



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:53 AM UTC

PDB ID : 5Z1G / pdb_00005z1g
Title : Structure of the Brx1 and Ebp2 complex
Authors : Zheng, S.; Ye, K.
Deposited on : 2017-12-26
Resolution : 2.29 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

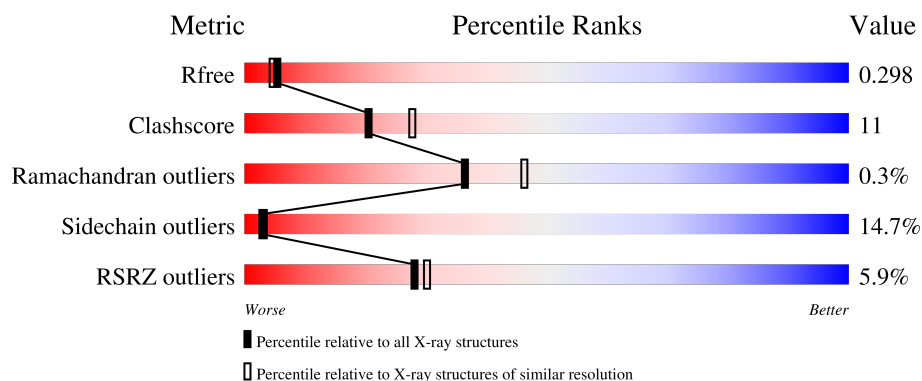
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	110	8% 67% 19% • 10%
1	C	110	8% 58% 28% • 10%
2	B	234	6% 58% 27% 6% 9%
2	D	234	2% 60% 27% • 9%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5459 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.

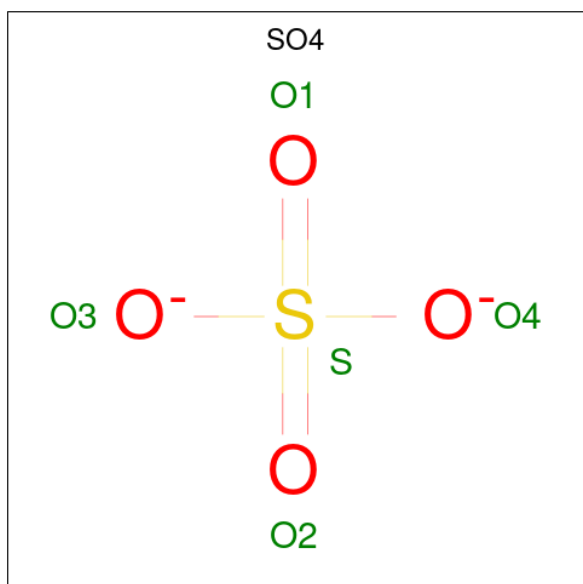
- Molecule 1 is a protein called rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	99	Total	C	N	O	S	0	0	0
			826	523	145	155	3			
1	C	99	Total	C	N	O	S	0	0	0
			826	523	145	155	3			

- Molecule 2 is a protein called Ribosome biogenesis protein BRX1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1747	1125	309	307	6			
2	D	212	Total	C	N	O	S	0	0	0
			1747	1125	309	307	6			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		

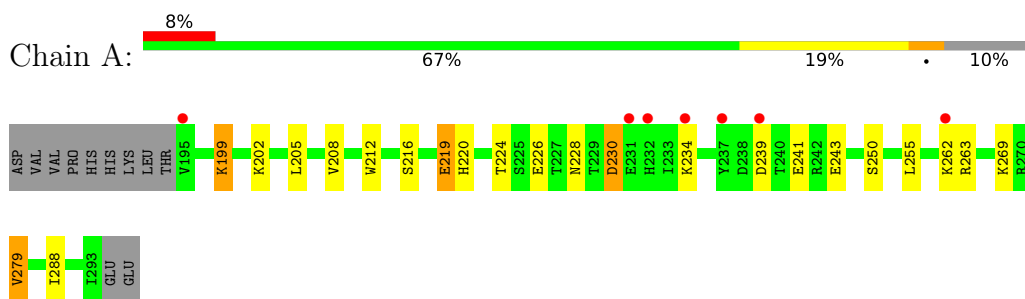
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	59	Total	O	0	0
			59	59		
4	B	98	Total	O	0	0
			98	98		
4	C	57	Total	O	0	0
			57	57		
4	D	94	Total	O	0	0
			94	94		

