES	J	505	-	12,12,12	2.24	1 (8%)	15,16,16	1.47	2 (13%)
2	BRJ	B	402	-	3,3,3	0.28	0	2,2,2	0.34	0
2	BRJ	G	403	-	3,3,3	0.29	0	2,2,2	0.58	0
2	BRJ	G	402	-	3,3,3	0.26	0	2,2,2	1.03	0
2	BRJ	J	503	-	3,3,3	0.29	0	2,2,2	0.37	0
2	BRJ	E	503	-	3,3,3	0.29	0	2,2,2	0.40	0
2	BRJ	H	401	-	3,3,3	0.28	0	2,2,2	0.62	0
2	BRJ	H	403	-	3,3,3	0.29	0	2,2,2	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MES	G	405	-	12,12,12	2.25	1 (8%)	15,16,16	1.60	5 (33%)
2	BRJ	B	401	-	3,3,3	0.25	0	2,2,2	0.39	0
2	BRJ	B	403	-	3,3,3	0.32	0	2,2,2	0.11	0
3	3CN	F	405	-	3,3,3	0.72	0	2,2,2	0.20	0
4	MES	E	505	-	12,12,12	2.30	1 (8%)	15,16,16	1.44	2 (13%)
2	BRJ	A	401	-	3,3,3	0.33	0	2,2,2	0.59	0
2	BRJ	E	504	-	3,3,3	0.31	0	2,2,2	0.22	0
4	MES	I	405	-	12,12,12	2.31	1 (8%)	15,16,16	1.32	2 (13%)
2	BRJ	G	401	-	3,3,3	0.29	0	2,2,2	0.27	0
3	3CN	D	404	-	3,3,3	0.70	0	2,2,2	0.18	0
3	3CN	G	404	-	3,3,3	0.88	0	2,2,2	0.07	0
4	MES	A	406	-	12,12,12	2.23	1 (8%)	15,16,16	1.40	2 (13%)
4	MES	C	405	-	12,12,12	2.19	1 (8%)	15,16,16	1.68	3 (20%)
2	BRJ	A	403	-	3,3,3	0.31	0	2,2,2	0.36	0
2	BRJ	C	402	-	3,3,3	0.31	0	2,2,2	0.16	0
2	BRJ	I	402	-	3,3,3	0.28	0	2,2,2	0.43	0
2	BRJ	F	402	-	3,3,3	0.29	0	2,2,2	0.39	0
2	BRJ	H	402	-	3,3,3	0.27	0	2,2,2	0.58	0

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
3	3CN	B	404	-	-	1/1/1/1	-
4	MES	D	405	-	-	1/6/14/14	0/1/1/1
3	3CN	J	501	-	-	1/1/1/1	-
2	BRJ	A	404	-	-	0/1/1/1	-
2	BRJ	D	401	-	-	0/1/1/1	-
2	BRJ	F	403	-	-	0/1/1/1	-
2	BRJ	D	403	-	-	0/1/1/1	-
4	MES	B	405	-	-	2/6/14/14	0/1/1/1
2	BRJ	J	502	-	-	0/1/1/1	-
3	3CN	I	404	-	-	0/1/1/1	-
3	3CN	C	404	-	-	1/1/1/1	-
2	BRJ	I	401	-	-	0/1/1/1	-
2	BRJ	A	402	-	-	0/1/1/1	-
2	BRJ	F	404	-	-	0/1/1/1	-
2	BRJ	F	401	-	-	0/1/1/1	-
3	3CN	E	501	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	3CN	H	404	-	-	0/1/1/1	-
2	BRJ	I	403	-	-	0/1/1/1	-
4	MES	H	405	-	-	4/6/14/14	0/1/1/1
2	BRJ	C	403	-	-	0/1/1/1	-
2	BRJ	D	402	-	-	0/1/1/1	-
4	MES	F	406	-	-	4/6/14/14	0/1/1/1
2	BRJ	E	502	-	-	0/1/1/1	-
2	BRJ	J	504	-	-	0/1/1/1	-
3	3CN	A	405	-	-	0/1/1/1	-
2	BRJ	C	401	-	-	0/1/1/1	-
4	MES	J	505	-	-	4/6/14/14	0/1/1/1
2	BRJ	B	402	-	-	0/1/1/1	-
