



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 01:54 AM EDT

PDB ID : 5UL9
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 : 2.78 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	:	4.02b-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

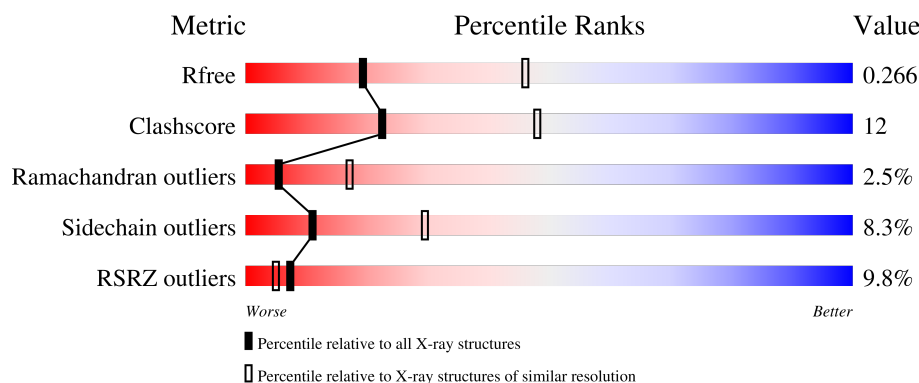
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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	<div> <div>9%</div> <div>73%</div> <div>22%</div> <div>.</div> </div>
1	B	445	<div> <div>11%</div> <div>72%</div> <div>22%</div> <div>5%</div> </div>
1	C	445	<div> <div>10%</div> <div>72%</div> <div>23%</div> <div>5%</div> </div>
1	D	445	<div> <div>9%</div> <div>72%</div> <div>23%</div> <div>5%</div> </div>

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
3	CIT	B	503	-	-	-	X
3	CIT	C	503	-	-	-	X
3	CIT	D	503	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13408 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
			3337	2225	522	564	26			
1	B	445	Total	C	N	O	S	0	0	0
			3337	2225	522	564	26			
1	C	445	Total	C	N	O	S	0	0	0
			3337	2225	522	564	26			
1	D	445	Total	C	N	O	S	0	0	0
			3337	2225	522	564	26			

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

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

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).

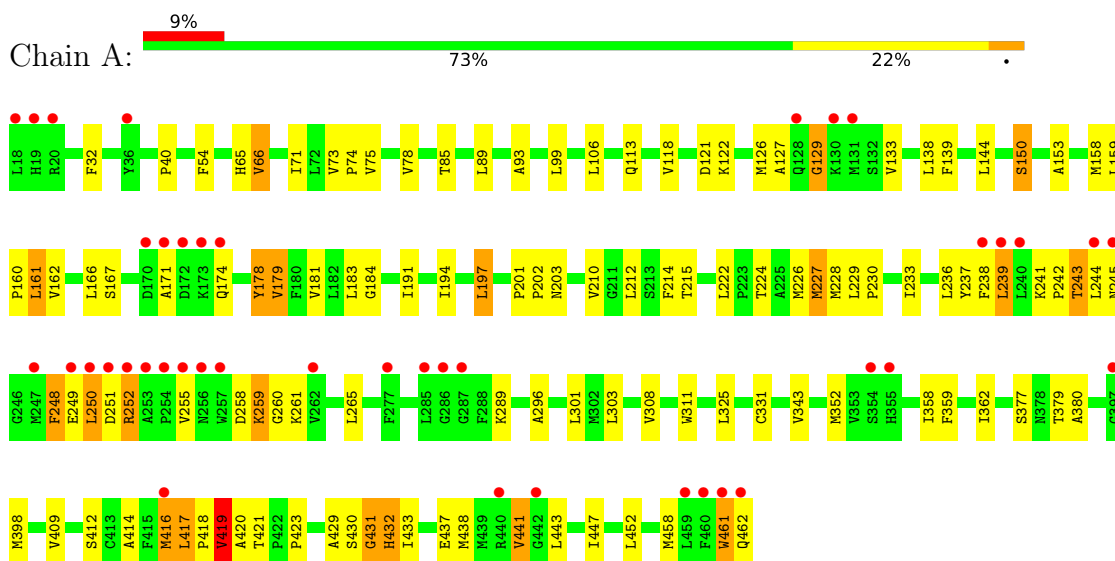


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		
3	D	1	Total	C	O	0	0
			13	6	7		

