



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 8, 2016 – 05:57 PM EDT

PDB ID : 5K5D  
Title : Structure of the C2221 form of Pnob8-like ParB-N domain  
Authors : Schumacher, M.  
Deposited on : 2016-05-23  
Resolution : 2.45 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027674  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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-20027674

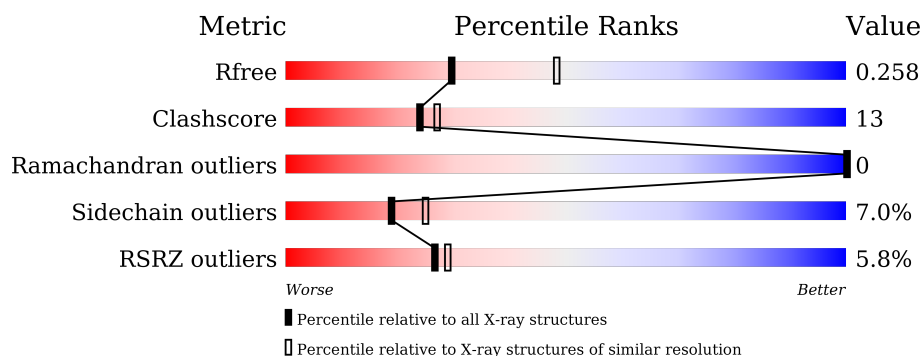
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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))
$R_{free}$	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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  $\geq 3$ , 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	300	 2% 58% 23% • 16%
1	B	300	 2% 56% 25% • 17%
1	C	300	 10% 53% 27% • 17%

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	CIT	C	302	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6407 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 ParB domain protein nuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	250	Total	C	N	O	Se	0	0	0
			2080	1318	353	402	7			
1	A	252	Total	C	N	O	Se	0	0	0
			2097	1329	356	405	7			
1	C	249	Total	C	N	O	Se	0	0	0
			2075	1316	352	400	7			

There are 24 discrepancies between the modelled and reference sequences:

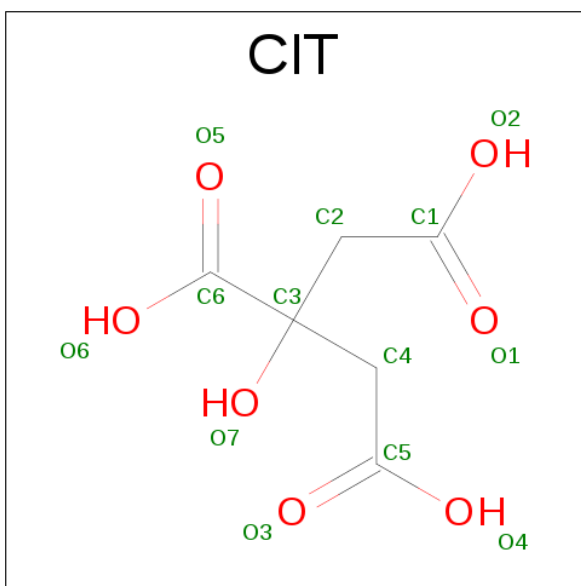
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP D0KSP7
B	-1	SER	-	expression tag	UNP D0KSP7
B	0	HIS	-	expression tag	UNP D0KSP7
B	25	MSE	LEU	engineered mutation	UNP D0KSP7
B	123	MSE	ILE	engineered mutation	UNP D0KSP7
B	228	MSE	LEU	engineered mutation	UNP D0KSP7
B	264	MSE	LEU	engineered mutation	UNP D0KSP7
B	?	-	GLU	deletion	UNP D0KSP7
A	-2	GLY	-	expression tag	UNP D0KSP7
A	-1	SER	-	expression tag	UNP D0KSP7
A	0	HIS	-	expression tag	UNP D0KSP7
A	25	MSE	LEU	engineered mutation	UNP D0KSP7
A	123	MSE	ILE	engineered mutation	UNP D0KSP7
A	228	MSE	LEU	engineered mutation	UNP D0KSP7
A	264	MSE	LEU	engineered mutation	UNP D0KSP7
A	?	-	GLU	deletion	UNP D0KSP7
C	-2	GLY	-	expression tag	UNP D0KSP7
C	-1	SER	-	expression tag	UNP D0KSP7
C	0	HIS	-	expression tag	UNP D0KSP7
C	25	MSE	LEU	engineered mutation	UNP D0KSP7
C	123	MSE	ILE	engineered mutation	UNP D0KSP7
C	228	MSE	LEU	engineered mutation	UNP D0KSP7
C	264	MSE	LEU	engineered mutation	UNP D0KSP7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLU	deletion	UNP D0KSP7