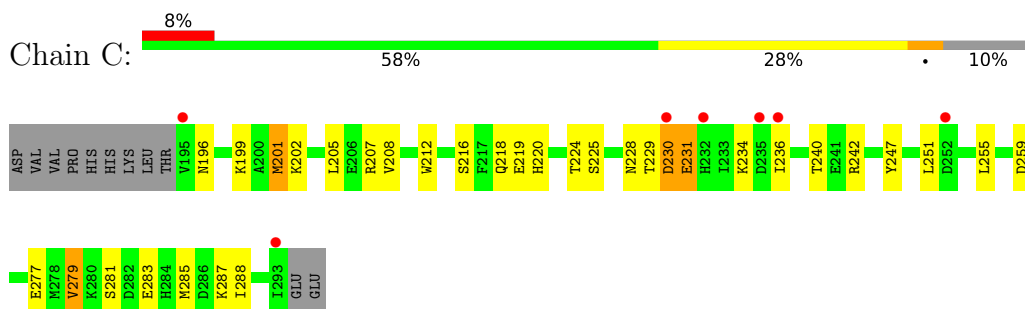
3 Residue-property plots [i](#)

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.

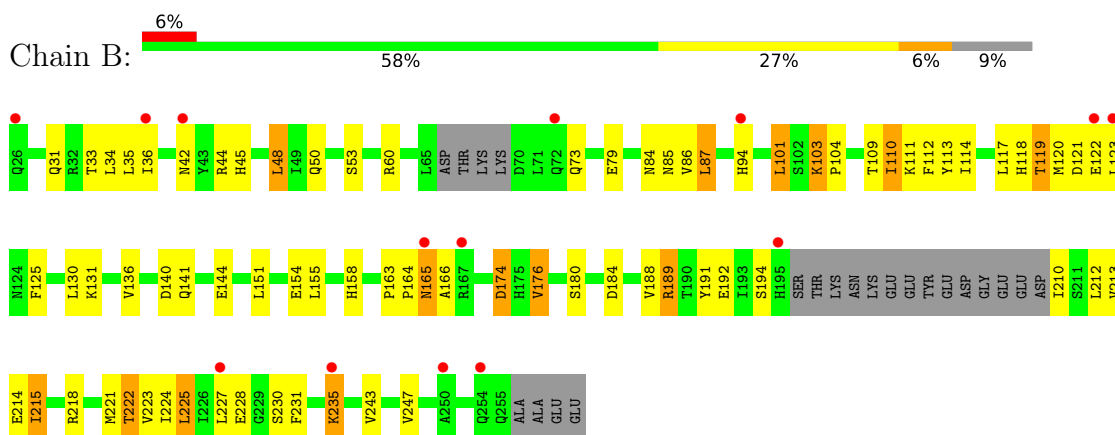
- Molecule 1: rRNA-processing protein EBP2



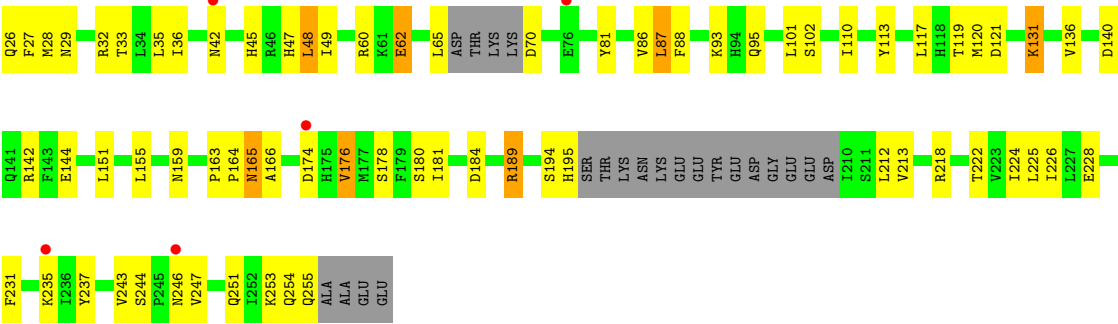
- Molecule 1: rRNA-processing protein EBP2