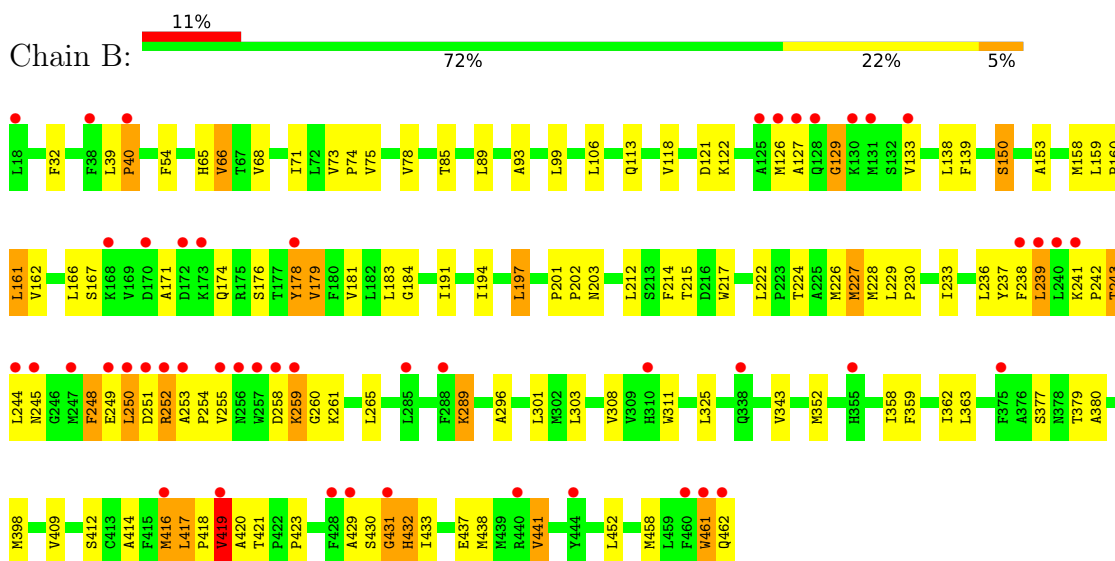
3 Residue-property plots [i](#)

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.

