



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 02:20 AM EDT

PDB ID : 5ULE  
Title : Structure and function of the divalent anion/Na<sup>+</sup> symporter from *Vibrio cholerae* and a humanized variant  
Authors : Lu, M.  
Deposited on : 2017-01-24  
Resolution : 2.80 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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

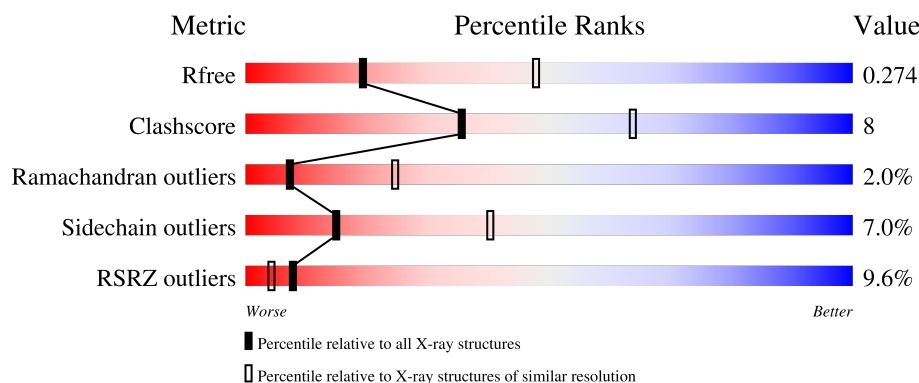
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	445	
1	B	445	
1	C	445	
1	D	445	

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	NA	B	502	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13436 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 Transporter, NadC family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3349	2234	523	566	26			
1	B	445	Total	C	N	O	S	0	0	0
			3349	2234	523	566	26			
1	C	445	Total	C	N	O	S	0	0	0
			3349	2234	523	566	26			
1	D	445	Total	C	N	O	S	0	0	0
			3349	2234	523	566	26			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	200	THR	SER	conflict	UNP Q9KNE0
A	201	GLY	PRO	conflict	UNP Q9KNE0
A	322	ILE	VAL	conflict	UNP Q9KNE0
A	376	THR	ALA	conflict	UNP Q9KNE0
A	379	VAL	THR	conflict	UNP Q9KNE0
A	381	THR	SER	conflict	UNP Q9KNE0
A	382	THR	ALA	conflict	UNP Q9KNE0
A	383	THR	ALA	conflict	UNP Q9KNE0
B	200	THR	SER	conflict	UNP Q9KNE0
B	201	GLY	PRO	conflict	UNP Q9KNE0
B	322	ILE	VAL	conflict	UNP Q9KNE0
B	376	THR	ALA	conflict	UNP Q9KNE0
B	379	VAL	THR	conflict	UNP Q9KNE0
B	381	THR	SER	conflict	UNP Q9KNE0
B	382	THR	ALA	conflict	UNP Q9KNE0
B	383	THR	ALA	conflict	UNP Q9KNE0
C	200	THR	SER	conflict	UNP Q9KNE0
C	201	GLY	PRO	conflict	UNP Q9KNE0
C	322	ILE	VAL	conflict	UNP Q9KNE0
C	376	THR	ALA	conflict	UNP Q9KNE0
C	379	VAL	THR	conflict	UNP Q9KNE0

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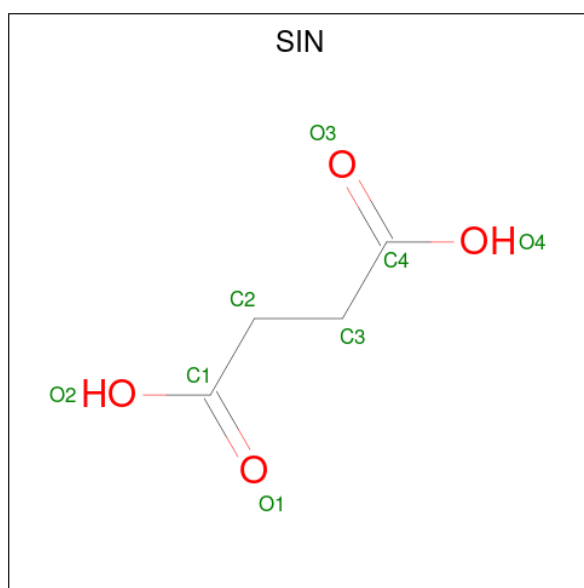
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Chain	Residue	Modelled	Actual	Comment	Reference
C	381	THR	SER	conflict	UNP Q9KNE0
C	382	THR	ALA	conflict	UNP Q9KNE0
C	383	THR	ALA	conflict	UNP Q9KNE0
D	200	THR	SER	conflict	UNP Q9KNE0
D	201	GLY	PRO	conflict	UNP Q9KNE0
D	322	ILE	VAL	conflict	UNP Q9KNE0
D	376	THR	ALA	conflict	UNP Q9KNE0
D	379	VAL	THR	conflict	UNP Q9KNE0
D	381	THR	SER	conflict	UNP Q9KNE0
D	382	THR	ALA	conflict	UNP Q9KNE0
D	383	THR	ALA	conflict	UNP Q9KNE0

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Na 2 2	0	0
2	B	2	Total Na 2 2	0	0
2	C	2	Total Na 2 2	0	0
2	D	2	Total Na 2 2	0	0

- Molecule 3 is SUCCINIC ACID (three-letter code: SIN) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>4</sub>).