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 13 6 7	0	0
2	A	1	Total C O 13 6 7	0	0
2	C	1	Total C O 13 6 7	0	0
2	C	1	Total C O 13 6 7	0	0

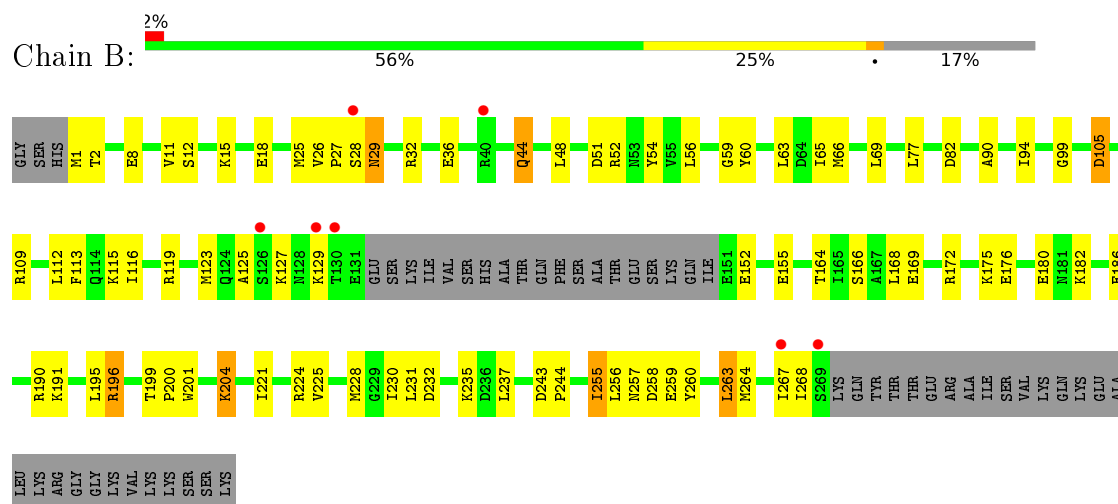
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	41	Total O 41 41	0	0
3	A	44	Total O 44 44	0	0
3	C	18	Total O 18 18	0	0

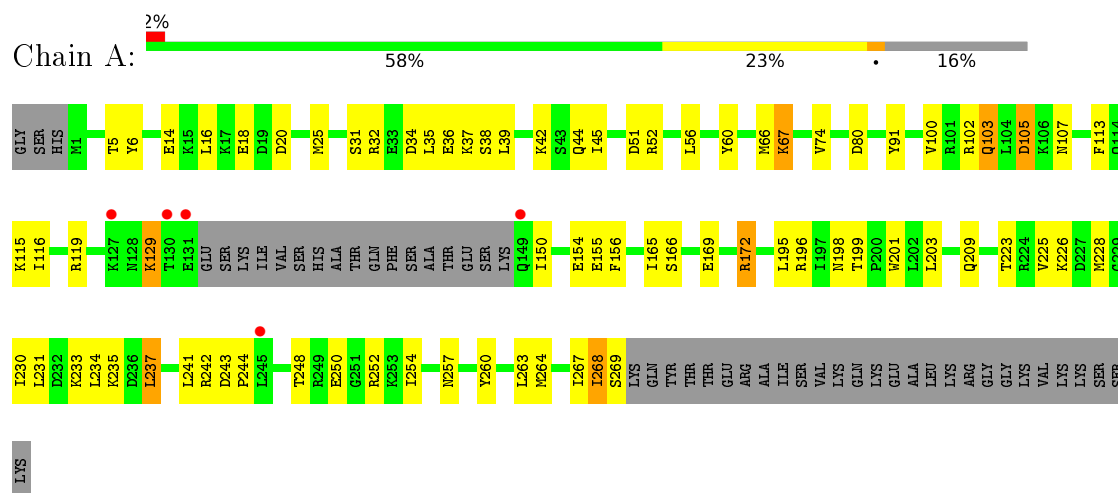
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: ParB domain protein nuclease

