



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2017 – 04:28 PM EST

PDB ID : 5SXU
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 : unknown
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

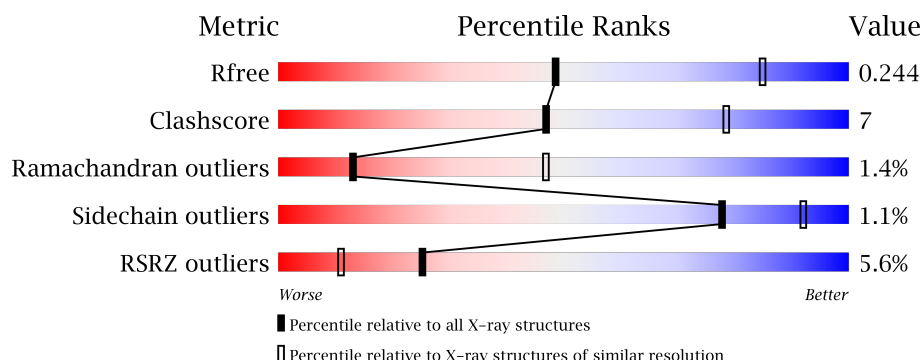
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>7%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>..</div> </div> </div>
1	B	322	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>..</div> </div> </div>
1	C	322	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>14%</div> <div>..</div> </div> </div>
1	D	322	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>..</div> </div> </div>
1	E	322	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>..</div> </div> </div>

Continued on next page...

Continued from previous page...

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	X
2	BRJ	A	402	-	-	-	X
2	BRJ	A	403	-	-	-	X
2	BRJ	A	404	-	-	-	X
2	BRJ	B	401	-	-	-	X
2	BRJ	B	402	-	-	-	X
2	BRJ	B	403	-	-	-	X
2	BRJ	C	401	-	-	X	X
2	BRJ	C	402	-	-	-	X
2	BRJ	C	403	-	-	-	X
2	BRJ	D	401	-	-	-	X
2	BRJ	D	402	-	-	-	X
2	BRJ	D	403	-	-	-	X
2	BRJ	E	502	-	-	-	X
2	BRJ	E	503	-	-	-	X
2	BRJ	E	504	-	-	-	X
2	BRJ	F	401	-	-	X	X
2	BRJ	F	402	-	-	-	X
2	BRJ	F	403	-	-	-	X
2	BRJ	F	404	-	-	-	X
2	BRJ	G	401	-	-	-	X
2	BRJ	G	402	-	-	-	X
2	BRJ	H	401	-	-	X	X
2	BRJ	H	402	-	-	-	X
2	BRJ	H	403	-	-	-	X
2	BRJ	I	401	-	-	-	X
2	BRJ	I	402	-	-	-	X
2	BRJ	I	403	-	-	X	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BRJ	J	502	-	-	-	X
2	BRJ	J	503	-	-	-	X
2	BRJ	J	504	-	-	-	X
3	3CN	G	404	-	-	-	X

2 Entry composition

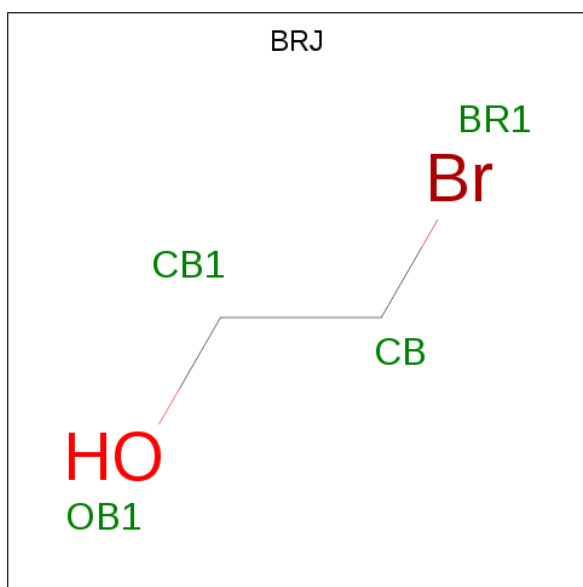
There are 6 unique types of molecules in this entry. The entry contains 25453 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: BRJ) (formula: C₂H₅BrO).



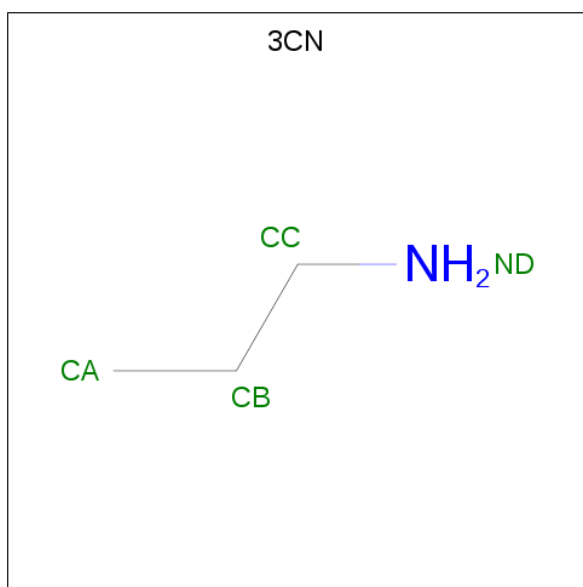
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	Br	C	O	0	0
			4	1	2	1		
2	A	1	Total	Br	C	O	0	0
			4	1	2	1		
2	A	1	Total	Br	C	O	0	0
			4	1	2	1		
2	A	1	Total	Br	C	O	0	0
			4	1	2	1		
2	B	1	Total	Br	C	O	0	0
			4	1	2	1		
2	B	1	Total	Br	C	O	0	0
			4	1	2	1		
2	B	1	Total	Br	C	O	0	0
			4	1	2	1		
2	C	1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

Continued on next page...

Continued from previous page...

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 (three-letter code: 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 (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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 (three-letter code: CL) (formula: Cl).

