



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 6, 2023 – 05:22 pm BST

PDB ID : 8BBY  
Title : VarB H/L (SLPL/SLPH) complex from *C. difficile* SlpA (R20291 strain)  
Authors : Barwinska-Sendra, A.; Salgado, P.S.  
Deposited on : 2022-10-14  
Resolution : 2.90 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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  
Xtrriage (Phenix) : 1.13  
EDS : 2.34  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.34

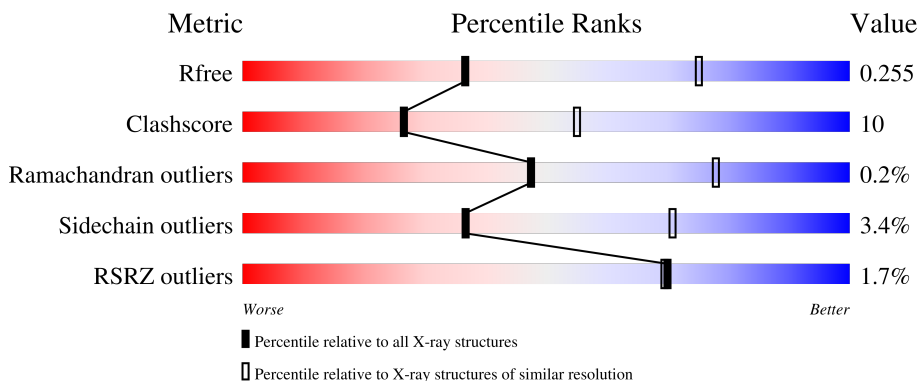
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	320	
1	C	320	
2	B	416	
2	D	416	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 8384 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 S-layer protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	143	1133	718	186	227	2	0	0	0
1	C	131	1045	661	172	210	2	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	LEU	ALA	conflict	UNP B3GV24
A	61	VAL	GLU	conflict	UNP B3GV24
A	62	GLN	ASP	conflict	UNP B3GV24
A	63	LYS	ALA	conflict	UNP B3GV24
A	64	MET	SER	conflict	UNP B3GV24
A	65	GLN	LYS	conflict	UNP B3GV24
A	66	VAL	LEU	conflict	UNP B3GV24
A	67	ASN	-	insertion	UNP B3GV24
A	68	TYR	-	insertion	UNP B3GV24
A	69	CYS	LEU	conflict	UNP B3GV24
A	70	LEU	PHE	conflict	UNP B3GV24
A	71	HIS	THR	conflict	UNP B3GV24
A	72	LYS	GLN	conflict	UNP B3GV24
C	60	LEU	ALA	conflict	UNP B3GV24
C	61	VAL	GLU	conflict	UNP B3GV24
C	62	GLN	ASP	conflict	UNP B3GV24
C	63	LYS	ALA	conflict	UNP B3GV24
C	64	MET	SER	conflict	UNP B3GV24
C	65	GLN	LYS	conflict	UNP B3GV24
C	66	VAL	LEU	conflict	UNP B3GV24
C	67	ASN	-	insertion	UNP B3GV24
C	68	TYR	-	insertion	UNP B3GV24
C	69	CYS	LEU	conflict	UNP B3GV24
C	70	LEU	PHE	conflict	UNP B3GV24
C	71	HIS	THR	conflict	UNP B3GV24

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Chain	Residue	Modelled	Actual	Comment	Reference
C	72	LYS	GLN	conflict	UNP B3GV24

- Molecule 2 is a protein called S-layer protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	416	Total	C	N	O	S	0	0	0
			3100	1910	525	660	5			
2	D	412	Total	C	N	O	S	0	0	0
			3072	1893	520	655	4			