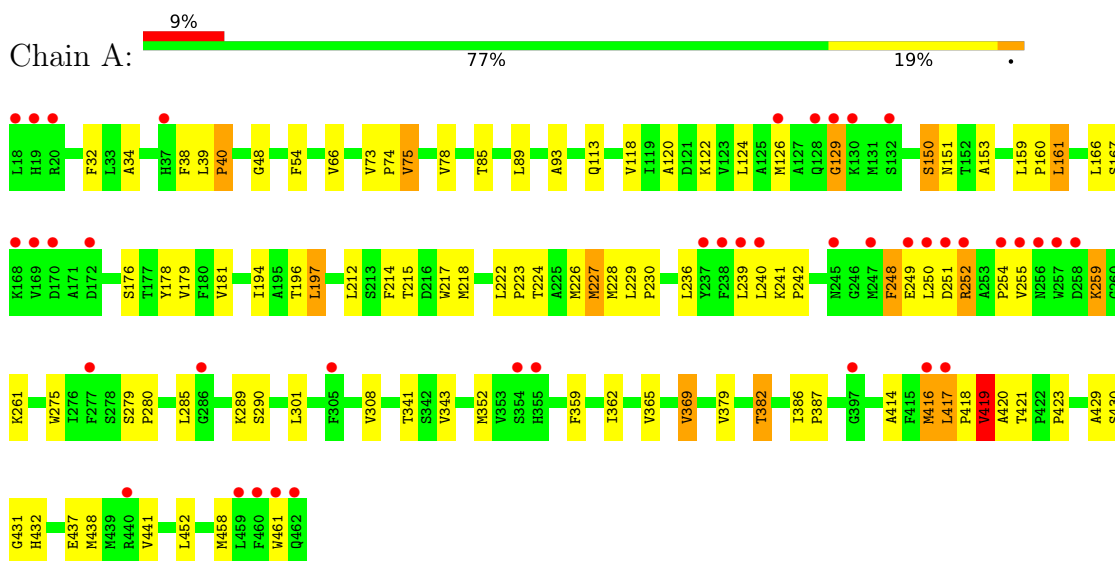


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 8	C 4	O 4	0	0
3	B	1	Total 8	C 4	O 4	0	0
3	C	1	Total 8	C 4	O 4	0	0
3	D	1	Total 8	C 4	O 4	0	0

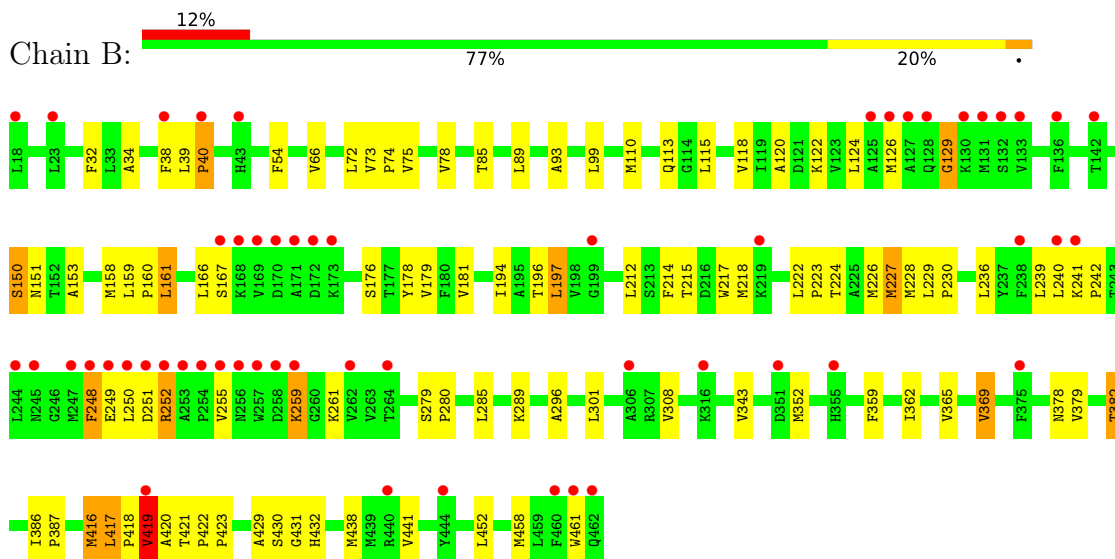
### 3 Residue-property plots

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.