2	BRJ	G	403	-	-	0/1/1/1	-
2	BRJ	G	402	-	-	0/1/1/1	-
2	BRJ	J	503	-	-	0/1/1/1	-
2	BRJ	E	503	-	-	0/1/1/1	-
2	BRJ	H	401	-	-	0/1/1/1	-
2	BRJ	H	403	-	-	0/1/1/1	-
4	MES	G	405	-	-	5/6/14/14	0/1/1/1
2	BRJ	B	401	-	-	0/1/1/1	-
2	BRJ	B	403	-	-	0/1/1/1	-
3	3CN	F	405	-	-	0/1/1/1	-
4	MES	E	505	-	-	1/6/14/14	0/1/1/1
2	BRJ	A	401	-	-	0/1/1/1	-
2	BRJ	E	504	-	-	0/1/1/1	-
4	MES	I	405	-	-	1/6/14/14	0/1/1/1
2	BRJ	G	401	-	-	0/1/1/1	-
3	3CN	D	404	-	-	0/1/1/1	-
3	3CN	G	404	-	-	1/1/1/1	-
4	MES	A	406	-	-	5/6/14/14	0/1/1/1
4	MES	C	405	-	-	4/6/14/14	0/1/1/1
2	BRJ	A	403	-	-	0/1/1/1	-
2	BRJ	C	402	-	-	0/1/1/1	-
2	BRJ	I	402	-	-	0/1/1/1	-
2	BRJ	F	402	-	-	0/1/1/1	-
2	BRJ	H	402	-	-	0/1/1/1	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	405	MES	C8-S	-7.74	1.66	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	505	MES	C8-S	-7.72	1.66	1.77
4	D	405	MES	C8-S	-7.61	1.66	1.77
4	H	405	MES	C8-S	-7.59	1.66	1.77
4	B	405	MES	C8-S	-7.57	1.67	1.77
4	G	405	MES	C8-S	-7.50	1.67	1.77
4	J	505	MES	C8-S	-7.47	1.67	1.77
4	A	406	MES	C8-S	-7.45	1.67	1.77
4	F	406	MES	C8-S	-7.42	1.67	1.77
4	C	405	MES	C8-S	-7.28	1.67	1.77

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	505	MES	O2S-S-C8	3.44	111.93	106.73
4	C	405	MES	O1S-S-C8	3.27	111.67	106.73
4	C	405	MES	C6-C5-N4	-3.04	105.51	110.12
4	B	405	MES	C5-N4-C3	2.86	115.01	108.84
4	E	505	MES	C5-N4-C3	2.83	114.94	108.84
4	I	405	MES	C5-N4-C3	2.83	114.94	108.84
4	A	406	MES	O1S-S-C8	2.72	110.84	106.73
4	F	406	MES	O3S-S-C8	2.67	111.22	106.00
4	D	405	MES	C5-N4-C3	2.55	114.34	108.84
4	F	406	MES	C7-N4-C5	2.45	117.76	111.24
4	D	405	MES	O1S-S-C8	2.41	110.37	106.73
4	A	406	MES	C5-N4-C3	2.39	114.00	108.84
4	J	505	MES	C5-N4-C3	2.34	113.89	108.84
4	G	405	MES	C5-N4-C3	2.32	113.85	108.84
4	G	405	MES	C6-C5-N4	-2.32	106.60	110.12
4	D	405	MES	C7-N4-C5	2.29	117.33	111.24
4	G	405	MES	O1S-S-C8	2.20	110.05	106.73
4	C	405	MES	O2S-S-C8	2.19	110.04	106.73
4	I	405	MES	O3S-S-C8	2.18	110.26	106.00
4	H	405	MES	O2S-S-C8	2.17	110.01	106.73
4	H	405	MES	C5-N4-C3	2.16	113.50	108.84
4	H	405	MES	O3S-S-C8	2.15	110.21	106.00
4	B	405	MES	O3S-S-C8	2.13	110.16	106.00