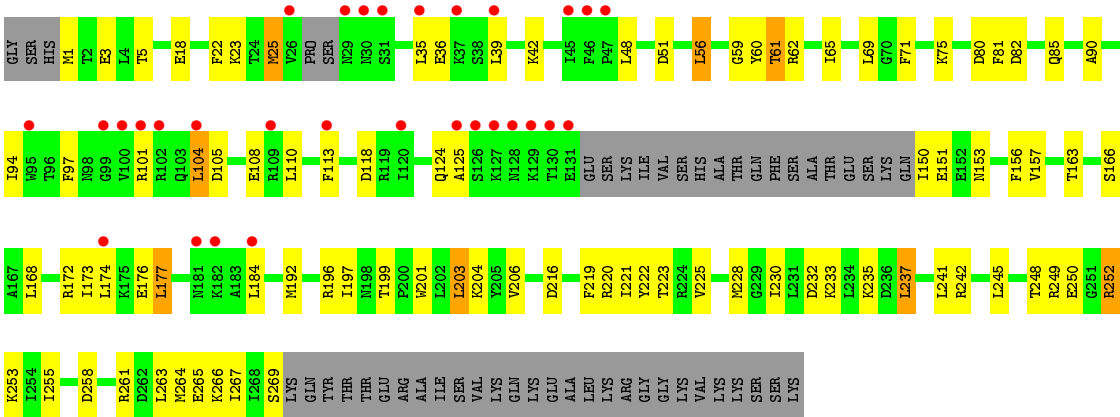


- Molecule 1: ParB domain protein nuclease



- Molecule 1: ParB domain protein nuclease





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.03 Å 98.70 Å 307.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.11 – 2.45 46.11 – 2.45	Depositor EDS
% Data completeness (in resolution range)	95.6 (46.11-2.45) 95.4 (46.11-2.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 2.45 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.222 , 0.262 0.217 , 0.258	Depositor DCC
$R_{free}$ test set	1998 reflections (5.21%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.5	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 53.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6407	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: CIT

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	0.24	0/2117	0.41	0/2828
1	B	0.25	0/2100	0.41	0/2805
1	C	0.23	0/2093	0.39	0/2793
All	All	0.24	0/6310	0.40	0/8426

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2097	0	2157	51	0
1	B	2080	0	2138	60	0
1	C	2075	0	2136	58	0
2	A	13	0	5	0	0
2	B	13	0	5	1	0
2	C	26	0	10	5	0
3	A	44	0	0	0	0
3	B	41	0	0	1	0
3	C	18	0	0	0	0
All	All	6407	0	6451	167	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 13.