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

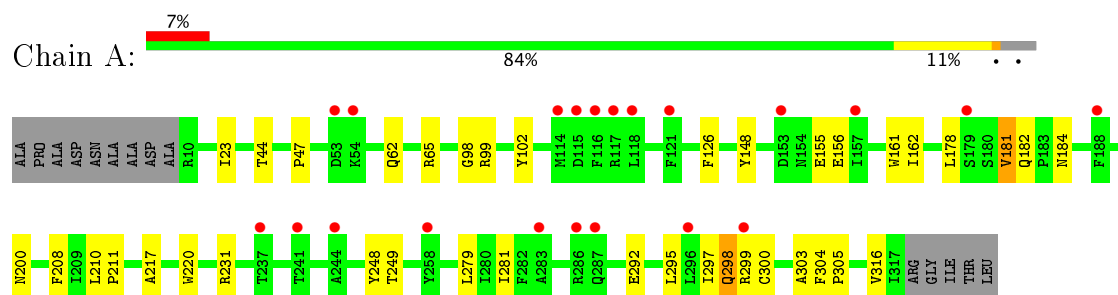
- Molecule 6 is water.

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

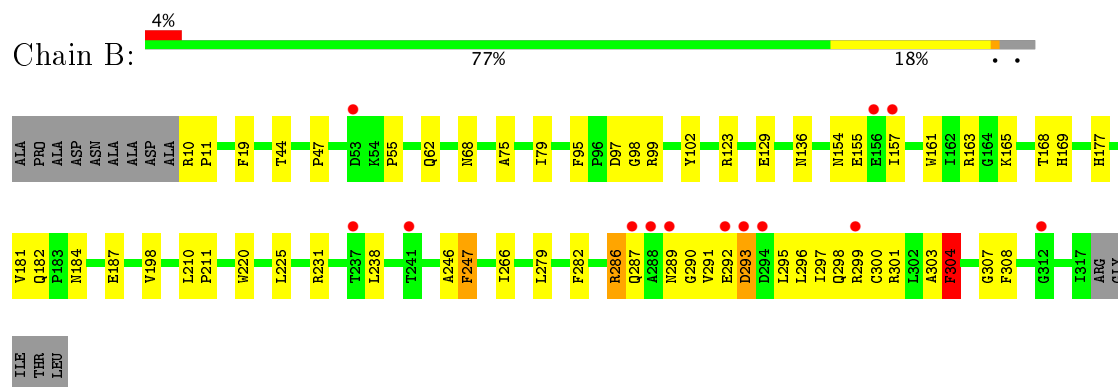
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

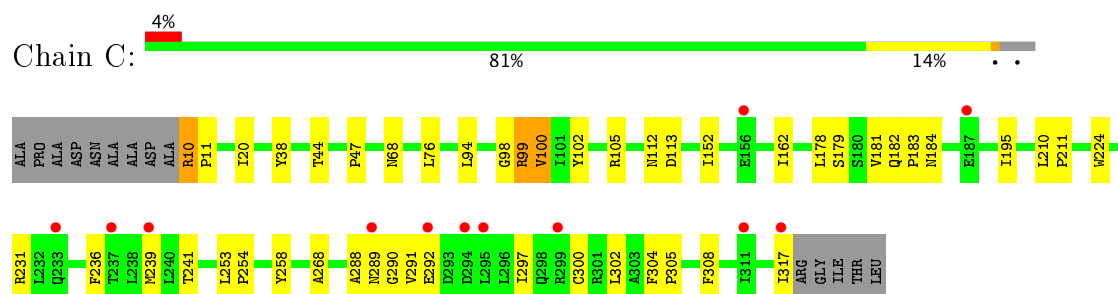
- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1



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

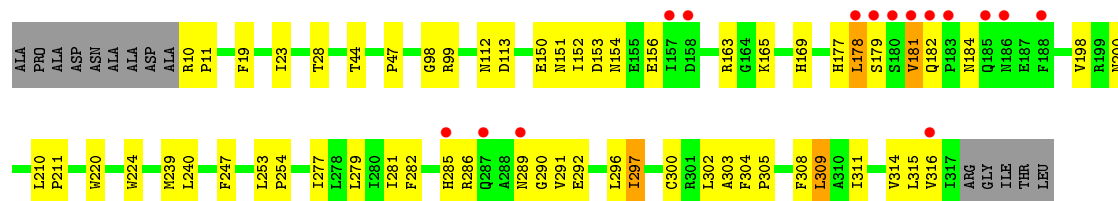


- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

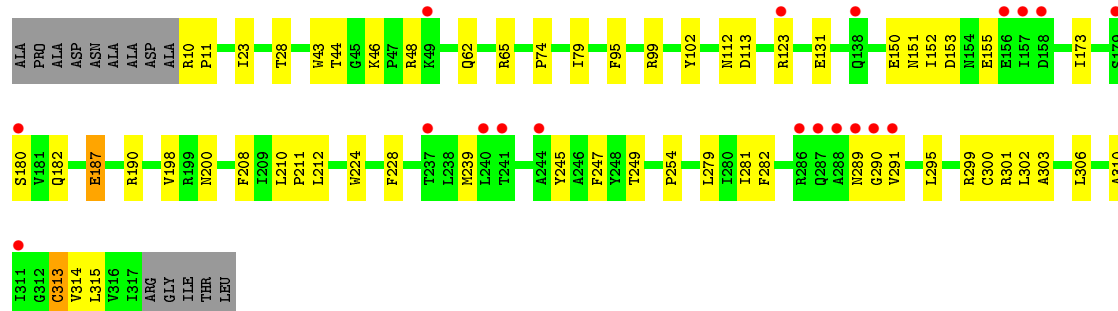
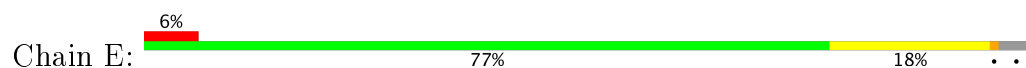


- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

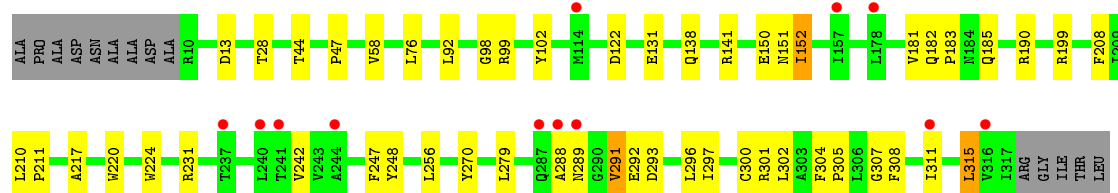
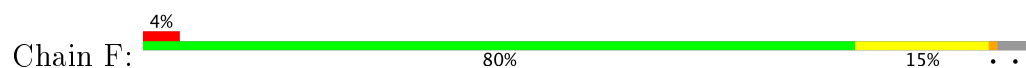