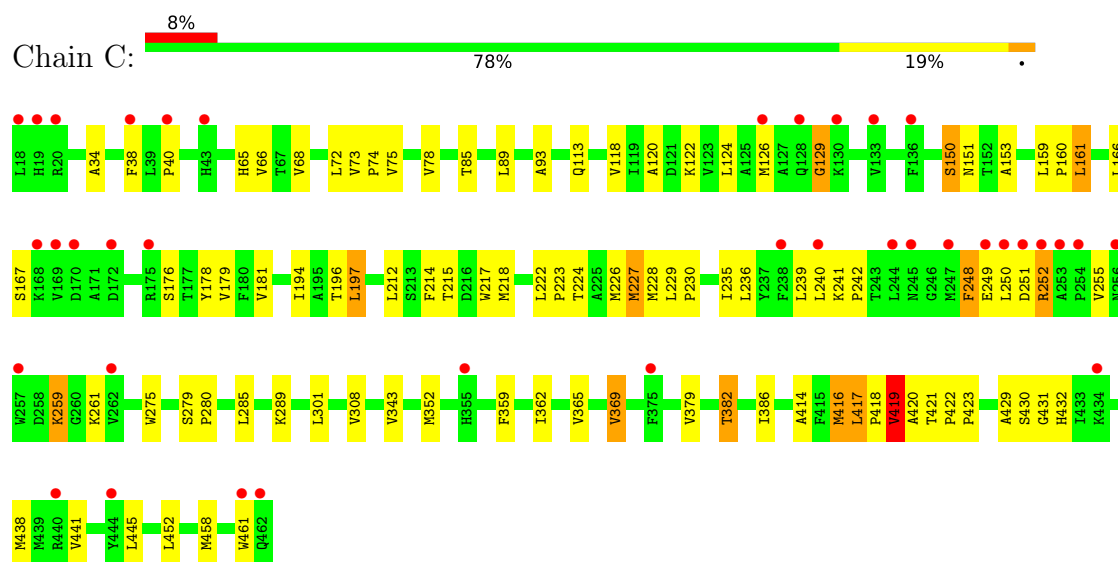
- Molecule 1: Transporter, NadC family



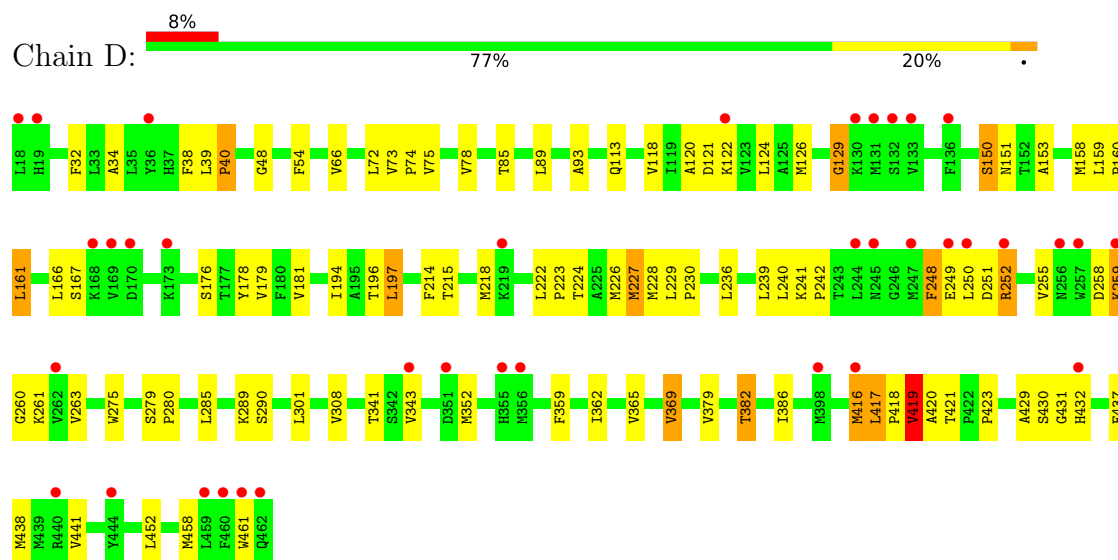
- Molecule 1: Transporter, NadC family



- Molecule 1: Transporter, NadC family



- Molecule 1: Transporter, NadC family





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.14Å 102.28Å 170.86Å 90.00° 98.31° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 14.99 – 2.81	Depositor EDS
% Data completeness (in resolution range)	90.4 (15.00-2.80) 90.5 (14.99-2.81)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.247 , 0.266 0.258 , 0.274	Depositor DCC
$R_{free}$ test set	4041 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	77.6	Xtriage
Anisotropy	0.600	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 74.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13436	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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: SIN, 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	0.32	0/3427	0.49	0/4673
1	B	0.32	0/3427	0.49	0/4673
1	C	0.33	0/3427	0.50	0/4673
1	D	0.33	0/3427	0.50	0/4673
All	All	0.33	0/13708	0.49	0/18692

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	3349	0	3504	59	0
1	B	3349	0	3504	57	0
1	C	3349	0	3504	59	0
1	D	3349	0	3504	59	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	8	0	4	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	8	0	4	2	0
3	C	8	0	4	1	0
3	D	8	0	4	1	0
All	All	13436	0	14032	222	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 8.