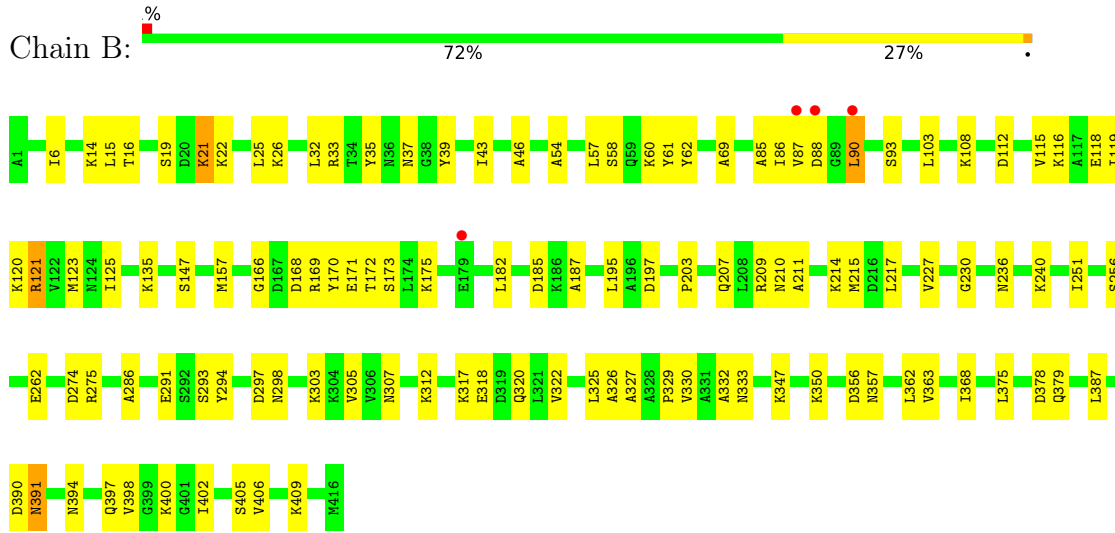
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		

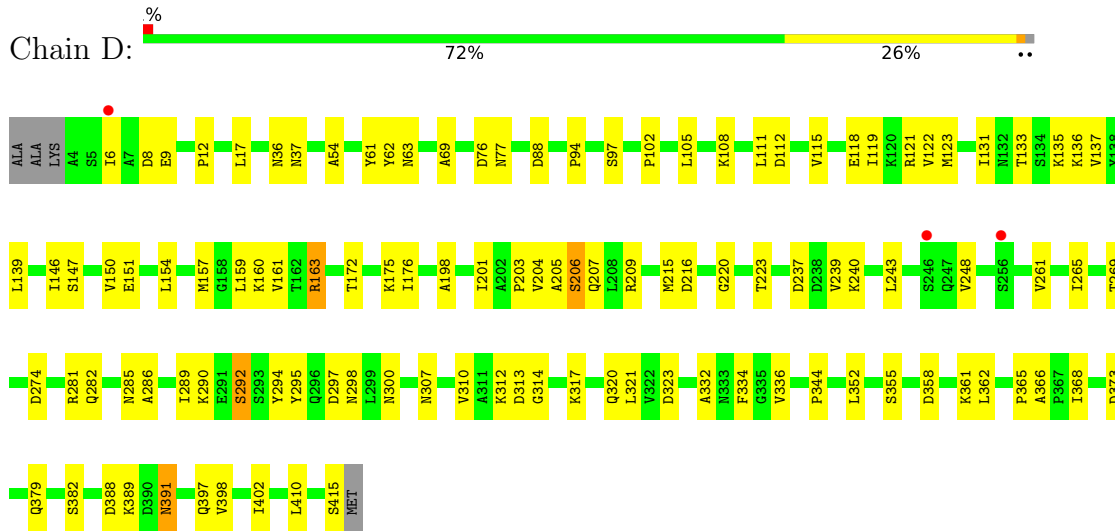
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	B	13	Total	O	0	0
			13	13		
4	C	1	Total	O	0	0
			1	1		
4	D	15	Total	O	0	0
			15	15		





• Molecule 2: S-layer protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.93Å 131.29Å 138.27Å 90.00° 108.78° 90.00°	Depositor
Resolution (Å)	36.23 – 2.90 37.21 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.8 (36.23-2.90) 88.7 (37.21-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 2.90Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.244 , 0.287 0.248 , 0.255	Depositor DCC
$R_{free}$ test set	1951 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.3	Xtrriage
Anisotropy	1.253	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 27.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	8384	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.58% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.25	0/1143	0.47	0/1534
1	C	0.26	0/1054	0.50	0/1413
2	B	0.25	0/3125	0.48	0/4221
2	D	0.24	0/3097	0.45	0/4186
All	All	0.25	0/8419	0.47	0/11354

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 [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	1133	0	1145	19	0
1	C	1045	0	1044	26	0
2	B	3100	0	3119	75	0
2	D	3072	0	3084	67	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	3	0	0	0	0
4	B	13	0	0	1	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	15	0	0	0	0
All	All	8384	0	8392	173	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 10.