- Molecule 2: Ribosome biogenesis protein BRX1



- Molecule 2: Ribosome biogenesis protein BRX1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.93Å 47.35Å 100.69Å 90.00° 94.10° 90.00°	Depositor
Resolution (Å)	24.91 – 2.29 24.91 – 2.29	Depositor EDS
% Data completeness (in resolution range)	96.1 (24.91-2.29) 96.2 (24.91-2.29)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.28Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.230 , 0.297 0.231 , 0.298	Depositor DCC
R_{free} test set	1685 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5459	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.02 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9126e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.33	0/842	0.54	0/1130
1	C	0.35	0/842	0.55	0/1130
2	B	0.38	0/1790	0.68	0/2418
2	D	0.38	0/1790	0.65	0/2418
All	All	0.37	0/5264	0.63	0/7096

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	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	230	ASP	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	826	0	828	14	0
1	C	826	0	828	20	0
2	B	1747	0	1759	52	0
2	D	1747	0	1759	41	0
3	D	5	0	0	0	0
4	A	59	0	0	5	0
4	B	98	0	0	7	0
4	C	57	0	0	9	0
4	D	94	0	0	10	0
All	All	5459	0	5174	116	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 11.

All (116) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:GLN:HE21	2:B:85:ASN:HD21	1.27	0.79
2:D:142:ARG:HB3	2:D:181:ILE:HD12	1.62	0.79
2:B:44:ARG:NH2	2:B:122:GLU:OE2	2.16	0.79
2:D:164:PRO:O	4:D:401:HOH:O	2.02	0.76
1:A:262:LYS:NZ	4:A:303:HOH:O	2.20	0.74
2:B:210:ILE:N	4:B:303:HOH:O	2.21	0.73
1:C:285:MET:SD	4:C:309:HOH:O	2.46	0.73
2:D:101:LEU:HD11	2:D:159:ASN:ND2	2.04	0.72
2:D:60:ARG:NH2	4:D:403:HOH:O	2.19	0.72
2:B:164:PRO:O	4:B:301:HOH:O	2.08	0.71
2:B:103:LYS:NZ	2:B:158:HIS:HD2	1.89	0.70
2:B:42:ASN:H	2:B:45:HIS:CD2	2.11	0.67
2:B:119:THR:O	2:B:122:GLU:HG2	1.95	0.67
2:D:131:LYS:NZ	4:D:407:HOH:O	2.29	0.65
2:D:70:ASP:OD2	4:D:402:HOH:O	2.15	0.65
2:D:26:GLN:HG3	2:D:27:PHE:H	1.62	0.65
2:B:235:LYS:H	2:B:235:LYS:HE3	1.61	0.65
1:C:277:GLU:OE2	4:C:301:HOH:O	2.14	0.64
2:B:42:ASN:HB2	2:B:45:HIS:CD2	2.32	0.64
2:B:111:LYS:HB3	2:B:225:LEU:HD22	1.79	0.64
2:B:60:ARG:NH2	4:B:306:HOH:O	2.32	0.63