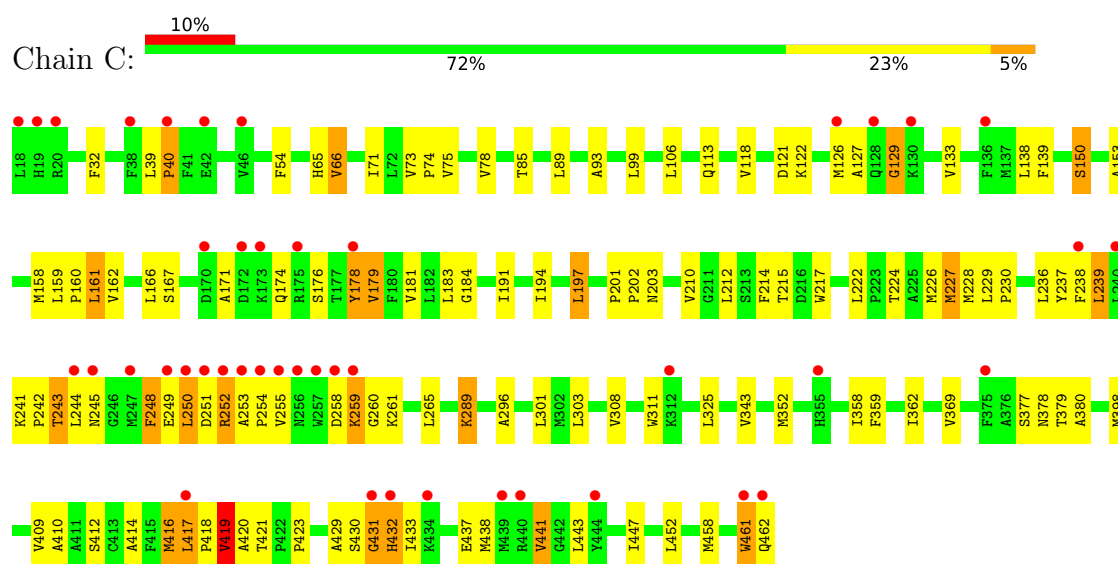
- Molecule 1: Transporter, NadC family



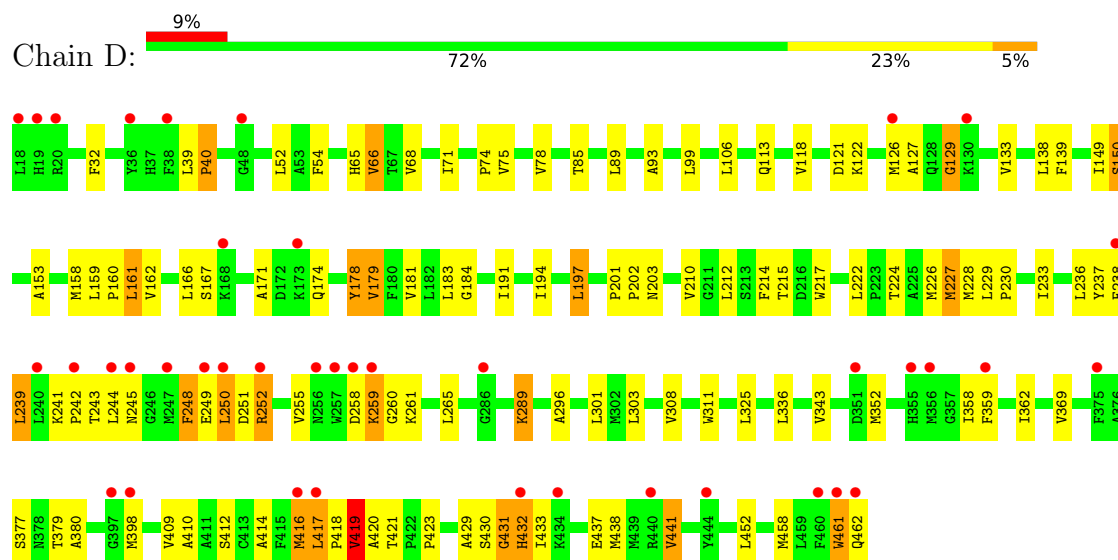
- Molecule 1: Transporter, NadC family



- 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	106.12Å 102.11Å 167.99Å 90.00° 99.52° 90.00°	Depositor
Resolution (Å)	15.00 – 2.78 14.99 – 2.78	Depositor EDS
% Data completeness (in resolution range)	87.3 (15.00-2.78) 87.4 (14.99-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.242 , 0.261 0.256 , 0.266	Depositor DCC
R_{free} test set	3927 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	72.3	Xtriage
Anisotropy	0.526	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 29.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13408	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% 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: CIT, 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	0.34	0/3416	0.55	2/4659 (0.0%)
1	B	0.33	0/3416	0.55	2/4659 (0.0%)
1	C	0.33	0/3416	0.55	2/4659 (0.0%)
1	D	0.33	0/3416	0.56	1/4659 (0.0%)
All	All	0.33	0/13664	0.55	7/18636 (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	239	LEU	CB-CA-C	7.23	123.94	110.20
1	C	239	LEU	CB-CA-C	7.19	123.87	110.20
1	D	239	LEU	CB-CA-C	7.09	123.67	110.20
1	A	239	LEU	CB-CA-C	7.07	123.62	110.20
1	C	239	LEU	N-CA-C	-5.50	96.14	111.00
1	B	239	LEU	N-CA-C	-5.35	96.55	111.00
1	A	239	LEU	N-CA-C	-5.04	97.39	111.00

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	3337	0	3476	79	0
1	B	3337	0	3477	83	0
1	C	3337	0	3477	86	0
1	D	3337	0	3477	85	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	13	0	5	2	0
3	B	13	0	5	2	0
3	C	13	0	5	3	0
3	D	13	0	5	2	0
All	All	13408	0	13927	317	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 12.