All (222) 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:B:421:THR:HG22	1:B:423:PRO:HD2	1.14	1.14
1:D:421:THR:HG22	1:D:423:PRO:HD2	1.15	1.11
1:C:421:THR:HG22	1:C:423:PRO:HD2	1.13	1.10
1:A:421:THR:HG22	1:A:423:PRO:HD2	1.12	1.05
1:C:416:MET:O	1:C:438:MET:HG2	1.80	0.81
1:A:78:VAL:HG11	1:A:85:THR:HG22	1.63	0.81
1:C:78:VAL:HG11	1:C:85:THR:HG22	1.62	0.81
1:A:416:MET:O	1:A:438:MET:HG2	1.82	0.78
1:B:416:MET:O	1:B:438:MET:HG2	1.83	0.77
1:D:78:VAL:HG11	1:D:85:THR:HG22	1.66	0.77
1:D:416:MET:O	1:D:438:MET:HG2	1.85	0.77
1:B:78:VAL:HG11	1:B:85:THR:HG22	1.65	0.76
1:A:421:THR:CG2	1:A:423:PRO:HD2	2.07	0.74
1:D:73:VAL:HB	1:D:74:PRO:HD3	1.72	0.71
1:B:421:THR:CG2	1:B:423:PRO:HD2	2.09	0.70
1:B:73:VAL:HB	1:B:74:PRO:HD3	1.74	0.69
1:A:73:VAL:HB	1:A:74:PRO:HD3	1.75	0.69
1:C:421:THR:CG2	1:C:423:PRO:HD2	2.08	0.69
1:A:166:LEU:HD11	1:A:181:VAL:HB	1.76	0.68
1:C:166:LEU:HD11	1:C:181:VAL:HB	1.75	0.68
1:C:73:VAL:HB	1:C:74:PRO:HD3	1.76	0.68
1:D:166:LEU:HD11	1:D:181:VAL:HB	1.77	0.67
1:C:222:LEU:O	1:C:226:MET:HG2	1.95	0.67
1:A:159:LEU:HB3	1:A:160:PRO:HD3	1.78	0.66
1:C:93:ALA:HB2	1:D:93:ALA:HB2	1.76	0.66
1:B:159:LEU:HB3	1:B:160:PRO:HD3	1.77	0.66
1:A:222:LEU:O	1:A:226:MET:HG2	1.96	0.66
1:B:166:LEU:HD11	1:B:181:VAL:HB	1.76	0.66
1:D:159:LEU:HB3	1:D:160:PRO:HD3	1.78	0.65
1:B:222:LEU:O	1:B:226:MET:HG2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:ILE:HD11	1:C:458:MET:HE2	1.79	0.65
1:C:159:LEU:HB3	1:C:160:PRO:HD3	1.78	0.64
1:D:421:THR:CG2	1:D:423:PRO:HD2	2.10	0.64
1:B:382:THR:HG22	1:B:386:ILE:HG13	1.80	0.63
1:A:382:THR:HG22	1:A:386:ILE:HG13	1.80	0.62
1:D:194:ILE:HG22	1:D:194:ILE:O	1.99	0.62
1:D:222:LEU:O	1:D:226:MET:HG2	1.98	0.62
1:A:421:THR:HG22	1:A:423:PRO:CD	2.08	0.62
1:B:362:ILE:HD11	1:B:458:MET:HE2	1.82	0.62
1:C:194:ILE:O	1:C:194:ILE:HG22	1.99	0.61
1:C:382:THR:HG22	1:C:386:ILE:HG13	1.83	0.61
1:D:382:THR:HG22	1:D:386:ILE:HG13	1.82	0.61
1:A:194:ILE:O	1:A:194:ILE:HG22	1.99	0.61
1:A:418:PRO:C	1:A:420:ALA:H	2.05	0.60
1:B:194:ILE:HG22	1:B:194:ILE:O	2.01	0.59
1:D:362:ILE:HD11	1:D:458:MET:HE2	1.85	0.59
1:D:418:PRO:C	1:D:420:ALA:H	2.05	0.59
1:D:227:MET:HG2	1:D:452:LEU:HD11	1.85	0.58
1:A:254:PRO:HG2	1:C:429:ALA:HA	1.86	0.58
1:C:418:PRO:C	1:C:420:ALA:H	2.07	0.58
1:D:421:THR:HG22	1:D:423:PRO:CD	2.10	0.58
1:B:418:PRO:C	1:B:420:ALA:H	2.06	0.58
1:D:197:LEU:HD12	1:D:214:PHE:HA	1.86	0.57
1:A:227:MET:HG2	1:A:452:LEU:HD11	1.87	0.57
1:B:176:SER:HA	1:B:179:VAL:HG12	1.86	0.56
1:C:122:LYS:O	1:C:126:MET:HG2	2.05	0.56
1:C:197:LEU:HD12	1:C:214:PHE:HA	1.87	0.56
1:B:227:MET:HG2	1:B:452:LEU:HD11	1.86	0.56
1:C:176:SER:HA	1:C:179:VAL:HG12	1.87	0.56
1:B:197:LEU:HD12	1:B:214:PHE:HA	1.87	0.56
1:B:122:LYS:O	1:B:126:MET:HG2	2.06	0.55
1:A:197:LEU:HD12	1:A:214:PHE:HA	1.88	0.55
1:A:93:ALA:HB2	1:B:93:ALA:HB2	1.89	0.55
1:A:122:LYS:O	1:A:126:MET:HG2	2.06	0.54
1:D:122:LYS:O	1:D:126:MET:HG2	2.06	0.54
1:A:75:VAL:HG11	1:B:301:LEU:HD11	1.88	0.54
1:C:421:THR:HG22	1:C:423:PRO:CD	2.09	0.54
1:C:75:VAL:HG11	1:D:301:LEU:HD11	1.88	0.54
1:C:227:MET:HG2	1:C:452:LEU:HD11	1.88	0.54
1:C:151:ASN:HB2	3:C:503:SIN:C4	2.38	0.53
1:D:176:SER:HA	1:D:179:VAL:HG12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:ILE:HD11	1:A:458:MET:HE2	1.90	0.53
1:A:176:SER:HA	1:A:179:VAL:HG12	1.89	0.53
1:B:34:ALA:O	1:B:38:PHE:HB2	2.09	0.53
1:D:34:ALA:O	1:D:38:PHE:HB2	2.09	0.52