2:D:47:HIS:CE1	2:D:121:ASP:HB2	2.34	0.62
1:C:287:LYS:NZ	4:C:302:HOH:O	2.18	0.61
2:D:42:ASN:HB2	2:D:45:HIS:CG	2.36	0.61
2:D:29:ASN:O	4:D:401:HOH:O	2.16	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:136:VAL:HB	2:D:176:VAL:HG13	1.84	0.60
1:A:219:GLU:HG2	2:D:28:MET:HE3	1.83	0.59
2:B:31:GLN:NE2	2:B:85:ASN:HD21	1.99	0.59
2:B:42:ASN:HB2	2:B:45:HIS:CG	2.39	0.58
2:B:192:GLU:HB2	2:B:215:ILE:HD11	1.87	0.57
2:D:33:THR:HG21	2:D:87:LEU:HD22	1.86	0.57
1:C:196:ASN:N	4:C:307:HOH:O	2.38	0.57
2:D:87:LEU:HD13	2:D:101:LEU:HD13	1.86	0.57
2:B:163:PRO:HG2	2:B:166:ALA:HB2	1.88	0.55
1:A:234:LYS:N	4:A:301:HOH:O	2.16	0.55
1:A:228:ASN:ND2	4:A:309:HOH:O	2.40	0.54
2:D:189:ARG:NH2	4:D:415:HOH:O	2.40	0.54
2:B:103:LYS:HZ3	2:B:158:HIS:HD2	1.53	0.54
2:B:114:ILE:HD13	2:B:221:MET:HG2	1.90	0.54
2:D:246:ASN:ND2	4:D:412:HOH:O	2.34	0.54
1:C:234:LYS:NZ	4:C:303:HOH:O	2.27	0.53
1:C:231:GLU:N	4:C:310:HOH:O	2.41	0.52
2:B:140:ASP:HB2	2:B:180:SER:HA	1.92	0.52
2:B:48:LEU:HG	2:B:117:LEU:HD11	1.92	0.51
1:A:241:GLU:OE1	4:A:301:HOH:O	2.19	0.51
2:B:120:MET:HE1	1:C:279:VAL:HG22	1.92	0.51
1:A:271:PRO:HG2	1:A:274:TYR:HB2	1.92	0.50
2:B:113:TYR:HB3	2:B:222:THR:HG23	1.93	0.50
2:D:163:PRO:HG2	2:D:166:ALA:HB2	1.94	0.50
2:D:120:MET:HE2	4:D:408:HOH:O	2.12	0.50
1:C:228:ASN:C	1:C:230:ASP:H	2.19	0.49
2:B:109:THR:HB	2:B:227:LEU:HD13	1.95	0.49
2:D:189:ARG:CZ	2:D:218:ARG:HG3	2.42	0.49
2:D:165:ASN:OD1	2:D:165:ASN:N	2.42	0.49
2:B:86:VAL:HG21	2:B:231:PHE:CE2	2.47	0.49
2:D:140:ASP:HB2	2:D:180:SER:HA	1.94	0.49
2:B:136:VAL:HB	2:B:176:VAL:HG13	1.94	0.49
2:B:222:THR:HG22	4:B:335:HOH:O	2.12	0.48
1:C:218:GLN:NE2	4:C:308:HOH:O	2.39	0.48
2:D:62:GLU:HG2	2:D:81:TYR:CE2	2.48	0.48
2:D:32:ARG:HH11	2:D:60:ARG:HE	1.62	0.48
2:B:110:ILE:HG12	2:B:112:PHE:CZ	2.49	0.47
2:B:130:LEU:N	2:B:174:ASP:OD2	2.34	0.47
2:B:53:SER:OG	4:B:302:HOH:O	2.13	0.47
2:B:34:LEU:HG	2:B:36:ILE:HG13	1.96	0.47
2:B:73:GLN:HA	4:B:305:HOH:O	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:GLU:OE1	2:B:158:HIS:HE1	1.98	0.46
2:B:164:PRO:HA	2:B:165:ASN:HA	1.61	0.46
2:D:247:VAL:O	2:D:251:GLN:HG2	2.15	0.46
1:C:207:ARG:NH2	4:C:315:HOH:O	2.48	0.46
2:B:33:THR:HG21	2:B:87:LEU:HD22	1.97	0.46
2:B:44:ARG:HG2	2:B:117:LEU:HD23	1.98	0.45
2:B:174:ASP:OD1	1:C:270:ARG:NH1	2.36	0.45