All (317) 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:D:421:THR:CG2	1:D:423:PRO:HD2	1.80	1.11
1:A:421:THR:CG2	1:A:423:PRO:HD2	1.80	1.09
1:C:421:THR:CG2	1:C:423:PRO:HD2	1.81	1.09
1:B:421:THR:CG2	1:B:423:PRO:HD2	1.83	1.08
1:D:421:THR:HG22	1:D:423:PRO:CD	1.84	1.07
1:C:421:THR:HG22	1:C:423:PRO:CD	1.86	1.06
1:A:421:THR:HG22	1:A:423:PRO:CD	1.85	1.06
1:B:421:THR:HG22	1:B:423:PRO:CD	1.87	1.04
1:D:379:THR:HG23	3:D:503:CIT:H21	1.56	0.87
1:C:379:THR:HG23	3:C:503:CIT:H21	1.56	0.85
1:C:78:VAL:HG11	1:C:85:THR:HG22	1.60	0.84
1:A:202:PRO:HD3	1:A:379:THR:HG22	1.60	0.83
1:B:379:THR:HG23	3:B:503:CIT:H21	1.59	0.83
1:A:78:VAL:HG11	1:A:85:THR:HG22	1.59	0.83
1:B:78:VAL:HG11	1:B:85:THR:HG22	1.60	0.82
1:D:78:VAL:HG11	1:D:85:THR:HG22	1.62	0.82
1:B:421:THR:HG22	1:B:423:PRO:HD2	0.90	0.81
1:B:202:PRO:HD3	1:B:379:THR:HG22	1.63	0.81
1:A:379:THR:HG23	3:A:503:CIT:H21	1.61	0.81
1:D:150:SER:HB3	1:D:153:ALA:HB3	1.62	0.81
1:C:421:THR:HG22	1:C:423:PRO:HD2	0.89	0.81
1:C:202:PRO:HD3	1:C:379:THR:HG22	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:TRP:HB3	1:D:65:HIS:HD2	1.45	0.80
1:D:202:PRO:HD3	1:D:379:THR:HG22	1.62	0.80
1:C:65:HIS:HD2	1:D:311:TRP:HB3	1.45	0.79
1:A:150:SER:HB3	1:A:153:ALA:HB3	1.64	0.79
1:C:65:HIS:CD2	1:D:311:TRP:HB3	2.20	0.77
1:A:421:THR:HG22	1:A:423:PRO:HD2	0.88	0.77
1:C:150:SER:HB3	1:C:153:ALA:HB3	1.66	0.76
1:A:129:GLY:HA2	1:A:248:PHE:HB2	1.69	0.75
1:D:421:THR:HG22	1:D:423:PRO:HD2	0.88	0.75
1:B:129:GLY:HA2	1:B:248:PHE:HB2	1.69	0.74
1:B:150:SER:HB3	1:B:153:ALA:HB3	1.69	0.74
1:B:379:THR:CG2	3:B:503:CIT:H21	2.18	0.73
1:D:129:GLY:HA2	1:D:248:PHE:HB2	1.69	0.73
1:C:75:VAL:HG11	1:D:301:LEU:HD11	1.70	0.73
1:C:129:GLY:HA2	1:C:248:PHE:HB2	1.69	0.73
1:A:311:TRP:HB3	1:B:65:HIS:HD2	1.53	0.73
1:D:379:THR:CG2	3:D:503:CIT:H21	2.18	0.72
1:C:379:THR:CG2	3:C:503:CIT:H21	2.19	0.71
1:A:65:HIS:HD2	1:B:311:TRP:HB3	1.55	0.71
1:C:222:LEU:O	1:C:226:MET:HG2	1.91	0.70
1:A:379:THR:CG2	3:A:503:CIT:H21	2.21	0.70
1:C:311:TRP:HB3	1:D:65:HIS:CD2	2.27	0.68
1:B:222:LEU:O	1:B:226:MET:HG2	1.95	0.66
1:A:311:TRP:HB3	1:B:65:HIS:CD2	2.30	0.66
1:A:301:LEU:HD11	1:B:75:VAL:HG11	1.78	0.66
1:A:71:ILE:O	1:A:74:PRO:HD2	1.96	0.64
1:D:377:SER:HB3	1:D:380:ALA:HB3	1.80	0.64
1:A:236:LEU:HD23	1:A:441:VAL:HG11	1.80	0.63
1:A:222:LEU:O	1:A:226:MET:HG2	1.97	0.63
1:D:113:GLN:HG3	1:D:261:LYS:HG2	1.80	0.63
1:C:416:MET:O	1:C:438:MET:HG2	1.98	0.63
1:C:236:LEU:HD23	1:C:441:VAL:HG11	1.81	0.62
1:B:236:LEU:HD23	1:B:441:VAL:HG11	1.82	0.62
1:D:416:MET:O	1:D:438:MET:HG2	2.00	0.62
1:B:416:MET:O	1:B:438:MET:HG2	1.99	0.61
1:D:222:LEU:O	1:D:226:MET:HG2	2.00	0.61
1:A:113:GLN:HG3	1:A:261:LYS:HG2	1.82	0.61
1:D:66:VAL:HG12	1:D:325:LEU:HD13	1.82	0.61
1:A:65:HIS:CD2	1:B:311:TRP:HB3	2.36	0.60
1:A:416:MET:O	1:A:438:MET:HG2	2.00	0.60
