



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:49 PM UTC

PDB ID : 5ULE / pdb_00005ule
Title : Structure and function of the divalent anion/Na⁺ 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

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

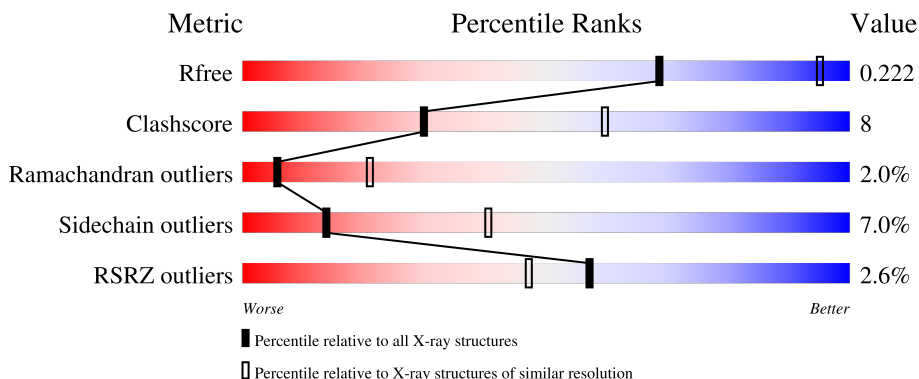
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 ≥ 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	0% 77% 20% .
1	B	445	4% 76% 20% .
1	C	445	2% 78% 19% .
1	D	445	3% 76% 20% .

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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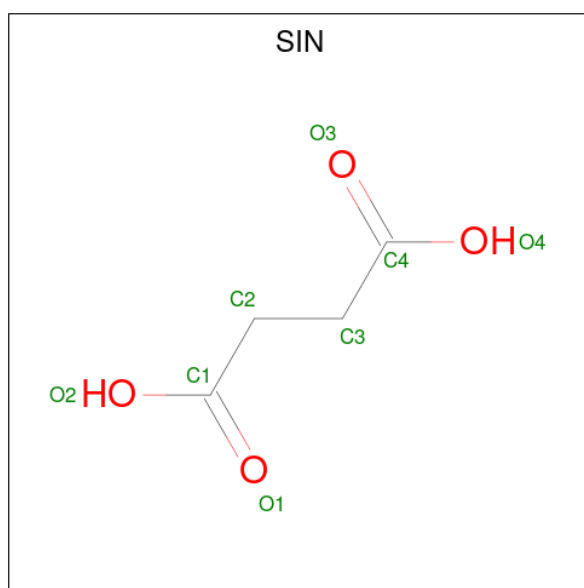
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Chain	Residue	Modelled	Actual	Comment	Reference
C	381	THR	SER	conflict	UNP Q9KNE0
C	382	THR	ALA	conflict	UNP Q9KNE0
C	383	THR	ALA	conflict	UNP Q9KNE0
D	200	THR	SER	conflict	UNP Q9KNE0
D	201	GLY	PRO	conflict	UNP Q9KNE0
D	322	ILE	VAL	conflict	UNP Q9KNE0
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 (CCD ID: 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 (CCD ID: SIN) (formula: C₄H₆O₄).