All (173) 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:347:LYS:HD2	2:B:347:LYS:H	1.29	0.96
1:C:76:LYS:O	1:C:79:ASN:ND2	2.15	0.80
2:B:87:VAL:HG21	2:B:169:ARG:NE	1.97	0.80
2:B:197:ASP:HB3	2:B:251:ILE:HG22	1.65	0.79
2:B:86:ILE:HD13	2:B:322:VAL:HG12	1.66	0.78
2:B:182:LEU:HD21	2:B:187:ALA:HB2	1.67	0.75
2:D:312:LYS:HG2	2:D:320:GLN:HE21	1.54	0.73
1:A:255:THR:HG23	2:B:16:THR:HB	1.71	0.72
2:D:63:ASN:ND2	2:D:121:ARG:O	2.22	0.72
2:B:19:SER:HB3	2:B:25:LEU:HD23	1.74	0.69
1:C:73:VAL:O	1:C:77:LEU:N	2.17	0.67
2:B:118:GLU:OE1	2:B:121:ARG:NH1	2.28	0.67
2:B:375:LEU:HB2	2:B:406:VAL:HG13	1.75	0.67
1:A:12:GLN:H	1:A:12:GLN:CD	1.98	0.67
2:D:312:LYS:HG2	2:D:320:GLN:NE2	2.10	0.66
2:D:282:GLN:NE2	2:D:379:GLN:OE1	2.28	0.66
2:B:33:ARG:O	2:B:37:ASN:ND2	2.29	0.66
2:B:347:LYS:H	2:B:347:LYS:CD	2.05	0.66
2:B:327:ALA:HB2	2:B:398:VAL:HG11	1.78	0.65
2:B:209:ARG:HH22	2:B:294:TYR:HA	1.61	0.65
1:C:9:THR:HA	2:D:6:ILE:HD11	1.78	0.65
2:D:215:MET:HE3	2:D:298:ASN:HB2	1.78	0.65
1:A:17:VAL:HG12	1:A:19:SER:H	1.61	0.64
2:B:326:ALA:O	4:B:601:HOH:O	2.15	0.64
2:D:139:LEU:HD22	2:D:146:ILE:HG21	1.80	0.64
1:C:247:ARG:NH1	2:D:9:GLU:HB3	2.14	0.62
1:A:310:TYR:CZ	2:B:14:LYS:HG3	2.34	0.62
1:C:283:LEU:HD22	1:C:309:LEU:HD21	1.81	0.61
2:B:357:ASN:HA	2:B:362:LEU:HD21	1.82	0.61
2:B:87:VAL:HG21	2:B:169:ARG:CZ	2.30	0.61
1:C:41:LYS:HB3	1:C:43:PHE:CZ	2.37	0.60
2:D:137:VAL:HG11	2:D:154:LEU:HD13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:VAL:CG2	2:B:169:ARG:HG3	2.32	0.60
2:B:85:ALA:HB1	2:B:88:ASP:HB2	1.86	0.58
1:C:48:LEU:HD12	1:C:49:ALA:H	1.70	0.57
1:C:311:PRO:HG2	2:D:12:PRO:HD2	1.87	0.57
1:C:17:VAL:HG12	1:C:19:SER:H	1.70	0.56
1:C:16:VAL:HG13	1:C:248:ILE:HG23	1.87	0.56
2:B:347:LYS:HD2	2:B:347:LYS:N	2.12	0.56
2:B:108:LYS:O	2:B:147:SER:OG	2.22	0.56
2:B:58:SER:HA	2:B:62:TYR:HD2	1.72	0.55
1:A:267:GLN:HG3	2:B:35:TYR:HD1	1.72	0.55
2:B:168:ASP:OD1	2:B:170:TYR:N	2.39	0.55
2:D:397:GLN:HG3	2:D:402:ILE:HD12	1.89	0.55
2:B:125:ILE:HD11	2:B:135:LYS:HG3	1.89	0.54
1:C:306:GLN:HA	2:D:17:LEU:O	2.07	0.54
2:B:90:LEU:HD13	2:B:195:LEU:HD22	1.89	0.54
2:B:217:LEU:HD21	2:B:363:VAL:HG21	1.90	0.54
2:D:203:PRO:HB2	2:D:295:TYR:HE2	1.73	0.54
2:B:207:GLN:HA	2:B:332:ALA:HB1	1.90	0.54
2:B:317:LYS:HB3	2:B:320:GLN:HE21	1.73	0.54
1:A:267:GLN:HG3	2:B:35:TYR:CD1	2.42	0.53
1:C:44:PHE:O	1:C:46:GLY:N	2.41	0.53
2:D:151:GLU:HG3	2:D:161:VAL:HG11	1.89	0.53
2:D:336:VAL:HG23	2:D:362:LEU:HD23	1.90	0.53
1:A:283:LEU:HD11	1:A:307:VAL:HG11	1.90	0.53
2:D:344:PRO:HB2	2:D:352:LEU:HD12	1.90	0.53
2:D:313:ASP:O	2:D:321:LEU:HD21	2.09	0.53
2:B:329:PRO:O	2:B:333:ASN:ND2	2.42	0.52
2:B:46:ALA:HB1	2:B:400:LYS:HG2	1.91	0.52