1:D:32:PHE:HB2	1:D:54:PHE:HD1	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:GLN:HG3	1:B:261:LYS:HG2	1.82	0.60
1:D:191:ILE:HG12	1:D:228:MET:HE2	1.84	0.60
1:D:236:LEU:HD23	1:D:441:VAL:HG11	1.83	0.60
1:C:66:VAL:HG12	1:C:325:LEU:HD13	1.83	0.60
1:B:32:PHE:HB2	1:B:54:PHE:HD1	1.65	0.59
1:C:113:GLN:HG3	1:C:261:LYS:HG2	1.83	0.59
1:C:32:PHE:HB2	1:C:54:PHE:HD1	1.67	0.59
1:A:32:PHE:HB2	1:A:54:PHE:HD1	1.67	0.59
1:A:66:VAL:HG12	1:A:325:LEU:HD13	1.85	0.58
1:A:377:SER:HB3	1:A:380:ALA:HB3	1.85	0.58
1:C:377:SER:HB3	1:C:380:ALA:HB3	1.85	0.58
1:A:414:ALA:HB1	1:A:420:ALA:HB1	1.86	0.58
1:D:227:MET:HG2	1:D:452:LEU:HD11	1.86	0.58
1:B:66:VAL:HG12	1:B:325:LEU:HD13	1.85	0.58
1:B:377:SER:HB3	1:B:380:ALA:HB3	1.85	0.58
1:B:227:MET:HG2	1:B:452:LEU:HD11	1.86	0.57
1:D:418:PRO:C	1:D:420:ALA:H	2.08	0.57
1:C:71:ILE:O	1:C:74:PRO:HD2	2.04	0.57
1:B:418:PRO:O	1:B:419:VAL:HG12	2.04	0.57
1:C:418:PRO:O	1:C:419:VAL:HG12	2.05	0.57
1:A:167:SER:HB3	1:A:249:GLU:OE2	2.04	0.57
1:C:183:LEU:HD13	1:C:433:ILE:CD1	2.35	0.57
1:C:301:LEU:HD11	1:D:75:VAL:HG11	1.85	0.57
1:B:159:LEU:HB3	1:B:160:PRO:HD3	1.88	0.56
1:A:418:PRO:C	1:A:420:ALA:H	2.08	0.56
1:D:201:PRO:HB2	1:D:379:THR:CG2	2.35	0.56
1:D:418:PRO:O	1:D:419:VAL:HG12	2.05	0.56
1:A:159:LEU:HB3	1:A:160:PRO:HD3	1.88	0.56
1:D:414:ALA:HB1	1:D:420:ALA:HB1	1.88	0.56
1:A:127:ALA:HB1	1:A:133:VAL:HG13	1.88	0.56
1:B:167:SER:HB3	1:B:249:GLU:OE2	2.06	0.56
1:C:227:MET:HG2	1:C:452:LEU:HD11	1.87	0.56
1:D:71:ILE:O	1:D:74:PRO:HD2	2.06	0.56
1:D:167:SER:HB3	1:D:249:GLU:OE2	2.06	0.56
1:A:227:MET:HG2	1:A:452:LEU:HD11	1.87	0.56
1:C:418:PRO:C	1:C:420:ALA:H	2.09	0.55
1:D:194:ILE:HG22	1:D:194:ILE:O	2.06	0.55
1:C:167:SER:HB3	1:C:249:GLU:OE2	2.06	0.55
1:C:414:ALA:HB1	1:C:420:ALA:HB1	1.87	0.55
1:B:127:ALA:HB1	1:B:133:VAL:HG13	1.89	0.55
1:C:127:ALA:HB1	1:C:133:VAL:HG13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ILE:HG12	1:A:228:MET:CE	2.36	0.55
1:A:418:PRO:HD3	1:A:438:MET:HE3	1.88	0.55
1:B:71:ILE:O	1:B:74:PRO:HD2	2.06	0.55
1:D:191:ILE:HG12	1:D:228:MET:CE	2.37	0.55
1:B:414:ALA:HB1	1:B:420:ALA:HB1	1.88	0.55
1:A:122:LYS:O	1:A:126:MET:HG2	2.07	0.55
1:A:201:PRO:HB2	1:A:379:THR:CG2	2.36	0.55
1:D:127:ALA:HB1	1:D:133:VAL:HG13	1.89	0.55
1:C:159:LEU:HB3	1:C:160:PRO:HD3	1.88	0.55
1:C:201:PRO:HB2	1:C:379:THR:CG2	2.37	0.55
1:C:418:PRO:HD3	1:C:438:MET:CE	2.36	0.55
1:D:159:LEU:HB3	1:D:160:PRO:HD3	1.89	0.54
1:D:229:LEU:HB3	1:D:230:PRO:HD3	1.89	0.54
1:C:191:ILE:HG12	1:C:228:MET:HE2	1.89	0.54
1:B:418:PRO:C	1:B:420:ALA:H	2.10	0.54
1:B:122:LYS:O	1:B:126:MET:HG2	2.08	0.54
1:A:183:LEU:HD13	1:A:433:ILE:CD1	2.38	0.54
1:B:191:ILE:HG12	1:B:228:MET:CE	2.37	0.54
1:A:194:ILE:O	1:A:194:ILE:HG22	2.06	0.54
1:B:201:PRO:HB2	1:B:379:THR:CG2	2.37	0.54
1:C:418:PRO:HD3	1:C:438:MET:HE3	1.90	0.54
1:A:417:LEU:HD23	1:A:417:LEU:H	1.73	0.53
1:A:418:PRO:HD3	1:A:438:MET:CE	2.39	0.53