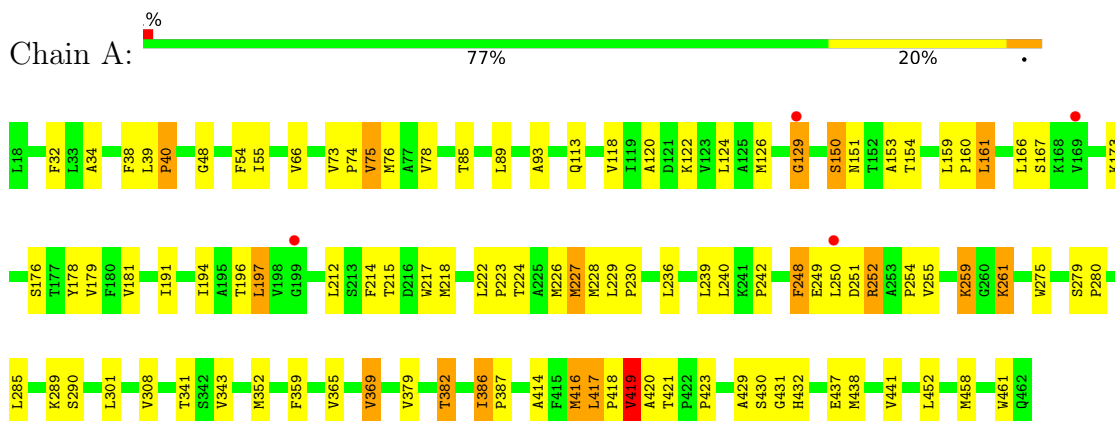


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 8	C 4	O 4	0	0
3	B	1	Total 8	C 4	O 4	0	0
3	C	1	Total 8	C 4	O 4	0	0
3	D	1	Total 8	C 4	O 4	0	0

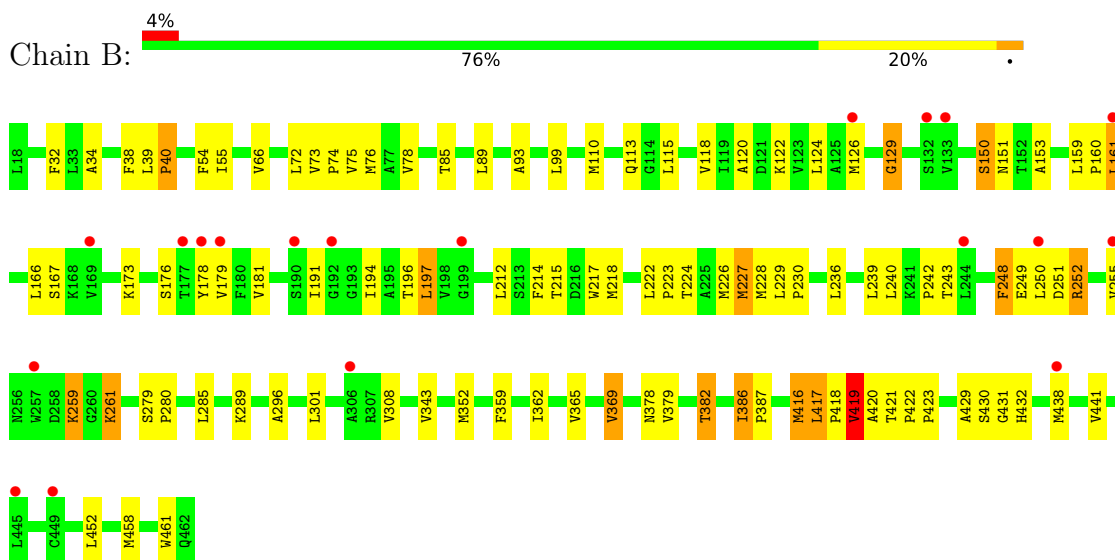
3 Residue-property plots [i](#)

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.