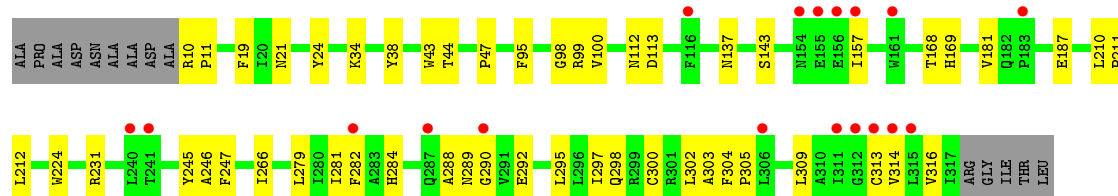
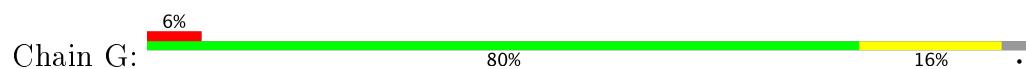
• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1



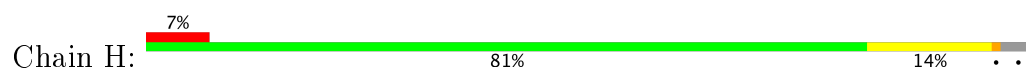
• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1



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

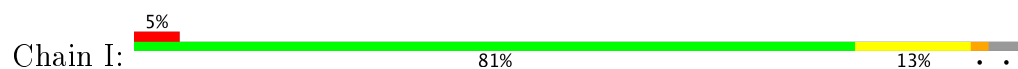


• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

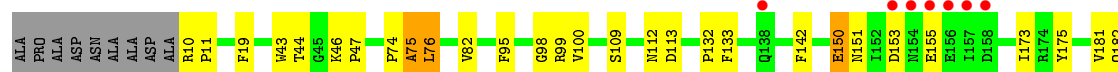
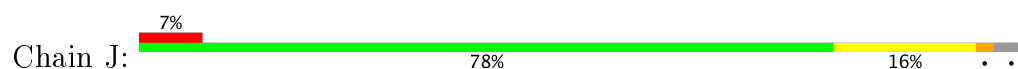




- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1



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



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 39.61 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.93-3.10) 99.9 (39.61-3.10)	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 0.207 , 0.244	Depositor DCC
R_{free} test set	5197 reflections (4.90%)	DCC
Wilson B-factor (Å ²)	108.7	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 81.7	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	0.92	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: 3CN, BRJ, MES, CL

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	0.31	0/2584	0.60	1/3522 (0.0%)
1	B	0.32	0/2584	0.66	2/3522 (0.1%)
1	C	0.33	0/2584	0.61	0/3522
1	D	0.35	0/2584	0.66	1/3522 (0.0%)
1	E	0.31	0/2584	0.62	0/3522
1	F	0.35	0/2584	0.63	0/3522
1	G	0.32	0/2584	0.61	0/3522
1	H	0.32	0/2584	0.62	1/3522 (0.0%)
1	I	0.31	0/2584	0.63	0/3522
1	J	0.34	0/2584	0.64	0/3522
All	All	0.33	0/25840	0.63	5/35220 (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
1	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	304	PHE	CB-CG-CD1	6.58	125.41	120.80
1	A	178	LEU	CA-CB-CG	6.10	129.33	115.30
1	B	304	PHE	CB-CG-CD2	-5.78	116.75	120.80
1	D	309	LEU	CA-CB-CG	5.58	128.14	115.30
1	H	178	LEU	CA-CB-CG	5.45	127.82	115.30