All (167) 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:A:225:VAL:HG13	1:A:230:ILE:HG13	1.55	0.86
1:B:25:MSE:HE2	1:B:25:MSE:HA	1.63	0.81
1:B:152:GLU:HG3	1:B:168:LEU:HB2	1.64	0.77
1:B:18:GLU:HB2	1:B:60:TYR:HE2	1.49	0.75
1:B:225:VAL:HG13	1:B:230:ILE:HG13	1.67	0.75
1:A:115:LYS:O	1:A:119:ARG:HG2	1.88	0.74
1:C:225:VAL:HG13	1:C:230:ILE:HG13	1.70	0.74
1:A:18:GLU:HB2	1:A:60:TYR:HE2	1.54	0.73
1:A:105:ASP:OD1	1:A:105:ASP:C	2.28	0.72
1:C:242:ARG:HH12	2:C:301:CIT:H41	1.55	0.72
1:A:254:ILE:HG22	1:A:264:MSE:HG2	1.71	0.71
1:C:245:LEU:HG	1:C:255:ILE:HD11	1.74	0.70
1:C:5:THR:HG23	1:C:80:ASP:HB3	1.74	0.69
1:A:248:THR:HG22	1:A:250:GLU:H	1.57	0.68
1:C:18:GLU:HG3	1:C:60:TYR:HE2	1.58	0.68
1:B:123:MSE:O	1:B:127:LYS:HG2	1.93	0.68
1:B:200:PRO:O	1:B:204:LYS:HE2	1.94	0.67
1:A:228:MSE:HB2	1:A:230:ILE:HG12	1.77	0.66
1:C:48:LEU:HD22	1:C:59:GLY:HA3	1.75	0.66
1:B:263:LEU:O	1:B:267:ILE:HG12	1.97	0.65
1:B:169:GLU:HA	1:B:172:ARG:HE	1.63	0.64
1:B:112:LEU:O	1:B:116:ILE:HG12	1.98	0.63
1:C:225:VAL:CG1	1:C:230:ILE:HG13	2.29	0.63
1:A:150:ILE:O	1:A:154:GLU:HG2	1.99	0.62
1:C:62:ARG:HH12	1:C:101:ARG:HH12	1.49	0.60
1:B:255:ILE:HA	1:B:264:MSE:SE	2.51	0.60
1:A:225:VAL:HG21	1:A:234:LEU:HD22	1.83	0.60
1:A:105:ASP:OD1	1:A:107:ASN:N	2.35	0.59
1:B:224:ARG:HG2	1:B:255:ILE:HD12	1.85	0.59
1:B:232:ASP:OD2	1:A:52:ARG:HD2	2.03	0.58
1:A:169:GLU:HG2	1:A:172:ARG:NH2	2.19	0.58
1:B:169:GLU:O	1:B:172:ARG:HG2	2.04	0.58
1:C:61:THR:O	1:C:65:ILE:HD12	2.02	0.58
1:C:51:ASP:HB2	1:C:81:PHE:O	2.03	0.57
1:B:11:VAL:HG11	1:B:54:TYR:HE2	1.67	0.57
1:C:252:ARG:HG2	1:C:252:ARG:HH11	1.70	0.57
1:C:204:LYS:HB3	2:C:301:CIT:O1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:SER:HB3	1:A:103:GLN:HB3	1.87	0.56
1:B:18:GLU:HB2	1:B:60:TYR:CE2	2.35	0.56
1:C:228:MSE:HE1	1:C:264:MSE:SE	2.56	0.56
1:B:190:ARG:HG3	3:B:405:HOH:O	2.05	0.56
1:C:153:ASN:HB2	1:C:168:LEU:HD13	1.88	0.56
1:A:32:ARG:O	1:A:36:GLU:HB2	2.07	0.55
1:A:248:THR:O	1:A:252:ARG:HG3	2.07	0.55
1:B:180:GLU:HB3	1:B:182:LYS:HG3	1.88	0.54
1:B:255:ILE:HG13	1:B:256:LEU:N	2.23	0.53
1:C:62:ARG:NH1	2:C:302:CIT:H41	2.24	0.53
1:C:35:LEU:CD2	1:C:62:ARG:HG2	2.38	0.53
1:A:199:THR:O	1:A:199:THR:HG23	2.09	0.53
1:B:52:ARG:HH21	1:B:82:ASP:HB2	1.74	0.53
1:B:225:VAL:CG1	1:B:230:ILE:HG13	2.38	0.52
1:A:248:THR:HG22	1:A:250:GLU:N	2.25	0.52
1:A:155:GLU:HG2	1:A:198:ASN:OD1	2.10	0.52
1:C:261:ARG:O	1:C:265:GLU:HG2	2.08	0.52
1:B:169:GLU:HA	1:B:172:ARG:NE	2.26	0.51
1:C:248:THR:HB	1:C:250:GLU:OE1	2.10	0.51
1:B:196:ARG:O	1:B:196:ARG:HD3	2.10	0.51
1:C:216:ASP:O	1:C:220:ARG:HG3	2.11	0.51
1:A:237:LEU:HD22	1:A:241:LEU:HB2	1.93	0.51