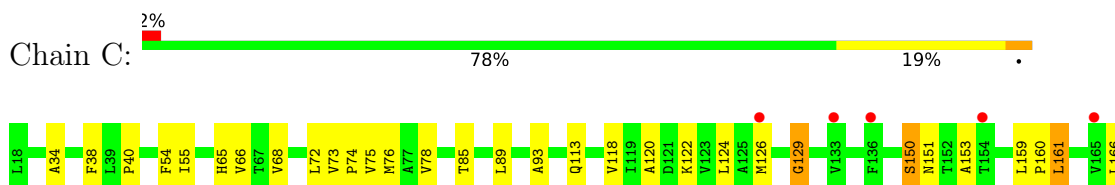
- Molecule 1: Transporter, NadC family



- Molecule 1: Transporter, NadC family

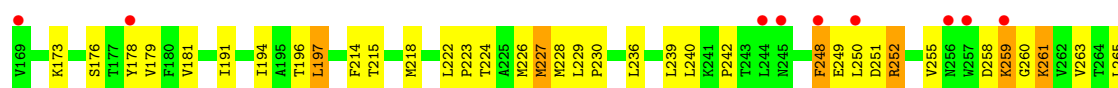
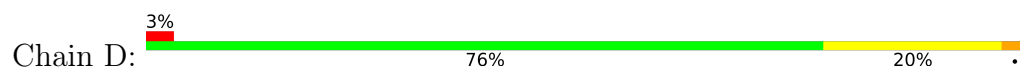


- Molecule 1: Transporter, NadC family





● 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, α , β , γ	107.14Å 102.28Å 170.86Å 90.00° 98.31° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	90.4 (15.00-2.80) 89.8 (15.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.247 , 0.266 (Not available) , 0.222	Depositor DCC
R_{free} test set	4041 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	77.6	Xtriage
Anisotropy	0.600	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 66.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.42	0/3427	0.86	2/4673 (0.0%)
1	B	0.42	0/3427	0.86	2/4673 (0.0%)
1	C	0.43	0/3427	0.87	1/4673 (0.0%)
1	D	0.44	0/3427	0.88	2/4673 (0.0%)
All	All	0.43	0/13708	0.87	7/18692 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	261	LYS	N-CA-C	-5.93	104.94	111.82
1	A	261	LYS	N-CA-C	-5.86	105.03	111.82
1	C	261	LYS	N-CA-C	-5.63	105.29	111.82
1	D	261	LYS	N-CA-C	-5.43	105.52	111.82
1	D	173	LYS	N-CA-C	-5.19	106.45	112.89
1	B	173	LYS	N-CA-C	-5.09	106.58	112.89
1	A	173	LYS	N-CA-C	-5.02	106.42	112.54