4	G	405	MES	C2-C3-N4	-2.11	106.91	110.12
4	E	505	MES	O1S-S-C8	2.05	109.83	106.73
4	G	405	MES	O2S-S-C8	2.04	109.81	106.73
4	F	406	MES	C5-N4-C3	2.01	113.17	108.84

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	405	MES	N4-C7-C8-S
4	C	405	MES	N4-C7-C8-S
4	C	405	MES	C7-C8-S-O2S
4	C	405	MES	C7-C8-S-O3S
4	D	405	MES	C8-C7-N4-C5
4	F	406	MES	C8-C7-N4-C5
4	F	406	MES	C7-C8-S-O1S
4	F	406	MES	C7-C8-S-O3S
4	G	405	MES	C7-C8-S-O2S
4	H	405	MES	C7-C8-S-O2S
4	H	405	MES	C7-C8-S-O3S
4	J	505	MES	N4-C7-C8-S
4	J	505	MES	C7-C8-S-O1S
4	J	505	MES	C7-C8-S-O3S
3	G	404	3CN	CA-CB-CC-ND
4	A	406	MES	C7-C8-S-O3S
4	G	405	MES	C7-C8-S-O3S
3	J	501	3CN	CA-CB-CC-ND
4	G	405	MES	C8-C7-N4-C3
4	I	405	MES	C8-C7-N4-C3
4	A	406	MES	C7-C8-S-O1S
4	A	406	MES	C7-C8-S-O2S
4	C	405	MES	C7-C8-S-O1S
4	F	406	MES	C7-C8-S-O2S
4	G	405	MES	C7-C8-S-O1S
4	H	405	MES	C7-C8-S-O1S
4	J	505	MES	C7-C8-S-O2S
4	A	406	MES	N4-C7-C8-S
4	B	405	MES	C8-C7-N4-C3
4	E	505	MES	C8-C7-N4-C3
4	G	405	MES	C8-C7-N4-C5
3	B	404	3CN	CA-CB-CC-ND
3	C	404	3CN	CA-CB-CC-ND
4	A	406	MES	C8-C7-N4-C3
4	H	405	MES	C8-C7-N4-C3

There are no ring outliers.

17 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	403	BRJ	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	502	BRJ	1	0
2	I	401	BRJ	1	0
2	A	402	BRJ	1	0
2	F	401	BRJ	2	0
3	H	404	3CN	1	0
2	I	403	BRJ	3	0
2	C	403	BRJ	1	0
2	E	502	BRJ	1	0
2	C	401	BRJ	2	0
2	G	402	BRJ	1	0
2	H	401	BRJ	2	0
2	B	401	BRJ	1	0
2	A	401	BRJ	2	0
2	E	504	BRJ	1	0
2	G	401	BRJ	1	0
2	A	403	BRJ	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	308/322 (95%)	0.06	16 (5%) 33 17	72, 115, 167, 209	0
1	B	308/322 (95%)	-0.10	2 (0%) 85 70	69, 107, 178, 227	0
1	C	308/322 (95%)	0.06	8 (2%) 57 36	71, 110, 181, 204	0
1	D	308/322 (95%)	-0.02	7 (2%) 61 39	63, 102, 174, 222	0
1	E	308/322 (95%)	-0.07	10 (3%) 50 30	73, 113, 168, 198	0
1	F	308/322 (95%)	-0.05	6 (1%) 66 45	71, 121, 177, 209	0
1	G	308/322 (95%)	-0.02	8 (2%) 57 36	57, 106, 163, 204	0
1	H	308/322 (95%)	0.08	8 (2%) 57 36	70, 113, 185, 215	0
1	I	308/322 (95%)	0.11	8 (2%) 57 36	70, 110, 173, 210	0
1	J	308/322 (95%)	0.15	9 (2%) 53 32	84, 123, 187, 207	0