1:B:152:GLU:OE2	1:B:168:LEU:HD13	2.10	0.51
1:C:110:LEU:HB3	1:C:192:MSE:HE1	1.92	0.51
1:C:22:PHE:O	1:C:25:MSE:HB2	2.11	0.51
1:B:115:LYS:O	1:B:119:ARG:HG2	2.11	0.51
1:B:59:GLY:HA2	2:B:301:CIT:O3	2.11	0.51
1:A:25:MSE:HE1	1:A:115:LYS:HB3	1.94	0.50
1:C:113:PHE:CE2	1:C:174:LEU:HD22	2.47	0.49
1:C:36:GLU:HA	1:C:39:LEU:HB2	1.92	0.49
1:A:201:TRP:CZ2	1:A:235:LYS:HB2	2.48	0.49
1:B:172:ARG:HA	1:B:175:LYS:HE2	1.95	0.49
1:B:172:ARG:O	1:B:176:GLU:HG3	2.13	0.49
1:C:97:PHE:O	1:C:101:ARG:HB2	2.13	0.49
1:C:173:ILE:O	1:C:177:LEU:HB2	2.12	0.49
1:C:237:LEU:HD22	1:C:241:LEU:HB2	1.94	0.49
1:A:263:LEU:O	1:A:267:ILE:HG12	2.12	0.49
1:B:257:ASN:HB3	1:B:259:GLU:HG2	1.95	0.48
1:A:37:LYS:HG3	1:A:38:SER:N	2.28	0.48
1:B:48:LEU:HD11	1:B:66:MSE:HE1	1.96	0.48
1:C:104:LEU:HD13	1:C:104:LEU:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:LEU:HD21	1:C:184:LEU:HD21	1.95	0.48
1:A:233:LYS:HB3	1:A:268:ILE:HG13	1.94	0.48
1:C:221:ILE:O	1:C:225:VAL:HG23	2.13	0.48
1:B:125:ALA:O	1:B:129:LYS:HB2	2.14	0.48
1:B:199:THR:HG23	1:B:199:THR:O	2.13	0.48
1:C:192:MSE:HG3	1:C:203:LEU:HD11	1.96	0.48
1:C:172:ARG:O	1:C:176:GLU:HG2	2.14	0.47
1:C:18:GLU:CD	1:C:23:LYS:HD2	2.33	0.47
1:C:203:LEU:HD23	1:C:206:VAL:HB	1.96	0.47
1:C:62:ARG:HH12	1:C:101:ARG:NH1	2.11	0.47
1:C:69:LEU:HD23	1:C:71:PHE:HE1	1.77	0.47
1:B:221:ILE:O	1:B:225:VAL:HG23	2.15	0.47
1:A:254:ILE:O	1:A:264:MSE:HG2	2.14	0.47
1:C:157:VAL:HG12	1:C:197:ILE:HG13	1.96	0.47
1:B:225:VAL:HG12	1:B:231:LEU:N	2.29	0.47
1:B:29:ASN:HD22	1:B:29:ASN:H	1.62	0.47
1:A:233:LYS:HD3	1:A:268:ILE:CG2	2.45	0.46
1:B:155:GLU:O	1:B:166:SER:HA	2.15	0.46
1:B:25:MSE:HA	1:B:25:MSE:CE	2.40	0.46
1:B:225:VAL:HG12	1:B:231:LEU:HA	1.97	0.46
1:C:263:LEU:O	1:C:267:ILE:HG12	2.15	0.46
1:A:165:ILE:CG1	1:A:169:GLU:HB2	2.46	0.45
1:C:1:MSE:C	1:C:3:GLU:H	2.20	0.45
1:C:156:PHE:CE2	1:C:166:SER:HB3	2.50	0.45
1:A:237:LEU:O	1:A:242:ARG:NH1	2.50	0.45
1:A:42:LYS:HD2	1:A:45:ILE:HD11	1.97	0.45
1:A:268:ILE:O	1:A:269:SER:HB2	2.16	0.45
1:C:201:TRP:CE2	1:C:235:LYS:HG3	2.52	0.45
1:C:82:ASP:OD1	1:C:85:GLN:HB2	2.17	0.45
1:A:243:ASP:N	1:A:244:PRO:HD2	2.31	0.45
1:A:257:ASN:HB3	1:A:260:TYR:HD1	1.82	0.45
1:C:104:LEU:HB2	1:C:108:GLU:HB3	1.98	0.44
1:C:65:ILE:O	1:C:69:LEU:HB2	2.18	0.44
1:B:259:GLU:HG3	1:B:260:TYR:CE1	2.53	0.44
1:B:221:ILE:HA	1:B:255:ILE:HD11	2.00	0.44
1:B:1:MSE:HE3	1:B:2:THR:O	2.17	0.44
1:C:199:THR:O	1:C:199:THR:HG23	2.17	0.44
1:B:225:VAL:CG1	1:B:231:LEU:HA	2.48	0.44
1:C:219:PHE:O	1:C:222:TYR:HB3	2.17	0.44
1:A:223:THR:HA	1:A:226:LYS:HE3	2.00	0.44