1:A:199:LYS:NZ	4:A:313:HOH:O	2.50	0.45
2:B:214:GLU:OE2	2:B:218:ARG:HD2	2.15	0.45
2:D:244:SER:OG	4:D:404:HOH:O	2.21	0.45
2:B:118:HIS:NE2	4:B:304:HOH:O	2.26	0.45
2:B:192:GLU:HB3	2:B:213:VAL:HG13	1.99	0.45
1:A:271:PRO:HB3	1:C:271:PRO:HB3	1.99	0.45
2:D:189:ARG:NE	2:D:218:ARG:HG3	2.31	0.45
2:D:226:ILE:HB	2:D:237:TYR:HB3	1.99	0.45
2:B:188:VAL:C	2:B:189:ARG:HE	2.25	0.45
1:A:279:VAL:HG13	2:D:120:MET:CE	2.47	0.44
1:A:279:VAL:HG13	2:D:120:MET:SD	2.58	0.44
2:D:194:SER:O	2:D:195:HIS:HB2	2.16	0.44
1:C:242:ARG:NH2	4:C:312:HOH:O	2.45	0.44
2:D:113:TYR:HB2	2:D:224:ILE:HD11	1.99	0.44
2:B:174:ASP:CG	1:C:270:ARG:HH11	2.24	0.43
2:D:131:LYS:HE3	2:D:131:LYS:HB2	1.83	0.43
2:D:86:VAL:HG21	2:D:231:PHE:CE2	2.53	0.43
2:B:101:LEU:C	2:B:101:LEU:HD12	2.42	0.43
1:A:250:SER:OG	2:D:178:SER:HB3	2.17	0.43
1:C:199:LYS:HE2	1:C:199:LYS:HB2	1.80	0.43
2:B:110:ILE:CD1	2:B:223:VAL:HG13	2.48	0.43
1:A:263:ARG:HE	1:A:263:ARG:HB2	1.64	0.42
2:B:119:THR:CG2	2:B:121:ASP:HB2	2.49	0.42
1:C:281:SER:O	1:C:285:MET:HG2	2.18	0.42
2:B:110:ILE:HD11	2:B:223:VAL:HG13	2.00	0.42
2:D:101:LEU:HD11	2:D:159:ASN:HD21	1.80	0.42
2:D:246:ASN:ND2	4:D:423:HOH:O	2.51	0.42
2:B:176:VAL:HG23	2:B:191:TYR:HB2	2.01	0.42
2:B:113:TYR:HB2	2:B:224:ILE:HD11	2.01	0.41
2:B:212:LEU:HB2	1:C:247:TYR:CE2	2.55	0.41
2:B:125:PHE:HZ	2:B:218:ARG:HD3	1.84	0.41
2:B:141:GLN:HB2	1:C:225:SER:O	2.20	0.41
2:B:109:THR:OG1	2:B:230:SER:HA	2.21	0.41
2:D:93:LYS:O	2:D:95:GLN:HG2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:TRP:CZ3	1:A:220:HIS:HB3	2.56	0.41
2:B:84:ASN:O	2:B:104:PRO:HD2	2.21	0.41
1:C:212:TRP:CZ3	1:C:220:HIS:HB3	2.56	0.41
2:D:48:LEU:HG	2:D:117:LEU:HD11	2.02	0.41
1:A:243:GLU:OE1	2:D:189:ARG:NH1	2.54	0.40
2:D:235:LYS:HE3	2:D:235:LYS:HB2	1.91	0.40
2:D:36:ILE:O	2:D:88:PHE:HA	2.20	0.40
1:C:201:MET:HE2	1:C:201:MET:HB2	1.80	0.40
2:B:86:VAL:HG21	2:B:231:PHE:HE2	1.86	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	97/110 (88%)	93 (96%)	4 (4%)	0	100	100
1	C	97/110 (88%)	94 (97%)	1 (1%)	2 (2%)	5	4
2	B	206/234 (88%)	197 (96%)	9 (4%)	0	100	100
2	D	206/234 (88%)	201 (98%)	5 (2%)	0	100	100
All	All	606/688 (88%)	585 (96%)	19 (3%)	2 (0%)	36	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	229	THR
1	C	236	ILE