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 ⓘ

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	28	0
1	B	2516	0	2490	45	0
1	C	2516	0	2490	33	0
1	D	2516	0	2490	51	0
1	E	2516	0	2490	38	0
1	F	2516	0	2490	38	0
1	G	2516	0	2490	35	0
1	H	2516	0	2490	37	0
1	I	2516	0	2490	45	0
1	J	2516	0	2490	41	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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	359	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 (359) 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: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:B:168:THR:C	1:B:169:HIS:HD1	1.88	0.75
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:281:ILE:HD11	1:E:224:TRP:CG	2.36	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:G:168:THR:C	1:G:169:HIS:ND1	2.59	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:F:288:ALA:O	1:F:289:ASN:CG	2.44	0.56
1:E:306:LEU:O	1:E:310:ALA:N	2.38	0.56
1:I:186:ASN:OD1	1:I:186:ASN:O	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:ND1	1:D:285:HIS:O	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: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:D:44:THR:HA	1:D:99:ARG:HA	1.90	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: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: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:CD1	1:H:19:PHE:N	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: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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:75:ALA:CB	1:J:133:PHE:HB3	2.43	0.49
1:F:152:ILE:HG13	1:F:152:ILE:O	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:G:302:LEU:HD23	1:G:305:PRO:HG2	1.95	0.48
1:G:44:THR:HA	1:G:99:ARG:HA	1.94	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: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: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: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:C:288:ALA:O	1:C:289:ASN:CG	2.53	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:295:LEU:O	1:A:299:ARG:HG3	2.14	0.47
1:C:94:LEU:CD2	1:C:100:VAL:HG22	2.45	0.47
1:C:10:ARG:N	1:C:11:PRO:HD2	2.29	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:B:293:ASP:C	1:B:295:LEU:H	2.18	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: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: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
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: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:B:304:PHE:CD1	1:B:304:PHE:C	2.90	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:150:GLU:HG3	1:J:151:ASN:H	1.82	0.45
1:G:288:ALA:O	1:G:289:ASN:CG	2.55	0.45
1:I:224:TRP:CG	1:J:281:ILE:HD11	2.51	0.45
1:I:95:PHE:CD2	1:I:99:ARG:HG3	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: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
1:B:136:ASN:HB2	1:B:187:GLU:O	2.17	0.44
1:B:304:PHE:HD1	1:B:304:PHE:C	2.20	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:D:285:HIS:O	1:D:285:HIS:CG	2.71	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:102:TYR:CD1	2:F:401:BRJ:BR1	3.27	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:ND1	1:H:285:HIS:O	2.52	0.43
1:D:220:TRP:CE3	1:D:305:PRO:HG3	2.54	0.43
1:E:173:ILE:O	1:E:187:GLU:HA	2.18	0.43
1:H:241:THR:HA	1:I:240:LEU:HD12	2.01	0.43
1:H:19:PHE:CD2	3:H:404:3CN:HA2	2.54	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: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:175:TYR:O	1:J:186:ASN:ND2	2.52	0.43
1:J:44:THR:HG22	1:J:99:ARG:HB3	1.99	0.43
1:G:10:ARG:N	1:G:11:PRO:HD2	2.33	0.43
1:D:150:GLU:HG3	1:D:152:ILE:HG23	2.01	0.43
1:C:224:TRP:CE3	1:D:281:ILE:HD11	2.54	0.43
1:E:224:TRP:CD2	1:E:301:ARG:HD3	2.54	0.43
1:I:19:PHE:N	1:I:19:PHE:CD1	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
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:279:LEU:O	1:E:282:PHE:N	2.47	0.42
1:E:43:TRP:CH2	1:E:74:PRO:HD2	2.55	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:D:224:TRP:CD2	1:E:281:ILE:HD11	2.55	0.42
1:E:313:CYS:C	1:E:315:LEU:H	2.22	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: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
1:H:10:ARG:N	1:H:11:PRO:CD	2.83	0.41
1:I:11:PRO:HB3	1:I:138:GLN:C	2.40	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:B:308:PHE:C	1:B:308:PHE:CD1	2.93	0.41
1:E:212:LEU:HD13	1:E:245:TYR:CD2	2.55	0.41
1:F:122:ASP:OD2	1:F:199:ARG:NH1	2.53	0.41
1:F:47:PRO:HA	1:F:98:GLY:HA2	2.02	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:137:ASN:OD1	1:I:137:ASN:C	2.58	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: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:J:47:PRO:HA	1:J:98:GLY:HA2	2.02	0.41
1:E:23:ILE:HG13	2:E:504:BRJ:BR1	2.76	0.41
1:F:315:LEU:HD23	1:F:315:LEU:N	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: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:H:208:PHE:CE1	1:H:248:TYR:CE2	3.08	0.41
1:B:165:LYS:HE2	1:I:163:ARG:HE	1.85	0.41
1:C:162:ILE:HG13	2:C:403:BRJ:BR1	2.75	0.41
1:C:20:ILE:HD12	1:C:195:ILE:HD11	2.03	0.41
1:G:47:PRO:HA	1:G:98:GLY:HA2	2.01	0.41
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:E:301:ARG:O	1:E:302:LEU:HD12	2.21	0.41
1:D:152:ILE:C	1:D:152:ILE:HD12	2.42	0.40
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:ILE:HG13	1:C:152:ILE:O	2.22	0.40
1:E:123:ARG:HG2	1:E:198:VAL:HG12	2.02	0.40
1:E:28:THR:HG21	1:E:254:PRO:HB2	2.03	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: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:102:TYR:CG	2:B:401:BRJ:HB11	2.56	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: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 [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	306/322 (95%)	278 (91%)	25 (8%)	3 (1%)	18	57
1	B	306/322 (95%)	270 (88%)	28 (9%)	8 (3%)	6	31
1	C	306/322 (95%)	274 (90%)	27 (9%)	5 (2%)	11	43
1	D	306/322 (95%)	274 (90%)	28 (9%)	4 (1%)	14	48
1	E	306/322 (95%)	275 (90%)	26 (8%)	5 (2%)	11	43
1	F	306/322 (95%)	278 (91%)	26 (8%)	2 (1%)	25	64
1	G	306/322 (95%)	273 (89%)	30 (10%)	3 (1%)	18	57
1	H	306/322 (95%)	273 (89%)	30 (10%)	3 (1%)	18	57
1	I	306/322 (95%)	274 (90%)	28 (9%)	4 (1%)	14	48

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	306/322 (95%)	273 (89%)	27 (9%)	6 (2%)	9	37
All	All	3060/3220 (95%)	2742 (90%)	275 (9%)	43 (1%)	13	47

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 [i](#)

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%)	276 (100%)	0	100	100
1	B	276/284 (97%)	273 (99%)	3 (1%)	78	92
1	C	276/284 (97%)	272 (99%)	4 (1%)	71	90
1	D	276/284 (97%)	273 (99%)	3 (1%)	78	92
1	E	276/284 (97%)	273 (99%)	3 (1%)	78	92
1	F	276/284 (97%)	274 (99%)	2 (1%)	87	95
1	G	276/284 (97%)	274 (99%)	2 (1%)	87	95
1	H	276/284 (97%)	274 (99%)	2 (1%)	87	95
1	I	276/284 (97%)	272 (99%)	4 (1%)	71	90
1	J	276/284 (97%)	270 (98%)	6 (2%)	57	85
All	All	2760/2840 (97%)	2731 (99%)	29 (1%)	78	92

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	19	PHE
1	B	247	PHE
1	B	304	PHE
1	C	10	ARG
1	C	239	MET
1	C	258	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	317	ILE
1	D	19	PHE
1	D	169	HIS
1	D	239	MET
1	E	228	PHE
1	E	239	MET
1	E	313	CYS
1	F	291	VAL
1	F	315	LEU
1	G	19	PHE
1	G	143	SER
1	H	19	PHE
1	H	171	SER
1	I	19	PHE
1	I	156	GLU
1	I	169	HIS
1	I	239	MET
1	J	19	PHE
1	J	46	LYS
1	J	194	ARG
1	J	239	MET
1	J	247	PHE
1	J	293	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	177	HIS
1	D	233	GLN
1	F	185	GLN