1:B:52:ARG:NH2	1:B:82:ASP:HB2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:ILE:HG22	1:C:151:GLU:N	2.33	0.44
1:C:228:MSE:SE	1:C:264:MSE:HE1	2.68	0.43
1:B:201:TRP:CZ2	1:B:235:LYS:HB2	2.54	0.43
1:B:36:GLU:HA	1:B:65:ILE:HG21	1.99	0.43
1:B:237:LEU:HD11	1:B:268:ILE:HG22	1.99	0.43
1:B:99:GLY:O	1:B:109:ARG:HD3	2.18	0.43
1:A:234:LEU:O	1:A:237:LEU:HB2	2.17	0.43
1:C:125:ALA:HB2	1:C:163:THR:HG23	2.00	0.43
1:A:225:VAL:HG12	1:A:231:LEU:HA	2.01	0.43
1:B:26:VAL:HA	1:B:27:PRO:HD3	1.85	0.43
1:C:221:ILE:HD11	1:C:252:ARG:CD	2.49	0.43
1:A:233:LYS:HD3	1:A:268:ILE:HG21	2.01	0.43
1:B:105:ASP:O	1:B:109:ARG:HG3	2.18	0.43
1:A:257:ASN:HB3	1:A:260:TYR:CD1	2.54	0.43
1:A:129:LYS:NZ	1:A:129:LYS:HB2	2.33	0.43
1:A:195:LEU:HA	1:A:199:THR:HG22	2.00	0.43
1:C:252:ARG:HG2	1:C:252:ARG:NH1	2.34	0.43
1:C:266:LYS:O	1:C:269:SER:HB3	2.19	0.43
1:C:62:ARG:HG3	2:C:302:CIT:O3	2.19	0.43
1:C:242:ARG:HH12	2:C:301:CIT:C4	2.29	0.42
1:C:249:ARG:O	1:C:253:LYS:HG3	2.18	0.42
1:B:12:SER:OG	1:B:15:LYS:HG3	2.19	0.42
1:A:14:GLU:OE2	1:A:67:LYS:HD2	2.19	0.42
1:B:25:MSE:HE1	1:B:119:ARG:NH2	2.35	0.42
1:B:186:GLU:OE2	1:B:186:GLU:HA	2.20	0.42
1:A:91:TYR:CE1	1:A:119:ARG:HB3	2.54	0.42
1:B:191:LYS:O	1:B:195:LEU:HG	2.19	0.42
1:A:25:MSE:HE2	1:A:116:ILE:CD1	2.50	0.42
1:B:243:ASP:HB2	1:B:244:PRO:HD3	2.01	0.42
1:B:90:ALA:O	1:B:94:ILE:HG13	2.20	0.42
1:A:156:PHE:CE2	1:A:166:SER:HB3	2.55	0.41
1:B:44:GLN:HG2	1:B:66:MSE:SE	2.70	0.41
1:C:241:LEU:N	1:C:241:LEU:HD22	2.35	0.41
1:A:129:LYS:HD3	1:A:129:LYS:HA	1.90	0.41
1:B:164:THR:HG21	1:A:6:TYR:OH	2.20	0.41
1:C:56:LEU:HB3	1:C:60:TYR:CZ	2.55	0.41
1:A:51:ASP:OD1	1:A:51:ASP:C	2.59	0.41
1:A:5:THR:HG23	1:A:80:ASP:HB3	2.02	0.41
1:A:230:ILE:HG22	1:A:233:LYS:HD2	2.02	0.41
1:A:44:GLN:OE1	1:A:74:VAL:HG23	2.21	0.41
1:C:237:LEU:HB3	1:C:242:ARG:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:ASP:HB2	1:B:244:PRO:CD	2.51	0.41
1:B:63:LEU:HA	1:B:66:MSE:CE	2.51	0.41
1:A:39:LEU:HD13	1:A:66:MSE:HG3	2.03	0.40
1:B:228:MSE:SE	1:B:264:MSE:HE1	2.72	0.40
1:A:100:VAL:O	1:A:100:VAL:HG12	2.20	0.40
1:C:90:ALA:O	1:C:94:ILE:HG13	2.21	0.40
1:B:8:GLU:HB3	1:B:77:LEU:CD2	2.51	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	248/300 (83%)	233 (94%)	15 (6%)	0	100	100
1	B	246/300 (82%)	236 (96%)	10 (4%)	0	100	100
1	C	243/300 (81%)	222 (91%)	21 (9%)	0	100	100
All	All	737/900 (82%)	691 (94%)	46 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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	234/268 (87%)	217 (93%)	17 (7%)	17	23
1	B	232/268 (87%)	218 (94%)	14 (6%)	24	33
1	C	231/268 (86%)	213 (92%)	18 (8%)	16	20
All	All	697/804 (87%)	648 (93%)	49 (7%)	19	25