1:C:34:ALA:O	1:C:38:PHE:HB2	2.10	0.52
1:C:120:ALA:O	1:C:124:LEU:HB2	2.10	0.52
1:D:120:ALA:O	1:D:124:LEU:HB2	2.10	0.52
1:D:73:VAL:HB	1:D:74:PRO:CD	2.40	0.52
1:C:301:LEU:HD11	1:D:75:VAL:HG11	1.92	0.51
1:B:151:ASN:HB2	3:B:503:SIN:C4	2.39	0.51
1:B:120:ALA:O	1:B:124:LEU:HB2	2.11	0.51
1:D:176:SER:HB2	1:D:240:LEU:O	2.11	0.51
1:D:151:ASN:HB2	3:D:503:SIN:C4	2.41	0.51
1:A:151:ASN:HB2	3:A:503:SIN:C4	2.41	0.51
1:A:34:ALA:O	1:A:38:PHE:HB2	2.11	0.50
1:D:194:ILE:O	1:D:194:ILE:CG2	2.59	0.50
1:A:290:SER:H	1:B:85:THR:HG21	1.75	0.50
1:A:120:ALA:O	1:A:124:LEU:HB2	2.11	0.50
1:A:194:ILE:O	1:A:194:ILE:CG2	2.60	0.50
1:A:150:SER:HB3	1:A:153:ALA:HB3	1.92	0.50
1:B:176:SER:HB2	1:B:240:LEU:O	2.11	0.50
1:A:429:ALA:C	1:A:431:GLY:H	2.15	0.50
1:A:176:SER:HB2	1:A:240:LEU:O	2.12	0.49
1:C:418:PRO:O	1:C:419:VAL:HG12	2.12	0.49
1:B:421:THR:HG22	1:B:423:PRO:CD	2.09	0.49
1:D:429:ALA:C	1:D:431:GLY:H	2.16	0.49
1:A:417:LEU:HB2	1:A:418:PRO:HD2	1.95	0.49
1:B:429:ALA:C	1:B:431:GLY:H	2.16	0.49
1:D:150:SER:HB3	1:D:153:ALA:HB3	1.94	0.49
1:B:194:ILE:O	1:B:194:ILE:CG2	2.61	0.48
1:B:417:LEU:HB2	1:B:418:PRO:HD2	1.95	0.48
1:C:417:LEU:HB2	1:C:418:PRO:HD2	1.94	0.48
1:C:85:THR:HG21	1:D:290:SER:H	1.79	0.48
1:C:176:SER:HB2	1:C:240:LEU:O	2.12	0.48
1:D:417:LEU:HB2	1:D:418:PRO:HD2	1.96	0.48
1:C:359:PHE:HA	1:C:458:MET:HE1	1.95	0.48
1:C:429:ALA:C	1:C:431:GLY:H	2.16	0.48
1:B:118:VAL:HG12	1:B:255:VAL:HB	1.96	0.48
1:D:113:GLN:HG3	1:D:261:LYS:HG2	1.95	0.48
1:B:222:LEU:HB3	1:B:223:PRO:HD3	1.96	0.47
1:B:359:PHE:HA	1:B:458:MET:HE1	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:ILE:O	1:C:194:ILE:CG2	2.61	0.47
1:B:113:GLN:HG3	1:B:261:LYS:HG2	1.95	0.47
1:C:129:GLY:HA2	1:C:248:PHE:HB2	1.97	0.47
1:B:418:PRO:O	1:B:419:VAL:HG12	2.14	0.47
1:D:118:VAL:HG12	1:D:255:VAL:HB	1.96	0.47
1:A:129:GLY:HA2	1:A:248:PHE:HB2	1.96	0.47
1:C:113:GLN:HG3	1:C:261:LYS:HG2	1.97	0.47
1:A:196:THR:HG22	1:A:218:MET:HG3	1.97	0.47
1:B:129:GLY:HA2	1:B:248:PHE:HB2	1.97	0.47
1:C:150:SER:HB3	1:C:153:ALA:HB3	1.97	0.46
1:A:118:VAL:HG12	1:A:255:VAL:HB	1.97	0.46
1:B:229:LEU:HB3	1:B:230:PRO:HD3	1.97	0.46
1:D:129:GLY:HA2	1:D:248:PHE:HB2	1.96	0.46
1:C:118:VAL:HG12	1:C:255:VAL:HB	1.97	0.46
1:B:251:ASP:O	1:B:252:ARG:HB3	2.16	0.46
1:A:113:GLN:HG3	1:A:261:LYS:HG2	1.96	0.46
1:B:196:THR:HG22	1:B:218:MET:HG3	1.97	0.46
1:C:251:ASP:O	1:C:252:ARG:HB3	2.16	0.46
1:D:196:THR:HG22	1:D:218:MET:HG3	1.97	0.46
1:A:167:SER:HB3	1:A:249:GLU:OE2	2.16	0.46
1:A:229:LEU:HB3	1:A:230:PRO:HD3	1.97	0.45
1:D:222:LEU:HB3	1:D:223:PRO:HD3	1.98	0.45
1:C:236:LEU:HD23	1:C:441:VAL:HG11	1.97	0.45
1:A:301:LEU:HD11	1:B:75:VAL:HG11	1.99	0.45
1:D:224:THR:O	1:D:228:MET:HB2	2.16	0.45
1:D:359:PHE:HA	1:D:458:MET:HE1	1.98	0.45
1:D:167:SER:HB3	1:D:249:GLU:OE2	2.17	0.45
1:A:251:ASP:O	1:A:252:ARG:HB3	2.16	0.45
1:C:118:VAL:HA	1:C:255:VAL:HG21	1.98	0.45
1:A:222:LEU:HB3	1:A:223:PRO:HD3	1.98	0.45
1:C:229:LEU:HB3	1:C:230:PRO:HD3	1.97	0.45
1:D:418:PRO:O	1:D:419:VAL:HG12	2.17	0.45
1:A:224:THR:O	1:A:228:MET:HB2	2.17	0.45
1:B:279:SER:HB3	1:B:280:PRO:HD3	1.99	0.45
1:C:167:SER:HB3	1:C:249:GLU:OE2	2.17	0.45
1:C:196:THR:HG22	1:C:218:MET:HG3	1.98	0.45
1:D:229:LEU:HB3	1:D:230:PRO:HD3	1.97	0.44
1:D:251:ASP:O	1:D:252:ARG:HB3	2.17	0.44
1:A:418:PRO:O	1:A:420:ALA:N	2.51	0.44
1:C:73:VAL:HB	1:C:74:PRO:CD	2.47	0.44