1:B:194:ILE:HG22	1:B:194:ILE:O	2.07	0.53
1:D:418:PRO:HD3	1:D:438:MET:HE3	1.88	0.53
1:B:229:LEU:HB3	1:B:230:PRO:HD3	1.90	0.53
1:D:122:LYS:O	1:D:126:MET:HG2	2.09	0.53
1:C:122:LYS:O	1:C:126:MET:HG2	2.08	0.53
1:C:191:ILE:HG12	1:C:228:MET:CE	2.38	0.53
1:C:429:ALA:C	1:C:431:GLY:H	2.12	0.53
1:D:417:LEU:HD23	1:D:417:LEU:H	1.74	0.53
1:A:418:PRO:O	1:A:419:VAL:HG12	2.08	0.52
1:A:429:ALA:C	1:A:431:GLY:H	2.12	0.52
1:B:429:ALA:C	1:B:431:GLY:H	2.12	0.52
1:A:106:LEU:HD12	1:A:303:LEU:HD11	1.92	0.52
1:C:229:LEU:HB3	1:C:230:PRO:HD3	1.91	0.52
1:D:106:LEU:HD12	1:D:303:LEU:HD11	1.90	0.52
1:B:106:LEU:HD12	1:B:303:LEU:HD11	1.92	0.52
1:B:183:LEU:HD13	1:B:433:ILE:CD1	2.39	0.52
1:B:418:PRO:HD3	1:B:438:MET:CE	2.40	0.52
1:D:78:VAL:CG1	1:D:85:THR:HG22	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:418:PRO:HD3	1:D:438:MET:CE	2.39	0.51
1:B:359:PHE:CD1	1:B:458:MET:HE3	2.45	0.51
1:C:194:ILE:O	1:C:194:ILE:HG22	2.09	0.51
1:B:417:LEU:HD23	1:B:417:LEU:H	1.76	0.51
1:D:429:ALA:C	1:D:431:GLY:H	2.13	0.51
1:B:418:PRO:HD3	1:B:438:MET:HE3	1.93	0.51
1:C:417:LEU:HD23	1:C:417:LEU:H	1.76	0.51
1:A:229:LEU:HB3	1:A:230:PRO:HD3	1.91	0.50
1:A:78:VAL:CG1	1:A:85:THR:HG22	2.37	0.50
1:A:75:VAL:HG11	1:B:301:LEU:HD11	1.92	0.50
1:B:78:VAL:CG1	1:B:85:THR:HG22	2.37	0.50
1:A:93:ALA:HB2	1:B:93:ALA:HB2	1.94	0.50
1:C:139:PHE:CE2	1:C:184:GLY:HA3	2.47	0.50
1:C:93:ALA:HB2	1:D:93:ALA:HB2	1.94	0.49
1:D:183:LEU:HD13	1:D:433:ILE:CD1	2.43	0.49
1:C:106:LEU:HD12	1:C:303:LEU:HD11	1.95	0.49
1:B:139:PHE:CE2	1:B:184:GLY:HA3	2.48	0.49
1:A:139:PHE:CE2	1:A:184:GLY:HA3	2.48	0.48
1:C:78:VAL:CG1	1:C:85:THR:HG22	2.37	0.48
1:A:461:TRP:HE3	1:A:462:GLN:HG3	1.79	0.48
1:A:362:ILE:HD11	1:A:458:MET:HE2	1.96	0.48
1:D:138:LEU:HD13	1:D:162:VAL:HG22	1.95	0.48
1:D:52:LEU:HD13	1:D:336:LEU:HD21	1.95	0.48
1:B:461:TRP:HE3	1:B:462:GLN:HG3	1.78	0.47
1:A:194:ILE:O	1:A:194:ILE:CG2	2.62	0.47
1:D:139:PHE:CE2	1:D:184:GLY:HA3	2.49	0.47
1:C:194:ILE:HD13	1:C:409:VAL:HG13	1.96	0.47
1:A:237:TYR:HB3	1:A:238:PHE:HD1	1.79	0.47
1:A:437:GLU:O	1:A:441:VAL:HG23	2.15	0.47
1:C:74:PRO:O	1:C:78:VAL:HG23	2.15	0.47
1:C:461:TRP:HE3	1:C:462:GLN:HG3	1.79	0.47
1:B:191:ILE:HG12	1:B:228:MET:HE2	1.97	0.47
1:A:129:GLY:CA	1:A:248:PHE:HB2	2.43	0.47
1:C:437:GLU:O	1:C:441:VAL:HG23	2.14	0.47
1:D:194:ILE:O	1:D:194:ILE:CG2	2.62	0.46
1:D:461:TRP:HE3	1:D:462:GLN:HG3	1.79	0.46
1:D:74:PRO:O	1:D:78:VAL:HG23	2.15	0.46
1:D:243:THR:C	1:D:245:ASN:H	2.18	0.46
1:B:237:TYR:HB3	1:B:238:PHE:HD1	1.80	0.46
1:B:437:GLU:O	1:B:441:VAL:HG23	2.15	0.46
1:C:201:PRO:HG2	1:C:379:THR:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:PHE:CD1	1:C:458:MET:HE3	2.50	0.46
1:D:178:TYR:HE2	1:D:432:HIS:CG	2.34	0.46
1:D:359:PHE:CD1	1:D:458:MET:HE3	2.50	0.46
1:C:166:LEU:HD11	1:C:181:VAL:CB	2.45	0.46
1:D:258:ASP:O	1:D:260:GLY:N	2.49	0.46
1:C:99:LEU:HD12	1:C:296:ALA:HB2	1.97	0.46