All	All	3080/3220 (95%)	0.02	82 (2%) 56 35	57, 112, 177, 227	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	157	ILE	6.8
1	E	289	ASN	4.5
1	C	172	ASP	4.1
1	A	258	TYR	3.9
1	G	255	ARG	3.8
1	A	116	PHE	3.7
1	H	207	SER	3.6
1	J	29	LEU	3.5
1	E	156	GLU	3.5
1	E	179	SER	3.3
1	A	177	HIS	3.3
1	E	29	LEU	3.2
1	J	157	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	I	245	TYR	3.2
1	G	314	VAL	3.2
1	D	157	ILE	3.2
1	A	117	ARG	3.2
1	C	187	GLU	3.2
1	I	208	PHE	3.2
1	A	53	ASP	3.2
1	E	317	ILE	3.2
1	A	115	ASP	3.1
1	D	179	SER	3.1
1	A	175	TYR	3.1
1	C	156	GLU	3.0
1	G	235	SER	3.0
1	J	257	PRO	2.9
1	J	158	ASP	2.9
1	B	317	ILE	2.9
1	C	173	ILE	2.8
1	C	237	THR	2.8
1	G	157	ILE	2.8
1	A	118	LEU	2.7
1	H	157	ILE	2.7
1	H	297	ILE	2.7
1	A	181	VAL	2.6
1	J	283	ALA	2.6
1	F	252	ILE	2.6
1	C	188	PHE	2.6
1	G	22	LYS	2.6
1	C	180	SER	2.5
1	D	178	LEU	2.5
1	H	300	CYS	2.5
1	A	153	ASP	2.5
1	F	157	ILE	2.5
1	A	119	PHE	2.4
1	J	156	GLU	2.4
1	H	185	GLN	2.4
1	A	296	LEU	2.4
1	F	306	LEU	2.4
1	I	248	TYR	2.3
1	E	302	LEU	2.3
1	I	70	GLY	2.3
1	A	151	ASN	2.3
1	J	44	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	154	ASN	2.3
1	D	53	ASP	2.3
1	A	257	PRO	2.2
1	E	166	ALA	2.2
1	H	296	LEU	2.2
1	D	188	PHE	2.2
1	I	304	PHE	2.2
1	A	188	PHE	2.2
1	C	175	TYR	2.2
1	I	152	ILE	2.1
1	J	317	ILE	2.1
1	F	26	VAL	2.1
1	I	157	ILE	2.1
1	G	155	GLU	2.1
1	E	137	ASN	2.1
1	J	153	ASP	2.1
1	F	175	TYR	2.1
1	F	257	PRO	2.1
1	G	316	VAL	2.1
1	B	152	ILE	2.1
1	H	237	THR	2.1
1	E	138	GLN	2.1
1	H	138	GLN	2.1
1	I	251	ASN	2.1
1	A	176	ASP	2.1
1	D	317	ILE	2.0
1	D	236	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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(Å ²)	Q<0.9
2	BRJ	I	403	4/4	0.33	0.40	95,99,111,142	0
5	CL	J	506	1/1	0.41	0.12	166,166,166,166	0
2	BRJ	H	403	4/4	0.49	0.40	142,145,149,152	0
4	MES	J	505	12/12	0.50	0.18	158,170,183,184	0
2	BRJ	I	402	4/4	0.51	0.42	98,114,121,125	0
2	BRJ	D	403	4/4	0.51	0.41	93,99,105,145	0
2	BRJ	B	403	4/4	0.53	0.41	118,141,150,163	0
2	BRJ	C	403	4/4	0.55	0.34	121,147,151,177	0
2	BRJ	E	504	4/4	0.56	0.34	118,126,142,147	0
2	BRJ	J	502	4/4	0.59	0.51	109,116,118,139	0