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 carbohydrates 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
2	BRJ	A	401	-	3,3,3	0.48	0	2,2,2	1.00	0
2	BRJ	A	402	-	3,3,3	0.37	0	2,2,2	1.92	1 (50%)
2	BRJ	A	403	-	3,3,3	0.43	0	2,2,2	0.46	0
2	BRJ	A	404	-	3,3,3	0.42	0	2,2,2	0.59	0
3	3CN	A	405	-	3,3,3	0.81	0	2,2,2	0.31	0
4	MES	A	406	-	12,12,12	2.08	1 (8%)	14,16,16	1.95	4 (28%)
2	BRJ	B	401	-	3,3,3	0.37	0	2,2,2	0.65	0
2	BRJ	B	402	-	3,3,3	0.39	0	2,2,2	0.43	0
2	BRJ	B	403	-	3,3,3	0.46	0	2,2,2	0.13	0
3	3CN	B	404	-	3,3,3	0.74	0	2,2,2	0.28	0
4	MES	B	405	-	12,12,12	2.11	1 (8%)	14,16,16	1.82	4 (28%)
2	BRJ	C	401	-	3,3,3	0.46	0	2,2,2	0.53	0
2	BRJ	C	402	-	3,3,3	0.45	0	2,2,2	0.18	0
2	BRJ	C	403	-	3,3,3	0.41	0	2,2,2	0.61	0
3	3CN	C	404	-	3,3,3	0.76	0	2,2,2	0.23	0
4	MES	C	405	-	12,12,12	2.04	1 (8%)	14,16,16	2.36	5 (35%)
2	BRJ	D	401	-	3,3,3	0.44	0	2,2,2	0.49	0
2	BRJ	D	402	-	3,3,3	0.39	0	2,2,2	0.58	0
2	BRJ	D	403	-	3,3,3	0.46	0	2,2,2	0.26	0
3	3CN	D	404	-	3,3,3	0.75	0	2,2,2	0.23	0
4	MES	D	405	-	12,12,12	2.11	1 (8%)	14,16,16	1.93	5 (35%)
3	3CN	E	501	-	3,3,3	0.75	0	2,2,2	0.21	0
2	BRJ	E	502	-	3,3,3	0.45	0	2,2,2	0.61	0
2	BRJ	E	503	-	3,3,3	0.41	0	2,2,2	0.58	0
2	BRJ	E	504	-	3,3,3	0.44	0	2,2,2	0.28	0
4	MES	E	505	-	12,12,12	2.15	1 (8%)	14,16,16	1.86	5 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BRJ	F	401	-	3,3,3	0.39	0	2,2,2	0.38	0
2	BRJ	F	402	-	3,3,3	0.41	0	2,2,2	0.55	0
2	BRJ	F	403	-	3,3,3	0.42	0	2,2,2	0.85	0
2	BRJ	F	404	-	3,3,3	0.40	0	2,2,2	0.81	0
3	3CN	F	405	-	3,3,3	0.77	0	2,2,2	0.26	0
4	MES	F	406	-	12,12,12	2.07	1 (8%)	14,16,16	1.94	4 (28%)
2	BRJ	G	401	-	3,3,3	0.44	0	2,2,2	0.43	0
2	BRJ	G	402	-	3,3,3	0.31	0	2,2,2	1.61	1 (50%)
2	BRJ	G	403	-	3,3,3	0.39	0	2,2,2	0.87	0
3	3CN	G	404	-	3,3,3	0.92	0	2,2,2	0.10	0
4	MES	G	405	-	12,12,12	2.09	1 (8%)	14,16,16	2.08	6 (42%)
2	BRJ	H	401	-	3,3,3	0.41	0	2,2,2	1.07	0
2	BRJ	H	402	-	3,3,3	0.37	0	2,2,2	0.85	0
2	BRJ	H	403	-	3,3,3	0.41	0	2,2,2	0.42	0
3	3CN	H	404	-	3,3,3	0.89	0	2,2,2	0.14	0
4	MES	H	405	-	12,12,12	2.12	1 (8%)	14,16,16	1.86	4 (28%)
2	BRJ	I	401	-	3,3,3	0.45	0	2,2,2	0.46	0
2	BRJ	I	402	-	3,3,3	0.40	0	2,2,2	0.59	0
2	BRJ	I	403	-	3,3,3	0.42	0	2,2,2	0.64	0
3	3CN	I	404	-	3,3,3	0.79	0	2,2,2	0.21	0
4	MES	I	405	-	12,12,12	2.15	1 (8%)	14,16,16	1.72	4 (28%)
3	3CN	J	501	-	3,3,3	0.87	0	2,2,2	0.17	0
2	BRJ	J	502	-	3,3,3	0.36	0	2,2,2	0.93	0
2	BRJ	J	503	-	3,3,3	0.41	0	2,2,2	0.48	0
2	BRJ	J	504	-	3,3,3	0.33	0	2,2,2	1.99	1 (50%)
4	MES	J	505	-	12,12,12	2.08	1 (8%)	14,16,16	2.12	3 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BRJ	A	401	-	-	0/1/1/1	0/0/0/0
2	BRJ	A	402	-	-	0/1/1/1	0/0/0/0
2	BRJ	A	403	-	-	0/1/1/1	0/0/0/0
2	BRJ	A	404	-	-	0/1/1/1	0/0/0/0
3	3CN	A	405	-	-	0/1/1/1	0/0/0/0
4	MES	A	406	-	-	0/6/14/14	0/1/1/1
2	BRJ	B	401	-	-	0/1/1/1	0/0/0/0
2	BRJ	B	402	-	-	0/1/1/1	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BRJ	B	403	-	-	0/1/1/1	0/0/0/0
3	3CN	B	404	-	-	0/1/1/1	0/0/0/0
4	MES	B	405	-	-	0/6/14/14	0/1/1/1
2	BRJ	C	401	-	-	0/1/1/1	0/0/0/0
2	BRJ	C	402	-	-	0/1/1/1	0/0/0/0
2	BRJ	C	403	-	-	0/1/1/1	0/0/0/0
3	3CN	C	404	-	-	0/1/1/1	0/0/0/0
4	MES	C	405	-	-	0/6/14/14	0/1/1/1
2	BRJ	D	401	-	-	0/1/1/1	0/0/0/0
2	BRJ	D	402	-	-	0/1/1/1	0/0/0/0
2	BRJ	D	403	-	-	0/1/1/1	0/0/0/0
3	3CN	D	404	-	-	0/1/1/1	0/0/0/0
4	MES	D	405	-	-	0/6/14/14	0/1/1/1
3	3CN	E	501	-	-	0/1/1/1	0/0/0/0
2	BRJ	E	502	-	-	0/1/1/1	0/0/0/0
2	BRJ	E	503	-	-	0/1/1/1	0/0/0/0
2	BRJ	E	504	-	-	0/1/1/1	0/0/0/0
4	MES	E	505	-	-	0/6/14/14	0/1/1/1
2	BRJ	F	401	-	-	0/1/1/1	0/0/0/0
2	BRJ	F	402	-	-	0/1/1/1	0/0/0/0
2	BRJ	F	403	-	-	0/1/1/1	0/0/0/0
2	BRJ	F	404	-	-	0/1/1/1	0/0/0/0
3	3CN	F	405	-	-	0/1/1/1	0/0/0/0
4	MES	F	406	-	-	0/6/14/14	0/1/1/1
2	BRJ	G	401	-	-	0/1/1/1	0/0/0/0
2	BRJ	G	402	-	-	0/1/1/1	0/0/0/0
2	BRJ	G	403	-	-	0/1/1/1	0/0/0/0
3	3CN	G	404	-	-	0/1/1/1	0/0/0/0
4	MES	G	405	-	-	0/6/14/14	0/1/1/1
2	BRJ	H	401	-	-	0/1/1/1	0/0/0/0
2	BRJ	H	402	-	-	0/1/1/1	0/0/0/0
2	BRJ	H	403	-	-	0/1/1/1	0/0/0/0
3	3CN	H	404	-	-	0/1/1/1	0/0/0/0
4	MES	H	405	-	-	0/6/14/14	0/1/1/1
2	BRJ	I	401	-	-	0/1/1/1	0/0/0/0
2	BRJ	I	402	-	-	0/1/1/1	0/0/0/0
2	BRJ	I	403	-	-	0/1/1/1	0/0/0/0
3	3CN	I	404	-	-	0/1/1/1	0/0/0/0
4	MES	I	405	-	-	0/6/14/14	0/1/1/1
3	3CN	J	501	-	-	0/1/1/1	0/0/0/0
2	BRJ	J	502	-	-	0/1/1/1	0/0/0/0
2	BRJ	J	503	-	-	0/1/1/1	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BRJ	J	504	-	-	0/1/1/1	0/0/0/0
4	MES	J	505	-	-	0/6/14/14	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	-7.19	1.66	1.77
4	E	505	MES	C8-S	-7.16	1.66	1.77
4	D	405	MES	C8-S	-7.06	1.66	1.77
4	H	405	MES	C8-S	-7.05	1.66	1.77
4	B	405	MES	C8-S	-7.03	1.67	1.77
4	G	405	MES	C8-S	-6.96	1.67	1.77
4	J	505	MES	C8-S	-6.93	1.67	1.77
4	A	406	MES	C8-S	-6.91	1.67	1.77
4	F	406	MES	C8-S	-6.88	1.67	1.77
4	C	405	MES	C8-S	-6.75	1.67	1.77