2:B:87:VAL:HG22	2:B:169:ARG:HG3	1.91	0.52
2:B:21:LYS:HE3	2:B:22:LYS:H	1.75	0.52
2:D:172:THR:O	2:D:176:ILE:HG13	2.10	0.52
2:D:239:VAL:O	2:D:243:LEU:HG	2.09	0.52
2:D:237:ASP:HA	2:D:240:LYS:HD3	1.91	0.52
2:B:262:GLU:HB2	2:B:275:ARG:HH21	1.75	0.52
1:C:281:ASN:O	1:C:285:ARG:HG3	2.09	0.51
2:B:195:LEU:HD12	2:B:318:GLU:HG3	1.93	0.51
1:A:77:LEU:HA	1:A:80:LEU:HG	1.93	0.51
1:A:16:VAL:HB	1:A:248:ILE:HG12	1.93	0.50
2:D:62:TYR:CG	2:D:102:PRO:HB3	2.47	0.50
2:D:76:ASP:HA	2:D:135:LYS:HD2	1.92	0.50
1:A:5:SER:O	1:A:5:SER:OG	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:203:PRO:HG2	2:B:368:ILE:HB	1.92	0.50
2:D:118:GLU:O	2:D:122:VAL:HG22	2.11	0.50
2:D:198:ALA:HA	2:D:201:ILE:HG22	1.94	0.49
2:D:94:PRO:HA	2:D:206:SER:HA	1.95	0.49
1:A:43:PHE:HB2	1:A:87:ASP:HB2	1.94	0.49
1:C:283:LEU:HD11	1:C:307:VAL:HG21	1.95	0.49
2:D:61:TYR:HA	2:D:69:ALA:HA	1.95	0.49
2:D:292:SER:O	2:D:297:ASP:HB2	2.13	0.49
2:B:215:MET:HE2	2:B:298:ASN:HB2	1.95	0.49
2:D:307:ASN:HB2	2:D:366:ALA:HB2	1.95	0.49
2:B:291:GLU:OE2	2:B:293:SER:N	2.45	0.48
2:B:397:GLN:HG3	2:B:402:ILE:HD12	1.95	0.48
2:D:265:ILE:O	2:D:269:THR:OG1	2.27	0.48
2:B:123:MET:SD	2:B:135:LYS:HB3	2.53	0.48
1:C:256:ILE:HD12	1:C:264:LYS:HB2	1.96	0.48
2:D:157:MET:HE2	2:D:159:LEU:HD11	1.96	0.48
2:B:171:GLU:O	2:B:175:LYS:HG2	2.14	0.47
2:B:203:PRO:HG3	2:B:368:ILE:HD12	1.95	0.47
2:D:323:ASP:HB3	2:D:398:VAL:HG12	1.96	0.47
2:B:210:ASN:OD1	2:B:211:ALA:N	2.47	0.47
1:A:16:VAL:O	1:A:248:ILE:HA	2.14	0.47
1:C:4:MET:HG2	1:C:5:SER:H	1.78	0.47
2:D:216:ASP:HB3	2:D:220:GLY:HA3	1.97	0.47
2:B:116:LYS:HG2	2:B:120:LYS:HE3	1.97	0.46
2:D:8:ASP:O	2:D:9:GLU:HG2	2.16	0.46
2:D:77:ASN:HA	2:D:136:LYS:O	2.16	0.46
1:C:301:VAL:HB	1:C:306:GLN:HE21	1.80	0.46
2:D:131:ILE:HG13	2:D:133:THR:HG23	1.97	0.46
2:D:133:THR:O	2:D:160:LYS:HE3	2.16	0.46
2:B:307:ASN:OD1	2:B:394:ASN:HB2	2.16	0.45
1:A:287:LEU:HB3	2:B:26:LYS:HB2	1.98	0.45
1:C:252:LYS:HG2	1:C:253:GLU:N	2.32	0.45
2:B:286:ALA:HB2	2:B:379:GLN:HG3	1.98	0.44
2:B:312:LYS:HE3	2:B:320:GLN:HB3	1.99	0.44
2:D:248:VAL:HG11	2:D:265:ILE:HD13	1.99	0.44
2:B:112:ASP:HB2	2:B:115:VAL:HG23	1.98	0.44
1:C:77:LEU:HD11	1:C:248:ILE:HD12	1.98	0.44
2:D:358:ASP:HB3	2:D:361:LYS:HG3	2.00	0.44
2:D:108:LYS:O	2:D:147:SER:OG	2.22	0.44
2:D:310:VAL:HG13	2:D:397:GLN:HA	2.00	0.44
2:B:214:LYS:HE2	2:B:297:ASP:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:323:ASP:N	2:D:323:ASP:OD1	2.50	0.44
1:A:21:TYR:CD1	1:A:77:LEU:HD13	2.53	0.44
2:D:150:VAL:O	2:D:154:LEU:HG	2.18	0.44
2:D:285:ASN:O	2:D:289:ILE:HG13	2.17	0.44
1:A:254:GLU:O	2:B:15:LEU:HA	2.18	0.44
2:B:350:LYS:HA	2:B:350:LYS:HD2	1.73	0.44