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	28	SER
1	B	29	ASN
1	B	32	ARG
1	B	44	GLN
1	B	51	ASP
1	B	56	LEU
1	B	69	LEU
1	B	105	ASP
1	B	113	PHE
1	B	196	ARG
1	B	204	LYS
1	B	255	ILE
1	B	258	ASP
1	B	263	LEU
1	A	16	LEU
1	A	20	ASP
1	A	34	ASP
1	A	35	LEU
1	A	56	LEU
1	A	67	LYS
1	A	102	ARG
1	A	103	GLN
1	A	105	ASP
1	A	113	PHE
1	A	129	LYS
1	A	172	ARG
1	A	196	ARG
1	A	203	LEU
1	A	209	GLN
1	A	237	LEU
1	A	268	ILE
1	C	25	MSE
1	C	42	LYS
1	C	56	LEU

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Mol	Chain	Res	Type
1	C	61	THR
1	C	75	LYS
1	C	104	LEU
1	C	105	ASP
1	C	118	ASP
1	C	124	GLN
1	C	177	LEU
1	C	196	ARG
1	C	203	LEU
1	C	223	THR
1	C	232	ASP
1	C	233	LYS
1	C	237	LEU
1	C	252	ARG
1	C	258	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	GLN
1	A	128	ASN
1	C	198	ASN
1	C	217	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.