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	405	MES	C6-C5-N4	-3.28	105.51	110.11
2	J	504	BRJ	BR1-CB-CB1	-2.64	104.27	111.50
2	A	402	BRJ	BR1-CB-CB1	-2.63	104.29	111.50
4	G	405	MES	C6-C5-N4	-2.51	106.60	110.11
4	G	405	MES	C2-C3-N4	-2.28	106.91	110.11
2	G	402	BRJ	BR1-CB-CB1	-2.16	105.58	111.50
4	E	505	MES	C6-C5-N4	-2.03	107.26	110.11
4	C	405	MES	C7-N4-C5	2.02	116.43	111.26
4	H	405	MES	C5-N4-C3	2.04	113.50	108.87
4	C	405	MES	O3S-S-C8	2.17	108.73	106.06
4	G	405	MES	C5-N4-C3	2.20	113.85	108.87
4	J	505	MES	C5-N4-C3	2.22	113.89	108.87
4	A	406	MES	C5-N4-C3	2.26	114.00	108.87
4	D	405	MES	C7-N4-C5	2.37	117.33	111.26
4	D	405	MES	C5-N4-C3	2.41	114.34	108.87
4	F	406	MES	O2S-S-C8	2.43	108.88	106.79
4	D	405	MES	O3S-S-C8	2.45	109.07	106.06
4	F	406	MES	C7-N4-C5	2.54	117.76	111.26
4	I	405	MES	O2S-S-C8	2.64	109.06	106.79
4	I	405	MES	C5-N4-C3	2.68	114.94	108.87
4	E	505	MES	C5-N4-C3	2.68	114.94	108.87
4	B	405	MES	C5-N4-C3	2.71	115.01	108.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	406	MES	O3S-S-C8	2.78	109.47	106.06
4	H	405	MES	O1S-S-C8	2.80	109.19	106.79
4	A	406	MES	O2S-S-C8	2.83	109.22	106.79
4	E	505	MES	O2S-S-C8	2.93	109.31	106.79
4	I	405	MES	O1S-S-C8	2.93	109.31	106.79
4	B	405	MES	O2S-S-C8	2.95	109.32	106.79
4	E	505	MES	O3S-S-C8	2.95	109.68	106.06
4	J	505	MES	O1S-S-C8	2.98	109.35	106.79
4	G	405	MES	O3S-S-C8	3.08	109.85	106.06
4	D	405	MES	O2S-S-C8	3.30	109.62	106.79
4	B	405	MES	O3S-S-C8	3.34	110.16	106.06
4	H	405	MES	O3S-S-C8	3.38	110.21	106.06
4	F	406	MES	O1S-S-C8	3.40	109.72	106.79
4	B	405	MES	O1S-S-C8	3.41	109.72	106.79
4	I	405	MES	O3S-S-C8	3.42	110.26	106.06
4	G	405	MES	O2S-S-C8	3.51	109.81	106.79
4	E	505	MES	O1S-S-C8	3.53	109.83	106.79
4	H	405	MES	O2S-S-C8	3.75	110.01	106.79
4	C	405	MES	O2S-S-C8	3.78	110.04	106.79
4	G	405	MES	O1S-S-C8	3.79	110.05	106.79
4	D	405	MES	O1S-S-C8	4.17	110.37	106.79
4	F	406	MES	O3S-S-C8	4.20	111.22	106.06
4	A	406	MES	O1S-S-C8	4.72	110.84	106.79
4	C	405	MES	O1S-S-C8	5.68	111.67	106.79
4	J	505	MES	O2S-S-C8	5.98	111.93	106.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	BRJ	2	0
2	A	402	BRJ	1	0
2	A	403	BRJ	1	0
2	B	401	BRJ	1	0
2	C	401	BRJ	2	0
2	C	403	BRJ	1	0
2	D	403	BRJ	1	0
2	E	502	BRJ	1	0
2	E	504	BRJ	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	401	BRJ	2	0
2	G	401	BRJ	1	0
2	G	402	BRJ	1	0
2	H	401	BRJ	2	0
3	H	404	3CN	1	0
2	I	401	BRJ	1	0
2	I	403	BRJ	3	0
2	J	502	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%)	0.10	21 (6%) 18 7	72, 115, 167, 209	0
1	B	308/322 (95%)	0.00	13 (4%) 37 18	69, 107, 178, 227	0
1	C	308/322 (95%)	0.04	12 (3%) 40 19	71, 110, 181, 204	0
1	D	308/322 (95%)	0.06	15 (4%) 30 14	63, 102, 174, 222	0
1	E	308/322 (95%)	0.18	19 (6%) 21 8	73, 113, 168, 198	0
1	F	308/322 (95%)	0.01	12 (3%) 40 19	71, 121, 177, 209	0
1	G	308/322 (95%)	0.04	18 (5%) 24 10	57, 106, 163, 204	0
1	H	308/322 (95%)	0.18	23 (7%) 15 5	70, 113, 185, 215	0
1	I	308/322 (95%)	0.03	16 (5%) 28 12	70, 110, 173, 210	0
1	J	308/322 (95%)	0.19	22 (7%) 17 6	84, 123, 187, 207	0