1:D:48:GLY:HA3	1:D:341:THR:OG1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:LEU:HD11	1:D:252:ARG:HH22	1.82	0.44
1:B:150:SER:HB3	1:B:153:ALA:HB3	1.99	0.44
1:C:72:LEU:O	1:C:75:VAL:HG12	2.18	0.44
1:C:222:LEU:HB3	1:C:223:PRO:HD3	2.00	0.44
1:A:418:PRO:O	1:A:419:VAL:HG12	2.17	0.44
1:B:161:LEU:HD11	1:B:252:ARG:HH22	1.82	0.44
1:C:75:VAL:HG11	1:D:301:LEU:CD1	2.48	0.44
1:C:212:LEU:HD13	1:C:217:TRP:HD1	1.83	0.44
1:D:118:VAL:HA	1:D:255:VAL:HG21	2.00	0.44
1:A:359:PHE:HA	1:A:458:MET:HE1	2.00	0.43
1:A:236:LEU:HD23	1:A:441:VAL:HG11	1.99	0.43
1:B:118:VAL:HA	1:B:255:VAL:HG21	2.00	0.43
1:B:224:THR:O	1:B:228:MET:HB2	2.18	0.43
1:B:236:LEU:HD23	1:B:441:VAL:HG11	2.00	0.43
1:A:118:VAL:HA	1:A:255:VAL:HG21	1.99	0.43
1:A:279:SER:HB3	1:A:280:PRO:HD3	2.01	0.43
1:B:167:SER:HB3	1:B:249:GLU:OE2	2.18	0.43
1:A:418:PRO:C	1:A:420:ALA:N	2.72	0.43
1:C:161:LEU:HD11	1:C:252:ARG:HH22	1.83	0.43
1:D:365:VAL:O	1:D:369:VAL:HG22	2.18	0.43
1:A:73:VAL:HB	1:A:74:PRO:CD	2.47	0.43
1:B:32:PHE:HB2	1:B:54:PHE:HD1	1.84	0.43
1:A:75:VAL:HG11	1:B:301:LEU:CD1	2.49	0.42
1:D:279:SER:HB3	1:D:280:PRO:HD3	2.00	0.42
1:A:359:PHE:CD1	1:A:458:MET:HE3	2.54	0.42
1:D:236:LEU:HD23	1:D:441:VAL:HG11	2.01	0.42
1:D:418:PRO:C	1:D:420:ALA:N	2.72	0.42
1:B:212:LEU:HD13	1:B:217:TRP:HD1	1.84	0.42
1:D:418:PRO:O	1:D:420:ALA:N	2.52	0.42
1:B:39:LEU:HA	1:B:40:PRO:HD3	1.87	0.42
1:B:418:PRO:C	1:B:420:ALA:N	2.73	0.42
1:C:422:PRO:HB2	1:C:423:PRO:HD3	2.01	0.42
1:B:72:LEU:O	1:B:75:VAL:HG12	2.19	0.42
1:B:378:ASN:ND2	3:B:503:SIN:O1	2.53	0.42
1:A:365:VAL:O	1:A:369:VAL:HG22	2.19	0.42
1:C:365:VAL:O	1:C:369:VAL:HG22	2.19	0.42
1:A:39:LEU:HA	1:A:40:PRO:HD3	1.89	0.41
1:A:214:PHE:CD2	1:A:275:TRP:HB3	2.55	0.41
1:C:224:THR:O	1:C:228:MET:HB2	2.20	0.41
1:C:418:PRO:O	1:C:420:ALA:N	2.53	0.41
1:A:48:GLY:HA3	1:A:341:THR:OG1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:ASP:OD2	1:D:252:ARG:NH2	2.54	0.41
1:B:110:MET:HB2	1:B:115:LEU:HB3	2.02	0.41
1:A:161:LEU:HD11	1:A:252:ARG:HH22	1.84	0.41
1:C:214:PHE:CD2	1:C:275:TRP:HB3	2.56	0.41
1:C:78:VAL:CG1	1:C:85:THR:HG22	2.43	0.41
1:C:301:LEU:CD1	1:D:75:VAL:HG11	2.50	0.41
1:D:72:LEU:O	1:D:75:VAL:HG12	2.21	0.41
1:B:422:PRO:HB2	1:B:423:PRO:HD3	2.03	0.41
1:A:212:LEU:HD13	1:A:217:TRP:HD1	1.86	0.41
1:A:386:ILE:HB	1:A:387:PRO:HD3	2.01	0.41
1:B:99:LEU:HD12	1:B:296:ALA:HB2	2.03	0.41
1:C:65:HIS:HB3	1:C:68:VAL:HG23	2.03	0.41
1:B:386:ILE:HB	1:B:387:PRO:HD3	2.03	0.41
1:C:279:SER:HB3	1:C:280:PRO:HD3	2.02	0.41
1:C:418:PRO:C	1:C:420:ALA:N	2.73	0.41
1:D:39:LEU:HA	1:D:40:PRO:HD3	1.85	0.41
1:D:258:ASP:OD1	1:D:261:LYS:HG3	2.20	0.41
1:D:260:GLY:HA3	1:D:263:VAL:HB	2.03	0.41
1:A:414:ALA:HB1	1:A:420:ALA:HB1	2.03	0.40
1:A:437:GLU:O	1:A:441:VAL:HG23	2.21	0.40
1:C:414:ALA:HB1	1:C:420:ALA:HB1	2.03	0.40
1:B:365:VAL:O	1:B:369:VAL:HG22	2.21	0.40
1:D:214:PHE:CD2	1:D:275:TRP:HB3	2.56	0.40
1:D:437:GLU:O	1:D:441:VAL:HG23	2.21	0.40
1:B:418:PRO:O	1:B:420:ALA:N	2.54	0.40
1:D:32:PHE:HB2	1:D:54:PHE:HD1	1.87	0.40
1:A:32:PHE:HB2	1:A:54:PHE:HD1	1.86	0.40
1:C:235:ILE:HD12	1:C:445:LEU:HD13	2.04	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	443/445 (100%)	407 (92%)	27 (6%)	9 (2%)	7	24
1	B	443/445 (100%)	410 (93%)	24 (5%)	9 (2%)	7	24
1	C	443/445 (100%)	410 (93%)	24 (5%)	9 (2%)	7	24
1	D	443/445 (100%)	410 (93%)	24 (5%)	9 (2%)	7	24
All	All	1772/1780 (100%)	1637 (92%)	99 (6%)	36 (2%)	7	24