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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	CIT	A	301	-	3,12,12	1.51	0	3,17,17	1.22	0
2	CIT	B	301	-	3,12,12	1.45	0	3,17,17	3.63	1 (33%)
2	CIT	C	301	-	3,12,12	1.31	0	3,17,17	2.98	2 (66%)
2	CIT	C	302	-	3,12,12	1.42	0	3,17,17	2.94	2 (66%)

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	CIT	A	301	-	-	0/6/16/16	0/0/0/0
2	CIT	B	301	-	-	0/6/16/16	0/0/0/0
2	CIT	C	301	-	-	0/6/16/16	0/0/0/0
2	CIT	C	302	-	-	0/6/16/16	0/0/0/0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	CIT	C3-C4-C5	-5.96	105.63	114.95
2	C	302	CIT	C3-C4-C5	-4.49	107.94	114.95
2	C	301	CIT	C3-C2-C1	-4.08	108.58	114.95
2	C	301	CIT	C3-C4-C5	-3.14	110.05	114.95
2	C	302	CIT	C3-C2-C1	-2.41	111.19	114.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	CIT	1	0
2	C	301	CIT	3	0
2	C	302	CIT	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	245/300 (81%)	0.39	5 (2%) 68 71	31, 50, 85, 127	0
1	B	243/300 (81%)	0.50	7 (2%) 55 58	29, 49, 86, 139	0
1	C	242/300 (80%)	0.87	30 (12%) 5 5	37, 68, 116, 149	0
All	All	730/900 (81%)	0.59	42 (5%) 26 29	29, 54, 102, 149	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	30	ASN	6.1
1	C	29	ASN	5.9
1	C	130	THR	5.8
1	B	129	LYS	5.6
1	A	130	THR	5.2
1	B	269	SER	5.2
1	C	131	GLU	5.2
1	C	127	LYS	4.7
1	C	35	LEU	4.5
1	B	130	THR	4.4
1	C	182	LYS	4.3
1	C	37	LYS	4.0
1	C	129	LYS	4.0
1	B	267	ILE	3.9
1	C	104	LEU	3.8
1	C	101	ARG	3.4
1	C	102	ARG	3.2
1	C	46	PHE	3.1
1	C	45	ILE	3.1
1	A	127	LYS	2.9
1	C	128	ASN	2.9
1	C	184	LEU	2.9
1	C	39	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	99	GLY	2.7
1	C	125	ALA	2.7
1	C	126	SER	2.6
1	A	149	GLN	2.6
1	C	100	VAL	2.6
1	A	131	GLU	2.5
1	B	28	SER	2.5
1	C	47	PRO	2.4
1	C	113	PHE	2.4
1	C	174	LEU	2.3
1	C	26	VAL	2.2
1	C	181	ASN	2.2
1	C	31	SER	2.1
1	A	245	LEU	2.1
1	C	120	ILE	2.1
1	C	109	ARG	2.1
1	C	95	TRP	2.0
1	B	40	ARG	2.0
1	B	126	SER	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 carbohydrates 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. 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	CIT	C	302	13/13	0.76	0.49	2.39	129,139,144,146	0
2	CIT	C	301	13/13	0.83	0.22	1.18	74,78,85,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CIT	A	301	13/13	0.90	0.18	0.11	42,49,56,58	0
2	CIT	B	301	13/13	0.84	0.18	-0.33	55,65,76,85	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.