All	All	3080/3220 (95%)	0.08	171 (5%) 25 11	57, 112, 177, 227	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	289	ASN	15.2
1	D	179	SER	7.7
1	H	289	ASN	7.1
1	H	288	ALA	6.3
1	J	287	GLN	6.2
1	F	287	GLN	6.0
1	E	157	ILE	5.9
1	H	317	ILE	5.8
1	E	290	GLY	5.8
1	J	157	ILE	5.5
1	J	306	LEU	5.4
1	D	157	ILE	5.4
1	H	183	PRO	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	53	ASP	5.3
1	G	311	ILE	5.3
1	G	314	VAL	5.2
1	I	157	ILE	5.1
1	A	153	ASP	5.1
1	D	178	LEU	5.0
1	D	180	SER	5.0
1	B	288	ALA	4.9
1	I	289	ASN	4.9
1	A	299	ARG	4.8
1	E	288	ALA	4.8
1	G	157	ILE	4.6
1	J	154	ASN	4.6
1	J	294	ASP	4.5
1	J	289	ASN	4.5
1	H	181	VAL	4.5
1	J	288	ALA	4.4
1	A	287	GLN	4.4
1	J	237	THR	4.3
1	D	183	PRO	4.2
1	B	294	ASP	4.2
1	C	294	ASP	4.2
1	I	287	GLN	4.2
1	J	292	GLU	4.1
1	F	288	ALA	4.0
1	H	185	GLN	3.9
1	G	315	LEU	3.9
1	E	179	SER	3.8
1	E	49	LYS	3.8
1	J	290	GLY	3.7
1	G	154	ASN	3.7
1	D	181	VAL	3.7
1	G	156	GLU	3.7
1	E	156	GLU	3.6
1	D	289	ASN	3.6
1	F	237	THR	3.6
1	I	179	SER	3.5
1	H	174	ARG	3.5
1	J	305	PRO	3.5
1	J	156	GLU	3.5
1	I	237	THR	3.5
1	A	116	PHE	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	115	ASP	3.4
1	H	311	ILE	3.4
1	C	317	ILE	3.3
1	B	241	THR	3.2
1	G	312	GLY	3.2
1	C	289	ASN	3.2
1	H	241	THR	3.2
1	B	312	GLY	3.2
1	A	237	THR	3.1
1	J	240	LEU	3.1
1	A	286	ARG	3.1
1	J	241	THR	3.1
1	F	157	ILE	3.1
1	I	317	ILE	3.1
1	D	182	GLN	3.1
1	J	138	GLN	3.1
1	C	156	GLU	3.0
1	J	153	ASP	3.0
1	E	158	ASP	3.0
1	C	299	ARG	3.0
1	H	180	SER	3.0
1	I	292	GLU	2.9
1	I	290	GLY	2.9
1	E	123	ARG	2.9
1	H	186	ASN	2.8
1	H	49	LYS	2.8
1	A	244	ALA	2.8
1	G	183	PRO	2.8
1	E	287	GLN	2.7
1	G	161	TRP	2.7
1	E	291	VAL	2.7
1	I	180	SER	2.7
1	G	155	GLU	2.7
1	D	186	ASN	2.7
1	H	182	GLN	2.7
1	F	240	LEU	2.7
1	B	237	THR	2.7
1	I	293	ASP	2.7
1	E	311	ILE	2.7
1	I	285	HIS	2.6
1	J	234	THR	2.6
1	H	316	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	187	GLU	2.5
1	C	295	LEU	2.5
1	B	157	ILE	2.5
1	G	290	GLY	2.5
1	A	296	LEU	2.5
1	G	116	PHE	2.5
1	F	244	ALA	2.5
1	H	291	VAL	2.5
1	B	289	ASN	2.5
1	E	237	THR	2.5
1	F	241	THR	2.5
1	B	299	ARG	2.4
1	G	313	CYS	2.4
1	A	157	ILE	2.4
1	B	293	ASP	2.4
1	H	187	GLU	2.4
1	E	286	ARG	2.4
1	I	286	ARG	2.4
1	H	315	LEU	2.4
1	D	185	GLN	2.3
1	F	311	ILE	2.3
1	A	117	ARG	2.3
1	I	181	VAL	2.3
1	H	156	GLU	2.3
1	G	306	LEU	2.3
1	D	188	PHE	2.3
1	J	238	LEU	2.3
1	B	287	GLN	2.3
1	G	241	THR	2.3
1	J	303	ALA	2.3
1	H	244	ALA	2.3
1	A	114	MET	2.3
1	C	237	THR	2.3
1	F	114	MET	2.3
1	A	179	SER	2.3
1	C	239	MET	2.3
1	A	121	PHE	2.2
1	D	285	HIS	2.2
1	J	155	GLU	2.2
1	E	138	GLN	2.2
1	F	316	VAL	2.2
1	A	258	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	289	ASN	2.2
1	H	173	ILE	2.2
1	D	287	GLN	2.2
1	C	311	ILE	2.2
1	G	240	LEU	2.2
1	I	241	THR	2.2
1	C	292	GLU	2.2
1	B	292	GLU	2.2
1	D	316	VAL	2.2
1	G	287	GLN	2.2
1	J	158	ASP	2.1
1	H	292	GLU	2.1
1	A	241	THR	2.1
1	E	241	THR	2.1
1	B	156	GLU	2.1
1	C	233	GLN	2.1
1	A	188	PHE	2.1
1	J	293	ASP	2.1
1	G	282	PHE	2.1
1	A	54	LYS	2.1
1	H	240	LEU	2.1
1	B	53	ASP	2.1
1	A	283	ALA	2.1
1	E	244	ALA	2.1
1	I	224	TRP	2.0