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	92/103 (89%)	78 (85%)	14 (15%)	3	3
1	C	92/103 (89%)	76 (83%)	16 (17%)	2	2
2	B	198/217 (91%)	170 (86%)	28 (14%)	3	3
2	D	198/217 (91%)	171 (86%)	27 (14%)	3	4
All	All	580/640 (91%)	495 (85%)	85 (15%)	3	3

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

Mol	Chain	Res	Type
1	A	199	LYS
1	A	202	LYS
1	A	205	LEU
1	A	208	VAL
1	A	216	SER
1	A	219	GLU
1	A	224	THR
1	A	226	GLU
1	A	230	ASP
1	A	239	ASP
1	A	255	LEU
1	A	269	LYS
1	A	279	VAL
1	A	288	ILE
2	B	35	LEU
2	B	48	LEU
2	B	50	GLN
2	B	79	GLU
2	B	87	LEU
2	B	94	HIS
2	B	101	LEU
2	B	103	LYS
2	B	110	ILE
2	B	119	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	123	LEU
2	B	131	LYS
2	B	144	GLU
2	B	151	LEU
2	B	155	LEU
2	B	165	ASN
2	B	174	ASP
2	B	176	VAL
2	B	184	ASP
2	B	189	ARG
2	B	194	SER
2	B	215	ILE
2	B	222	THR
2	B	225	LEU
2	B	228	GLU
2	B	235	LYS
2	B	243	VAL
2	B	247	VAL
1	C	201	MET
1	C	202	LYS
1	C	205	LEU
1	C	208	VAL
1	C	216	SER
1	C	219	GLU
1	C	224	THR
1	C	230	ASP
1	C	231	GLU
1	C	240	THR
1	C	251	LEU
1	C	255	LEU
1	C	259	ASP
1	C	279	VAL
1	C	283	GLU
1	C	288	ILE
2	D	35	LEU
2	D	48	LEU
2	D	49	ILE
2	D	62	GLU
2	D	65	LEU
2	D	87	LEU
2	D	102	SER
2	D	110	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	119	THR
2	D	131	LYS
2	D	144	GLU
2	D	151	LEU
2	D	155	LEU
2	D	165	ASN
2	D	174	ASP
2	D	176	VAL
2	D	184	ASP
2	D	189	ARG
2	D	212	LEU
2	D	213	VAL
2	D	222	THR
2	D	225	LEU
2	D	228	GLU
2	D	243	VAL
2	D	253	LYS
2	D	254	GLN
2	D	255	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	HIS
1	A	228	ASN
2	B	31	GLN
2	B	45	HIS
2	B	50	GLN
2	B	116	ASN
2	B	158	HIS
2	B	165	ASN
2	B	254	GLN
1	C	218	GLN
1	C	228	ASN
2	D	50	GLN
2	D	95	GLN
2	D	241	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	D	301	-	4,4,4	0.31	0	6,6,6	0.26	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	99/110 (90%)	0.72	9 (9%) 15 16	18, 27, 48, 68	0
1	C	99/110 (90%)	0.87	9 (9%) 15 16	18, 29, 44, 73	0
2	B	212/234 (90%)	0.49	14 (6%) 24 26	14, 21, 41, 56	0
2	D	212/234 (90%)	0.37	5 (2%) 59 62	13, 21, 38, 44	0
All	All	622/688 (90%)	0.55	37 (5%) 28 30	13, 23, 43, 73	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	232	HIS	7.0
1	A	232	HIS	5.6
1	C	235	ASP	3.7
2	D	76	GLU	3.3
2	B	254	GLN	3.3
1	C	272	LEU	3.2
1	C	252	ASP	3.2
2	B	123	LEU	3.2
1	A	272	LEU	3.2
2	B	122	GLU	3.1
2	B	165	ASN	3.0
1	C	195	VAL	3.0
2	B	36	ILE	2.9
1	C	236	ILE	2.8
1	A	231	GLU	2.7
1	A	237	TYR	2.6
2	B	235	LYS	2.4
1	C	230	ASP	2.4
1	C	273	ASP	2.3
2	B	42	ASN	2.3
1	A	195	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	293	ILE	2.3
2	B	250	ALA	2.3
2	B	167	ARG	2.3
1	A	234	LYS	2.3
2	D	174	ASP	2.3
2	D	42	ASN	2.2
2	B	195	HIS	2.2
1	A	273	ASP	2.2
2	D	246	ASN	2.2
1	A	239	ASP	2.2
2	B	94	HIS	2.1
2	B	26	GLN	2.1
1	A	262	LYS	2.1
2	B	72	GLN	2.1
2	B	227	LEU	2.0
2	D	235	LYS	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($\text{\AA}^2$)	Q<0.9
3	SO4	D	301	5/5	0.81	0.26	39,41,49,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.