1:A:99:LEU:HD12	1:A:296:ALA:HB2	1.98	0.46
1:B:194:ILE:HD13	1:B:409:VAL:HG13	1.97	0.46
1:A:178:TYR:HE2	1:A:432:HIS:CG	2.33	0.46
1:C:171:ALA:O	1:C:174:GLN:HB3	2.16	0.46
1:C:237:TYR:HB3	1:C:238:PHE:HD1	1.80	0.46
1:D:437:GLU:O	1:D:441:VAL:HG23	2.16	0.46
1:A:243:THR:C	1:A:245:ASN:H	2.19	0.46
1:B:194:ILE:O	1:B:194:ILE:CG2	2.64	0.46
1:A:138:LEU:HD13	1:A:162:VAL:HG22	1.99	0.45
1:B:171:ALA:O	1:B:174:GLN:HB3	2.17	0.45
1:C:243:THR:C	1:C:245:ASN:H	2.19	0.45
1:C:178:TYR:HE2	1:C:432:HIS:CG	2.35	0.45
1:D:194:ILE:HD13	1:D:409:VAL:HG13	1.99	0.45
1:D:237:TYR:HB3	1:D:238:PHE:HD1	1.80	0.45
1:B:161:LEU:HD11	1:B:252:ARG:CZ	2.47	0.45
1:C:194:ILE:O	1:C:194:ILE:CG2	2.65	0.45
1:C:258:ASP:O	1:C:260:GLY:N	2.50	0.45
1:B:243:THR:C	1:B:245:ASN:H	2.19	0.45
1:C:358:ILE:O	1:C:362:ILE:HG23	2.17	0.45
1:C:39:LEU:HA	1:C:40:PRO:HD3	1.87	0.44
1:D:171:ALA:O	1:D:174:GLN:HB3	2.17	0.44
1:D:224:THR:O	1:D:228:MET:HB2	2.16	0.44
1:C:161:LEU:HD11	1:C:252:ARG:CZ	2.48	0.44
1:A:171:ALA:O	1:A:174:GLN:HB3	2.16	0.44
1:A:191:ILE:HG12	1:A:228:MET:HE3	1.99	0.44
1:B:178:TYR:HE2	1:B:432:HIS:CG	2.35	0.44
1:C:258:ASP:OD1	1:C:261:LYS:HG3	2.18	0.44
1:B:201:PRO:HG2	1:B:379:THR:HG21	2.00	0.44
1:D:99:LEU:HD12	1:D:296:ALA:HB2	1.98	0.44
1:A:358:ILE:O	1:A:362:ILE:HG23	2.17	0.44
1:A:191:ILE:HG12	1:A:228:MET:HE2	1.99	0.44
1:B:129:GLY:CA	1:B:248:PHE:HB2	2.44	0.44
1:B:161:LEU:HD11	1:B:252:ARG:NH2	2.32	0.44
1:B:258:ASP:O	1:B:260:GLY:N	2.51	0.43
1:C:65:HIS:CD2	1:D:311:TRP:CB	2.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:LEU:HD11	1:D:252:ARG:CZ	2.48	0.43
1:B:212:LEU:HD13	1:B:217:TRP:HD1	1.83	0.43
1:D:39:LEU:HA	1:D:40:PRO:HD3	1.86	0.43
1:B:99:LEU:HD12	1:B:296:ALA:HB2	2.01	0.43
1:D:161:LEU:HD11	1:D:252:ARG:NH2	2.33	0.43
1:B:461:TRP:HZ3	1:B:462:GLN:HE21	1.66	0.43
1:D:118:VAL:HG12	1:D:255:VAL:HB	2.00	0.43
1:A:461:TRP:HZ3	1:A:462:GLN:HE21	1.67	0.43
1:A:161:LEU:HD11	1:A:252:ARG:NH2	2.34	0.43
1:C:362:ILE:HD11	1:C:458:MET:HE2	1.99	0.43
1:D:201:PRO:HB2	1:D:379:THR:HG21	2.00	0.43
1:D:461:TRP:HZ3	1:D:462:GLN:HE21	1.67	0.43
1:A:161:LEU:HD11	1:A:252:ARG:CZ	2.49	0.43
1:C:138:LEU:HD13	1:C:162:VAL:HG22	2.01	0.43
1:C:161:LEU:HD11	1:C:252:ARG:NH2	2.33	0.43
1:A:73:VAL:HG12	1:A:331:CYS:SG	2.59	0.42
1:B:39:LEU:HA	1:B:40:PRO:HD3	1.87	0.42
1:C:461:TRP:HZ3	1:C:462:GLN:HE21	1.67	0.42
1:A:118:VAL:HG12	1:A:255:VAL:HB	2.00	0.42
1:A:210:VAL:HG23	1:A:212:LEU:HG	2.01	0.42
1:A:258:ASP:O	1:A:260:GLY:N	2.52	0.42
1:B:166:LEU:HD11	1:B:181:VAL:CB	2.49	0.42
1:B:179:VAL:HG23	1:B:432:HIS:CE1	2.55	0.42
1:B:289:LYS:HD2	1:B:289:LYS:HA	1.81	0.42
1:D:250:LEU:H	1:D:250:LEU:HD23	1.84	0.42
1:C:179:VAL:HG23	1:C:432:HIS:CE1	2.55	0.42
1:A:201:PRO:HG2	1:A:379:THR:HG21	2.01	0.42
1:B:251:ASP:O	1:B:252:ARG:HB3	2.20	0.42
1:C:73:VAL:HB	1:C:74:PRO:HD3	2.02	0.42
1:D:166:LEU:HD11	1:D:181:VAL:CB	2.49	0.42