1	E	180	SER	2.0
1	A	118	LEU	2.0
1	E	240	LEU	2.0
1	F	178	LEU	2.0
1	H	294	ASP	2.0
1	I	240	LEU	2.0
1	D	158	ASP	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 carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	BRJ	G	401	4/4	0.58	1.02	39.27	111,117,133,164	0
2	BRJ	H	401	4/4	0.62	0.99	21.37	98,101,128,154	0
2	BRJ	B	401	4/4	0.43	1.25	18.43	106,132,136,192	0
2	BRJ	I	401	4/4	0.32	0.84	16.75	103,131,137,169	0
2	BRJ	D	401	4/4	0.58	0.68	16.24	94,127,129,141	0
2	BRJ	G	402	4/4	0.87	0.84	14.30	122,125,135,135	0
2	BRJ	I	402	4/4	0.55	0.72	12.85	98,114,121,125	0
2	BRJ	C	401	4/4	0.47	0.60	12.84	86,91,113,146	0
2	BRJ	J	503	4/4	0.79	0.99	12.74	131,142,143,153	0
2	BRJ	D	402	4/4	0.71	0.58	12.56	112,112,120,122	0
2	BRJ	A	401	4/4	0.53	0.92	11.93	124,131,154,183	0
2	BRJ	B	402	4/4	0.83	0.82	11.71	125,130,137,151	0
2	BRJ	J	502	4/4	0.60	0.89	11.30	109,116,118,139	0
2	BRJ	E	502	4/4	0.50	0.72	10.61	102,126,131,160	0
2	BRJ	H	403	4/4	0.57	0.66	10.15	142,145,149,152	0
2	BRJ	E	504	4/4	0.50	0.73	9.38	118,126,142,147	0
2	BRJ	I	403	4/4	0.32	0.65	8.59	95,99,111,142	0
2	BRJ	H	402	4/4	0.78	0.63	8.32	93,117,125,131	0
2	BRJ	F	401	4/4	0.65	0.46	7.88	99,117,132,135	0
2	BRJ	E	503	4/4	0.84	0.54	7.28	130,130,148,165	0
2	BRJ	F	402	4/4	0.64	0.45	7.05	101,108,121,128	0
2	BRJ	D	403	4/4	0.24	0.57	6.45	93,99,105,145	0
2	BRJ	J	504	4/4	0.74	0.56	6.27	145,148,153,158	0
2	BRJ	A	402	4/4	0.89	0.70	5.98	102,110,127,154	0
2	BRJ	C	402	4/4	0.55	0.42	5.80	104,106,110,139	0
2	BRJ	A	404	4/4	0.88	0.68	5.27	137,154,169,175	0
2	BRJ	C	403	4/4	0.65	0.45	5.16	121,147,151,177	0
2	BRJ	B	403	4/4	0.58	0.48	4.39	118,141,150,163	0
2	BRJ	F	403	4/4	0.69	0.57	4.19	118,146,156,160	0
2	BRJ	F	404	4/4	0.81	0.81	3.65	149,152,155,157	0
2	BRJ	A	403	4/4	0.60	0.50	3.34	125,129,136,146	0
3	3CN	G	404	4/4	0.92	0.34	2.13	85,87,97,99	0
2	BRJ	G	403	4/4	0.87	0.33	1.67	105,115,119,129	0
3	3CN	F	405	4/4	0.84	0.37	1.34	91,93,98,112	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	3CN	J	501	4/4	0.89	0.22	-0.41	97,121,130,132	0
4	MES	E	505	12/12	0.88	0.13	-0.82	136,156,168,171	0
3	3CN	D	404	4/4	0.88	0.33	-	96,102,109,113	0
5	CL	C	406	1/1	0.96	0.24	-	107,107,107,107	0
4	MES	F	406	12/12	0.93	0.15	-	131,155,168,187	0
4	MES	C	405	12/12	0.90	0.19	-	115,134,160,166	0
3	3CN	H	404	4/4	0.73	0.52	-	83,94,100,122	0
4	MES	A	406	12/12	0.85	0.18	-	132,154,185,186	0
3	3CN	I	404	4/4	0.91	0.38	-	96,98,103,109	0
3	3CN	E	501	4/4	0.94	0.28	-	91,95,102,114	0
4	MES	J	505	12/12	0.88	0.16	-	158,170,183,184	0
4	MES	G	405	12/12	0.92	0.18	-	128,151,170,173	0
4	MES	H	405	12/12	0.92	0.14	-	113,135,158,179	0
4	MES	B	405	12/12	0.89	0.11	-	129,148,167,179	0
3	3CN	A	405	4/4	0.69	0.42	-	86,98,102,115	0
5	CL	J	506	1/1	0.77	0.35	-	166,166,166,166	0
4	MES	I	405	12/12	0.85	0.30	-	141,175,183,195	0
4	MES	D	405	12/12	0.80	0.18	-	126,147,174,178	0
3	3CN	B	404	4/4	0.89	0.35	-	79,96,99,105	0
3	3CN	C	404	4/4	0.84	0.35	-	84,92,119,127	0

6.5 Other polymers

There are no such residues in this entry.