2	BRJ	F	402	4/4	0.64	0.30	101,108,121,128	0
2	BRJ	C	402	4/4	0.66	0.27	104,106,110,139	0
2	BRJ	J	504	4/4	0.66	0.24	145,148,153,158	0
4	MES	I	405	12/12	0.67	0.15	141,175,183,195	0
2	BRJ	E	502	4/4	0.67	0.37	102,126,131,160	0
4	MES	G	405	12/12	0.67	0.16	128,151,170,173	0
2	BRJ	D	402	4/4	0.68	0.33	112,112,120,122	0
2	BRJ	F	401	4/4	0.69	0.27	99,117,132,135	0
2	BRJ	F	403	4/4	0.70	0.22	118,146,156,160	0
2	BRJ	D	401	4/4	0.70	0.33	94,127,129,141	0
4	MES	H	405	12/12	0.71	0.14	113,135,158,179	0
2	BRJ	G	401	4/4	0.71	0.50	111,117,133,164	0
4	MES	F	406	12/12	0.72	0.14	131,155,168,187	0
2	BRJ	H	401	4/4	0.72	0.41	98,101,128,154	0
2	BRJ	F	404	4/4	0.72	0.31	149,152,155,157	0
2	BRJ	H	402	4/4	0.73	0.29	93,117,125,131	0
2	BRJ	J	503	4/4	0.73	0.53	131,142,143,153	0
2	BRJ	A	404	4/4	0.73	0.38	137,154,169,175	0
2	BRJ	C	401	4/4	0.74	0.34	86,91,113,146	0
4	MES	D	405	12/12	0.74	0.13	126,147,174,178	0
2	BRJ	A	403	4/4	0.75	0.20	125,129,136,146	0
3	3CN	H	404	4/4	0.76	0.61	83,94,100,122	0
2	BRJ	I	401	4/4	0.76	0.30	103,131,137,169	0
2	BRJ	G	403	4/4	0.77	0.24	105,115,119,129	0
2	BRJ	G	402	4/4	0.78	0.35	122,125,135,135	0
2	BRJ	B	402	4/4	0.80	0.31	125,130,137,151	0
2	BRJ	E	503	4/4	0.80	0.29	130,130,148,165	0
2	BRJ	A	402	4/4	0.80	0.30	102,110,127,154	0
2	BRJ	A	401	4/4	0.81	0.29	124,131,154,183	0
4	MES	E	505	12/12	0.81	0.12	136,156,168,171	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BRJ	B	401	4/4	0.81	0.51	106,132,136,192	0
4	MES	A	406	12/12	0.81	0.12	132,154,185,186	0
3	3CN	A	405	4/4	0.82	0.64	86,98,102,115	0
4	MES	C	405	12/12	0.82	0.13	115,134,160,166	0
4	MES	B	405	12/12	0.86	0.12	129,148,167,179	0
3	3CN	G	404	4/4	0.88	0.44	85,87,97,99	0
3	3CN	C	404	4/4	0.89	0.50	84,92,119,127	0
3	3CN	I	404	4/4	0.91	0.62	96,98,103,109	0
3	3CN	D	404	4/4	0.91	0.41	96,102,109,113	0
3	3CN	J	501	4/4	0.92	0.62	97,121,130,132	0
3	3CN	F	405	4/4	0.93	0.40	91,93,98,112	0
3	3CN	E	501	4/4	0.93	0.25	91,95,102,114	0
5	CL	C	406	1/1	0.94	0.08	107,107,107,107	0
3	3CN	B	404	4/4	0.94	0.27	79,96,99,105	0

6.5 Other polymers [i](#)

There are no such residues in this entry.