2:B:390:ASP:O	2:B:391:ASN:HB2	2.17	0.44
2:B:61:TYR:HD1	2:B:69:ALA:HA	1.83	0.43
2:D:286:ALA:O	2:D:290:LYS:HG3	2.18	0.43
2:D:175:LYS:HD3	2:D:175:LYS:HA	1.72	0.43
2:D:204:VAL:HG11	2:D:294:TYR:CD1	2.53	0.43
1:A:28:LEU:HD23	1:A:40:ILE:HG21	2.00	0.43
2:B:298:ASN:OD1	2:B:298:ASN:N	2.50	0.43
1:C:285:ARG:HB3	1:C:291:GLU:HB2	2.01	0.43
2:D:139:LEU:HB2	2:D:163:ARG:HG3	2.00	0.43
2:D:205:ALA:HB1	2:D:223:THR:O	2.19	0.43
2:B:57:LEU:HD12	2:B:330:VAL:HG21	2.01	0.43
2:B:115:VAL:O	2:B:119:ILE:HG13	2.19	0.43
2:D:54:ALA:HB2	2:D:105:LEU:HD22	1.99	0.43
2:B:236:ASN:O	2:B:240:LYS:HG3	2.19	0.43
1:C:43:PHE:CE1	1:C:47:THR:HG23	2.54	0.42
1:C:258:ILE:HA	1:C:263:SER:HB2	2.01	0.42
1:C:315:ARG:NH2	2:D:36:ASN:OD1	2.51	0.42
2:D:388:ASP:OD1	2:D:389:LYS:N	2.52	0.42
1:A:48:LEU:HD12	1:A:48:LEU:HA	1.68	0.42
2:D:332:ALA:HA	2:D:365:PRO:HB3	2.00	0.42
1:A:8:GLU:C	2:B:6:ILE:HD11	2.40	0.42
1:A:266:ALA:HB1	2:B:32:LEU:HA	2.02	0.42
2:D:111:LEU:HB2	2:D:150:VAL:HG13	2.01	0.42
2:B:375:LEU:HD23	2:B:409:LYS:HG2	2.02	0.42
2:D:112:ASP:HB2	2:D:115:VAL:HG23	2.00	0.42
2:D:203:PRO:HG3	2:D:368:ILE:HD12	2.01	0.42
2:D:410:LEU:HD23	2:D:410:LEU:HA	1.83	0.42
2:B:37:ASN:N	2:B:37:ASN:HD22	2.18	0.41
2:B:305:VAL:O	2:B:387:LEU:HD12	2.20	0.41
2:B:230:GLY:HA3	2:B:256:SER:O	2.20	0.41
2:D:286:ALA:HB1	2:D:382:SER:OG	2.20	0.41
2:D:314:GLY:HA2	2:D:317:LYS:O	2.19	0.41
2:D:391:ASN:ND2	2:D:415:SER:O	2.53	0.41
2:B:87:VAL:CG2	2:B:169:ARG:NE	2.76	0.41
2:B:93:SER:OG	2:B:325:LEU:HD23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:207:GLN:OE1	2:D:209:ARG:NH2	2.53	0.41
2:B:86:ILE:O	2:B:90:LEU:HB2	2.21	0.41
2:D:119:ILE:O	2:D:123:MET:HG3	2.21	0.41
2:D:261:VAL:O	2:D:265:ILE:HG13	2.20	0.41
2:B:43:ILE:HG21	2:B:60:LYS:HE3	2.03	0.41
2:D:207:GLN:HB3	2:D:215:MET:HE1	2.01	0.41
2:D:355:SER:O	2:D:361:LYS:NZ	2.50	0.41
2:B:119:ILE:O	2:B:123:MET:HB2	2.20	0.41
2:B:303:LYS:HA	2:B:303:LYS:HD3	1.92	0.41
1:C:314:LYS:CE	2:D:12:PRO:HB3	2.51	0.41
2:D:215:MET:HB2	2:D:300:ASN:ND2	2.35	0.41
2:B:166:GLY:N	2:B:172:THR:OG1	2.50	0.40
2:B:262:GLU:HB2	2:B:275:ARG:NH2	2.36	0.40
1:C:309:LEU:HD23	1:C:309:LEU:HA	1.78	0.40
2:D:136:LYS:HG2	2:D:160:LYS:HB2	2.03	0.40
1:C:82:ASP:HA	1:C:250:ASN:HB3	2.03	0.40
2:B:54:ALA:HB1	2:B:103:LEU:O	2.22	0.40
2:B:116:LYS:HG3	2:B:157:MET:SD	2.62	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	135/320 (42%)	131 (97%)	4 (3%)	0	100	100
1	C	121/320 (38%)	114 (94%)	6 (5%)	1 (1%)	19	51
2	B	414/416 (100%)	403 (97%)	10 (2%)	1 (0%)	47	78
2	D	410/416 (99%)	397 (97%)	13 (3%)	0	100	100
All	All	1080/1472 (73%)	1045 (97%)	33 (3%)	2 (0%)	47	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	391	ASN
1	C	45	GLU