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	3349	0	3504	62	0
1	B	3349	0	3504	60	0
1	C	3349	0	3504	61	0
1	D	3349	0	3504	62	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
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	233	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 (233) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:418:PRO:C	1:A:420:ALA:H	2.05	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:D:418:PRO:C	1:D:420:ALA:H	2.05	0.63
1:B:382:THR:HG22	1:B:386:ILE:HG13	1.80	0.63
1:C:418:PRO:C	1:C:420:ALA:H	2.07	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:B:418:PRO:C	1:B:420:ALA:H	2.06	0.62
1:A:421:THR:HG22	1:A:423:PRO:CD	2.08	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:B:194:ILE:HG22	1:B:194:ILE:O	2.01	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:B:359:PHE:CD1	1:B:458:MET:HE3	2.39	0.58
1:D:421:THR:HG22	1:D:423:PRO:CD	2.10	0.58
1:C:359:PHE:CD1	1:C:458:MET:HE3	2.39	0.57
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:D:359:PHE:CD1	1:D:458:MET:HE3	2.41	0.56
1:A:359:PHE:CD1	1:A:458:MET:HE3	2.41	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:429:ALA:C	1:A:431:GLY:H	2.15	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:B:429:ALA:C	1:B:431:GLY:H	2.16	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:429:ALA:C	1:D:431:GLY:H	2.16	0.53
1:D:176:SER:HA	1:D:179:VAL:HG12	1.89	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:C:429:ALA:C	1:C:431:GLY:H	2.16	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:55:ILE:HD11	1:B:76:MET:HE3	1.93	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:55:ILE:HD11	1:A:76:MET:HE3	1.91	0.51
1:A:151:ASN:HB2	3:A:503:SIN:C4	2.41	0.51
1:C:55:ILE:HD11	1:C:76:MET:HE3	1.92	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: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:A:417:LEU:HB2	1:A:418:PRO:HD2	1.95	0.49
1:D:150:SER:HB3	1:D:153:ALA:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:D:55:ILE:HD11	1:D:76:MET:HE3	1.96	0.47
1:A:196:THR:HG22	1:A:218:MET:HG3	1.97	0.47
1:B:418:PRO:C	1:B:420:ALA:N	2.73	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:418:PRO:HD3	1:A:438:MET:HE3	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:A:418:PRO:C	1:A:420:ALA:N	2.72	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:418:PRO:HD3	1:D:438:MET:HE3	1.99	0.45
1:C:54:PHE:CD2	1:C:76:MET:HE1	2.51	0.44
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
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: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:B:418:PRO:HD3	1:B:438:MET:HE3	1.99	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:D:54:PHE:CD2	1:D:76:MET:HE1	2.54	0.43
1:B:167:SER:HB3	1:B:249:GLU:OE2	2.18	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:C:418:PRO:HD3	1:C:438:MET:HE3	2.00	0.42
1:D:236:LEU:HD23	1:D:441:VAL:HG11	2.01	0.42
1:B:212:LEU:HD13	1:B:217:TRP:HD1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:422:PRO:HB2	1:C:423:PRO:HD3	2.01	0.42
1:A:191:ILE:HG12	1:A:228:MET:HE2	2.02	0.42
1:A:54:PHE:CD2	1:A:76:MET:HE1	2.55	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:C:418:PRO:C	1:C:420:ALA:N	2.73	0.42
1:A:150:SER:O	1:A:154:THR:OG1	2.29	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:B:191:ILE:HG12	1:B:228:MET:HE2	2.02	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
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:362:ILE:HD11	1:B:458:MET:HE2	2.03	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:D:39:LEU:HA	1:D:40:PRO:HD3	1.85	0.41
1:D:191:ILE:HG12	1:D:228:MET:HE2	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:362:ILE:HD11	1:D:458:MET:HE2	2.03	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%)	6	21
1	B	443/445 (100%)	410 (93%)	24 (5%)	9 (2%)	6	21
1	C	443/445 (100%)	410 (93%)	24 (5%)	9 (2%)	6	21
1	D	443/445 (100%)	410 (93%)	24 (5%)	9 (2%)	6	21
All	All	1772/1780 (100%)	1637 (92%)	99 (6%)	36 (2%)	6	21

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

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Mol	Chain	Res	Type
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
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%)	14	40
1	B	355/355 (100%)	330 (93%)	25 (7%)	14	40
1	C	355/355 (100%)	330 (93%)	25 (7%)	14	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	355/355 (100%)	330 (93%)	25 (7%)	14	40
All	All	1420/1420 (100%)	1320 (93%)	100 (7%)	14	40

All (100) 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	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
1	A	369	VAL
1	A	379	VAL
1	A	382	THR
1	A	386	ILE
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	161	LEU
1	B	178	TYR
1	B	197	LEU
1	B	215	THR
1	B	227	MET
1	B	239	LEU
1	B	243	THR
1	B	248	PHE
1	B	250	LEU

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Mol	Chain	Res	Type
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	386	ILE
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	243	THR
1	C	248	PHE
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	386	ILE
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	161	LEU