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	PRO
1	A	419	VAL
1	B	242	PRO
1	B	419	VAL
1	C	242	PRO
1	C	419	VAL
1	D	242	PRO
1	D	419	VAL
1	A	150	SER
1	A	252	ARG
1	B	150	SER
1	B	252	ARG
1	C	150	SER
1	C	252	ARG
1	D	150	SER
1	D	252	ARG
1	A	416	MET
1	A	430	SER
1	B	259	LYS
1	B	416	MET
1	B	430	SER
1	C	259	LYS
1	C	416	MET
1	C	430	SER
1	D	259	LYS
1	D	416	MET
1	D	430	SER
1	A	259	LYS
1	A	40	PRO
1	B	40	PRO
1	D	40	PRO
1	C	40	PRO
1	D	129	GLY

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Mol	Chain	Res	Type
1	A	129	GLY
1	B	129	GLY
1	C	129	GLY

### 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	355/355 (100%)	330 (93%)	25 (7%)	15	40
1	B	355/355 (100%)	330 (93%)	25 (7%)	15	40
1	C	355/355 (100%)	331 (93%)	24 (7%)	16	42
1	D	355/355 (100%)	330 (93%)	25 (7%)	15	40
All	All	1420/1420 (100%)	1321 (93%)	99 (7%)	15	40

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	VAL
1	A	75	VAL
1	A	89	LEU
1	A	161	LEU
1	A	178	TYR
1	A	197	LEU
1	A	215	THR
1	A	227	MET
1	A	239	LEU
1	A	241	LYS
1	A	248	PHE
1	A	250	LEU
1	A	259	LYS
1	A	285	LEU
1	A	289	LYS
1	A	308	VAL
1	A	343	VAL
1	A	352	MET

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Mol	Chain	Res	Type
1	A	369	VAL
1	A	379	VAL
1	A	382	THR
1	A	417	LEU
1	A	419	VAL
1	A	432	HIS
1	A	461	TRP
1	B	66	VAL
1	B	89	LEU
1	B	158	MET
1	B	161	LEU
1	B	178	TYR
1	B	197	LEU
1	B	215	THR
1	B	227	MET
1	B	239	LEU
1	B	241	LYS
1	B	248	PHE
1	B	250	LEU
1	B	259	LYS
1	B	285	LEU
1	B	289	LYS
1	B	308	VAL
1	B	343	VAL
1	B	352	MET
1	B	369	VAL
1	B	379	VAL
1	B	382	THR
1	B	417	LEU
1	B	419	VAL
1	B	432	HIS
1	B	461	TRP
1	C	66	VAL
1	C	89	LEU
1	C	161	LEU
1	C	178	TYR
1	C	197	LEU
1	C	215	THR
1	C	227	MET
1	C	239	LEU
1	C	241	LYS
1	C	248	PHE

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Mol	Chain	Res	Type
1	C	250	LEU
1	C	259	LYS
1	C	285	LEU
1	C	289	LYS
1	C	308	VAL
1	C	343	VAL
1	C	352	MET
1	C	369	VAL
1	C	379	VAL
1	C	382	THR
1	C	417	LEU
1	C	419	VAL
1	C	432	HIS
1	C	461	TRP
1	D	66	VAL
1	D	89	LEU
1	D	158	MET
1	D	161	LEU
1	D	178	TYR
1	D	197	LEU
1	D	215	THR
1	D	227	MET
1	D	239	LEU
1	D	241	LYS
1	D	248	PHE
1	D	250	LEU
1	D	259	LYS
1	D	285	LEU
1	D	289	LYS
1	D	308	VAL
1	D	343	VAL
1	D	352	MET
1	D	369	VAL
1	D	379	VAL
1	D	382	THR
1	D	417	LEU
1	D	419	VAL
1	D	432	HIS
1	D	461	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	B	43	HIS
1	C	43	HIS
1	C	90	ASN
1	D	43	HIS
1	D	90	ASN

### 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 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SIN	B	503	-	7,7,7	1.03	0	8,8,8	1.22	0
3	SIN	D	503	-	7,7,7	1.03	0	8,8,8	1.33	0
3	SIN	A	503	-	7,7,7	1.03	0	8,8,8	1.25	0
3	SIN	C	503	-	7,7,7	1.03	0	8,8,8	1.25	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SIN	B	503	-	-	4/5/5/5	-
3	SIN	D	503	-	-	4/5/5/5	-
3	SIN	A	503	-	-	4/5/5/5	-
3	SIN	C	503	-	-	4/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	503	SIN	C2-C3-C4-O3
3	D	503	SIN	O1-C1-C2-C3
3	D	503	SIN	O2-C1-C2-C3
3	C	503	SIN	C2-C3-C4-O4
3	A	503	SIN	O2-C1-C2-C3
3	C	503	SIN	O2-C1-C2-C3
3	B	503	SIN	O2-C1-C2-C3
3	A	503	SIN	O1-C1-C2-C3
3	C	503	SIN	O1-C1-C2-C3
3	B	503	SIN	O1-C1-C2-C3
3	A	503	SIN	C2-C3-C4-O4
3	B	503	SIN	C2-C3-C4-O4
3	D	503	SIN	C2-C3-C4-O4
3	A	503	SIN	C2-C3-C4-O3
3	B	503	SIN	C2-C3-C4-O3
3	D	503	SIN	C2-C3-C4-O3

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	503	SIN	2	0
3	D	503	SIN	1	0
3	A	503	SIN	1	0
3	C	503	SIN	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	445/445 (100%)	0.07	41 (9%) <b>9</b> <b>5</b>	43, 94, 165, 210	0
1	B	445/445 (100%)	0.28	55 (12%) <b>4</b> <b>2</b>	54, 104, 189, 219	0
1	C	445/445 (100%)	0.14	37 (8%) <b>11</b> <b>6</b>	41, 90, 170, 218	0
1	D	445/445 (100%)	0.07	37 (8%) <b>11</b> <b>6</b>	18, 87, 156, 206	0
All	All	1780/1780 (100%)	0.14	170 (9%) <b>8</b> <b>4</b>	18, 94, 173, 219	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	462	GLN	12.3
1	A	168	LYS	10.4
1	A	462	GLN	9.7
1	B	168	LYS	9.2
1	B	133	VAL	9.1
1	B	462	GLN	8.6
1	D	168	LYS	8.6
1	C	462	GLN	8.2
1	C	254	PRO	8.2
1	B	245	ASN	7.8
1	C	250	LEU	7.8
1	A	130	LYS	7.1
1	A	128	GLN	6.3
1	D	245	ASN	6.2
1	B	355	HIS	6.2
1	B	126	MET	6.2
1	B	256	ASN	6.1
1	C	18	LEU	6.0
1	C	245	ASN	6.0
1	C	355	HIS	5.6
1	B	132	SER	5.5