### 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	126/269 (47%)	123 (98%)	3 (2%)	49 79
1	C	116/269 (43%)	109 (94%)	7 (6%)	19 49
2	B	347/347 (100%)	336 (97%)	11 (3%)	39 73
2	D	345/347 (99%)	334 (97%)	11 (3%)	39 73
All	All	934/1232 (76%)	902 (97%)	32 (3%)	37 71

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	68	TYR
1	A	78	ASP
2	B	21	LYS
2	B	39	TYR
2	B	90	LEU
2	B	121	ARG
2	B	173	SER
2	B	185	ASP
2	B	227	VAL
2	B	274	ASP
2	B	356	ASP
2	B	378	ASP
2	B	405	SER
1	C	8	GLU
1	C	18	GLN
1	C	23	LYS
1	C	75	ASN
1	C	78	ASP
1	C	249	LEU

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Mol	Chain	Res	Type
1	C	250	ASN
2	D	37	ASN
2	D	88	ASP
2	D	97	SER
2	D	163	ARG
2	D	206	SER
2	D	274	ASP
2	D	281	ARG
2	D	292	SER
2	D	334	PHE
2	D	373	ASP
2	D	391	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	ASN
2	B	37	ASN
2	B	59	GLN
2	B	68	ASN
1	C	79	ASN
1	C	306	GLN
2	D	320	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	143/320 (44%)	0.15	4 (2%) 53 49	33, 63, 95, 116	0
1	C	131/320 (40%)	0.37	8 (6%) 21 17	39, 74, 103, 130	0
2	B	416/416 (100%)	0.05	4 (0%) 82 82	19, 44, 74, 117	0
2	D	412/416 (99%)	0.05	3 (0%) 87 87	20, 48, 79, 115	0
All	All	1102/1472 (74%)	0.10	19 (1%) 70 69	19, 51, 89, 130	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	89	LEU	3.4
1	C	90	ILE	3.1
2	B	88	ASP	3.0
1	C	79	ASN	3.0
1	C	254	GLU	2.9
1	C	40	ILE	2.5
2	D	6	ILE	2.5
1	C	286	VAL	2.4
2	D	256	SER	2.4
1	C	298	VAL	2.4
1	A	292	ALA	2.3
1	C	68	TYR	2.3
1	A	30	LYS	2.3
2	B	90	LEU	2.2
1	A	40	ILE	2.2
1	A	51	THR	2.2
2	B	179	GLU	2.2
2	B	87	VAL	2.1
2	D	246	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 monosaccharides 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	NA	D	501	1/1	0.90	0.32	33,33,33,33	0
3	NA	B	501	1/1	0.94	0.24	46,46,46,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.