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Mol	Chain	Res	Type
1	D	178	TYR
1	D	197	LEU
1	D	215	THR
1	D	227	MET
1	D	239	LEU
1	D	248	PHE
1	D	250	LEU
1	D	259	LYS
1	D	265	LEU
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	386	ILE
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 (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	378	ASN
1	A	432	HIS
1	B	43	HIS
1	B	151	ASN
1	B	378	ASN
1	B	432	HIS
1	C	43	HIS
1	C	378	ASN
1	C	432	HIS
1	D	43	HIS
1	D	432	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	D	503	-	7,7,7	1.06	0	8,8,8	1.25	0
3	SIN	A	503	-	7,7,7	1.06	0	8,8,8	1.17	0
3	SIN	C	503	-	7,7,7	1.06	0	8,8,8	1.18	0
3	SIN	B	503	-	7,7,7	1.06	0	8,8,8	1.14	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	D	503	-	-	4/5/5/5	-
3	SIN	A	503	-	-	4/5/5/5	-
3	SIN	C	503	-	-	4/5/5/5	-
3	SIN	B	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	D	503	SIN	O1-C1-C2-C3
3	D	503	SIN	O2-C1-C2-C3
3	C	503	SIN	C2-C3-C4-O3
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	C	503	SIN	C2-C3-C4-O4
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	B	503	SIN	C2-C3-C4-O3
3	A	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	D	503	SIN	1	0
3	A	503	SIN	1	0
3	C	503	SIN	1	0
3	B	503	SIN	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, 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	445/445 (100%)	-0.29	4 (0%) 81 74	43, 94, 165, 210	0
1	B	445/445 (100%)	-0.03	19 (4%) 40 31	54, 104, 189, 219	0
1	C	445/445 (100%)	-0.10	11 (2%) 58 48	41, 90, 170, 218	0
1	D	445/445 (100%)	-0.25	13 (2%) 53 43	18, 87, 156, 206	0
All	All	1780/1780 (100%)	-0.17	47 (2%) 57 47	18, 94, 173, 219	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	169	VAL	7.0
1	A	169	VAL	5.2
1	B	133	VAL	4.7
1	D	169	VAL	4.7
1	B	169	VAL	3.8
1	B	190	SER	3.4
1	B	244	LEU	3.2
1	C	244	LEU	3.2
1	A	250	LEU	3.0
1	B	255	VAL	2.9
1	C	136	PHE	2.9
1	D	259	LYS	2.8
1	D	18	LEU	2.8
1	C	177	THR	2.7
1	B	177	THR	2.7
1	C	133	VAL	2.7
1	A	199	GLY	2.6
1	D	248	PHE	2.6
1	B	132	SER	2.6
1	B	161	LEU	2.6
1	B	257	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	257	TRP	2.5
1	D	244	LEU	2.5
1	B	192	GLY	2.4
1	D	133	VAL	2.4
1	A	129	GLY	2.4
1	B	449	CYS	2.4
1	C	168	LYS	2.4
1	B	126	MET	2.4
1	D	245	ASN	2.3
1	B	250	LEU	2.3
1	C	432	HIS	2.2
1	B	438	MET	2.2
1	D	178	TYR	2.2
1	C	165	VAL	2.2
1	B	445	LEU	2.1
1	D	250	LEU	2.1
1	C	154	THR	2.1
1	B	179	VAL	2.1
1	D	132	SER	2.1
1	C	126	MET	2.0
1	D	432	HIS	2.0
1	B	199	GLY	2.0
1	C	193	GLY	2.0
1	D	256	ASN	2.0
1	B	306	ALA	2.0
1	B	178	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 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
2	NA	B	502	1/1	0.79	0.13	147,147,147,147	0
3	SIN	D	503	8/8	0.81	0.12	95,97,99,104	0
3	SIN	A	503	8/8	0.86	0.10	88,98,100,104	0
3	SIN	B	503	8/8	0.88	0.14	89,96,103,108	0
2	NA	B	501	1/1	0.88	0.08	115,115,115,115	0
3	SIN	C	503	8/8	0.89	0.20	87,100,105,112	0
2	NA	C	502	1/1	0.91	0.11	92,92,92,92	0
2	NA	D	501	1/1	0.91	0.12	88,88,88,88	0
2	NA	A	501	1/1	0.95	0.04	64,64,64,64	0
2	NA	D	502	1/1	0.95	0.09	82,82,82,82	0
2	NA	A	502	1/1	0.97	0.07	70,70,70,70	0
2	NA	C	501	1/1	0.98	0.05	82,82,82,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.