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Mol	Chain	Res	Type	RSRZ
1	C	128	GLN	5.5
1	A	245	ASN	5.4
1	A	461	TRP	5.2
1	D	130	LYS	5.2
1	B	18	LEU	5.2
1	D	250	LEU	5.1
1	C	251	ASP	5.1
1	B	259	LYS	5.0
1	A	129	GLY	4.9
1	C	133	VAL	4.9
1	A	251	ASP	4.8
1	D	259	LYS	4.7
1	A	240	LEU	4.6
1	B	170	ASP	4.4
1	C	130	LYS	4.4
1	C	126	MET	4.3
1	A	355	HIS	4.3
1	B	255	VAL	4.3
1	B	244	LEU	4.2
1	C	19	HIS	4.2
1	D	355	HIS	4.1
1	C	257	TRP	4.1
1	B	128	GLN	4.0
1	A	18	LEU	3.9
1	C	253	ALA	3.9
1	D	257	TRP	3.9
1	B	241	LYS	3.9
1	C	168	LYS	3.9
1	B	43	HIS	3.9
1	C	247	MET	3.9
1	A	256	ASN	3.8
1	C	461	TRP	3.8
1	D	133	VAL	3.8
1	D	249	GLU	3.8
1	B	38	PHE	3.8
1	B	262	VAL	3.8
1	B	173	LYS	3.7
1	B	167	SER	3.7
1	D	444	TYR	3.7
1	B	131	MET	3.7
1	B	238	PHE	3.7
1	C	38	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	257	TRP	3.6
1	B	40	PRO	3.6
1	D	461	TRP	3.5
1	A	459	LEU	3.5
1	A	254	PRO	3.5
1	D	256	ASN	3.5
1	A	250	LEU	3.5
1	B	247	MET	3.4
1	D	19	HIS	3.3
1	C	244	LEU	3.2
1	B	250	LEU	3.2
1	C	136	PHE	3.2
1	B	171	ALA	3.1
1	B	351	ASP	3.1
1	D	173	LYS	3.1
1	C	238	PHE	3.1
1	A	247	MET	3.0
1	A	460	PHE	3.0
1	D	247	MET	3.0
1	B	375	PHE	3.0
1	B	461	TRP	3.0
1	B	172	ASP	3.0
1	C	444	TYR	2.9
1	B	136	PHE	2.9
1	D	132	SER	2.9
1	A	417	LEU	2.9
1	A	440	ARG	2.9
1	A	249	GLU	2.9
1	B	254	PRO	2.9
1	B	23	LEU	2.9
1	C	256	ASN	2.8
1	B	240	LEU	2.8
1	D	170	ASP	2.8
1	D	440	ARG	2.8
1	D	460	PHE	2.8
1	C	252	ARG	2.8
1	C	375	PHE	2.7
1	C	172	ASP	2.7
1	A	132	SER	2.7
1	D	432	HIS	2.6
1	B	142	THR	2.6
1	D	244	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	351	ASP	2.6
1	A	277	PHE	2.6
1	D	18	LEU	2.6
1	B	248	PHE	2.6
1	B	251	ASP	2.6
1	D	169	VAL	2.6
1	A	238	PHE	2.6
1	A	172	ASP	2.5
1	A	255	VAL	2.5
1	C	169	VAL	2.5
1	C	175	ARG	2.5
1	C	40	PRO	2.5
1	B	419	VAL	2.5
1	A	397	GLY	2.5
1	A	239	LEU	2.5
1	A	257	TRP	2.5
1	B	125	ALA	2.4
1	C	20	ARG	2.4
1	D	36	TYR	2.4
1	A	19	HIS	2.4
1	A	20	ARG	2.4
1	A	252	ARG	2.4
1	A	170	ASP	2.4
1	D	398	MET	2.4
1	B	460	PHE	2.4
1	B	219	LYS	2.4
1	A	305	PHE	2.4
1	D	219	LYS	2.4
1	D	262	VAL	2.3
1	D	343	VAL	2.3
1	C	170	ASP	2.3
1	B	264	THR	2.3
1	B	130	LYS	2.3
1	C	262	VAL	2.3
1	A	258	ASP	2.3
1	D	416	MET	2.3
1	A	286	GLY	2.3
1	A	37	HIS	2.3
1	B	444	TYR	2.3
1	B	252	ARG	2.3
1	B	169	VAL	2.2
1	A	126	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	356	MET	2.2
1	B	253	ALA	2.2
1	A	169	VAL	2.2
1	A	354	SER	2.2
1	B	316	LYS	2.2
1	C	440	ARG	2.2
1	B	127	ALA	2.2
1	D	252	ARG	2.2
1	B	258	ASP	2.1
1	C	240	LEU	2.1
1	B	249	GLU	2.1
1	A	416	MET	2.1
1	C	43	HIS	2.1
1	D	136	PHE	2.1
1	C	434	LYS	2.1
1	C	249	GLU	2.0
1	D	459	LEU	2.0
1	D	122	LYS	2.0
1	B	306	ALA	2.0
1	D	131	MET	2.0
1	B	440	ARG	2.0
1	B	199	GLY	2.0
1	A	237	TYR	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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NA	B	502	1/1	0.72	0.49	147,147,147,147	0
2	NA	B	501	1/1	0.76	0.25	115,115,115,115	0
3	SIN	D	503	8/8	0.81	0.27	95,97,99,104	0
3	SIN	B	503	8/8	0.83	0.38	89,96,103,108	0
2	NA	C	502	1/1	0.84	0.26	92,92,92,92	0
2	NA	A	502	1/1	0.85	0.20	70,70,70,70	0
3	SIN	C	503	8/8	0.89	0.54	87,100,105,112	0
2	NA	D	502	1/1	0.90	0.23	82,82,82,82	0
3	SIN	A	503	8/8	0.91	0.33	88,98,100,104	0
2	NA	D	501	1/1	0.94	0.37	88,88,88,88	0
2	NA	C	501	1/1	0.98	0.17	82,82,82,82	0
2	NA	A	501	1/1	0.98	0.14	64,64,64,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.