1:D:179:VAL:HG23	1:D:432:HIS:CE1	2.55	0.42
1:D:358:ILE:O	1:D:362:ILE:HG23	2.20	0.42
1:A:166:LEU:HD11	1:A:181:VAL:CB	2.50	0.42
1:B:250:LEU:HD23	1:B:250:LEU:H	1.85	0.42
1:A:194:ILE:HD13	1:A:409:VAL:HG13	2.02	0.42
1:D:129:GLY:CA	1:D:248:PHE:HB2	2.43	0.42
1:D:201:PRO:HG2	1:D:379:THR:HG21	2.02	0.42
1:D:258:ASP:OD1	1:D:261:LYS:HG3	2.20	0.42
1:A:250:LEU:H	1:A:250:LEU:HD23	1.85	0.42
1:C:224:THR:O	1:C:228:MET:HB2	2.20	0.42
1:A:179:VAL:HG23	1:A:432:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:PRO:HB2	1:A:379:THR:HG21	2.00	0.41
1:A:224:THR:O	1:A:228:MET:HB2	2.19	0.41
1:B:258:ASP:OD1	1:B:261:LYS:HG3	2.20	0.41
1:A:258:ASP:OD1	1:A:261:LYS:HG3	2.20	0.41
1:B:233:ILE:O	1:B:237:TYR:HB2	2.21	0.41
1:C:212:LEU:HD13	1:C:217:TRP:HD1	1.85	0.41
1:D:149:ILE:O	1:D:150:SER:HB2	2.21	0.41
1:B:253:ALA:HA	1:B:254:PRO:HD3	1.95	0.41
1:C:118:VAL:HG12	1:C:255:VAL:HB	2.02	0.41
1:D:251:ASP:O	1:D:252:ARG:HB3	2.20	0.41
1:D:289:LYS:HD2	1:D:289:LYS:HA	1.83	0.41
1:B:65:HIS:HB3	1:B:68:VAL:HG23	2.02	0.41
1:D:197:LEU:HD12	1:D:214:PHE:HA	2.02	0.41
1:B:118:VAL:HG12	1:B:255:VAL:HB	2.02	0.41
1:B:138:LEU:HD13	1:B:162:VAL:HG22	2.01	0.41
1:B:197:LEU:HD12	1:B:214:PHE:HA	2.02	0.41
1:C:197:LEU:HD12	1:C:214:PHE:HA	2.03	0.41
1:C:253:ALA:HA	1:C:254:PRO:HD3	1.96	0.41
1:D:212:LEU:HD13	1:D:217:TRP:HD1	1.86	0.41
1:D:233:ILE:O	1:D:237:TYR:HB2	2.20	0.41
1:C:176:SER:HA	1:C:179:VAL:HG12	2.03	0.41
1:C:250:LEU:HD23	1:C:250:LEU:H	1.85	0.41
1:C:311:TRP:CB	1:D:65:HIS:CD2	3.00	0.41
1:D:210:VAL:HG23	1:D:212:LEU:HG	2.02	0.41
1:A:359:PHE:CD1	1:A:458:MET:HE3	2.55	0.41
1:B:73:VAL:HB	1:B:74:PRO:HD3	2.03	0.41
1:B:358:ILE:O	1:B:362:ILE:HG23	2.21	0.41
1:D:227:MET:HB3	1:D:452:LEU:HD21	2.03	0.41
1:A:251:ASP:O	1:A:252:ARG:HB3	2.20	0.41
1:C:210:VAL:HG23	1:C:212:LEU:HG	2.02	0.41
1:B:224:THR:O	1:B:228:MET:HB2	2.21	0.40
1:C:289:LYS:HA	1:C:289:LYS:HD2	1.79	0.40
1:C:443:LEU:O	1:C:447:ILE:HD12	2.21	0.40
1:D:369:VAL:HG23	1:D:410:ALA:HB1	2.03	0.40
1:A:443:LEU:O	1:A:447:ILE:HD12	2.21	0.40
1:B:176:SER:HA	1:B:179:VAL:HG12	2.03	0.40
1:C:251:ASP:O	1:C:252:ARG:HB3	2.20	0.40
1:C:359:PHE:HA	1:C:458:MET:HE1	2.03	0.40
1:A:197:LEU:HD12	1:A:214:PHE:HA	2.03	0.40
1:B:74:PRO:O	1:B:78:VAL:HG23	2.21	0.40
1:B:201:PRO:HB2	1:B:379:THR:HG21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:VAL:HG23	1:C:410:ALA:HB1	2.03	0.40
1:C:378:ASN:HB2	3:C:503:CIT:C6	2.51	0.40
1:A:178:TYR:CE2	1:A:432:HIS:CG	3.10	0.40
1:A:233:ILE:O	1:A:237:TYR:HB2	2.22	0.40
1:B:183:LEU:HD12	1:B:183:LEU:HA	1.96	0.40
1:B:359:PHE:HE2	1:B:363:LEU:HD22	1.87	0.40
1:C:201:PRO:HB2	1:C:379:THR:HG21	2.03	0.40
1:D:65:HIS:HB3	1:D:68:VAL:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	401 (90%)	31 (7%)	11 (2%)	5	17
1	B	443/445 (100%)	400 (90%)	32 (7%)	11 (2%)	5	17
1	C	443/445 (100%)	399 (90%)	33 (7%)	11 (2%)	5	17
1	D	443/445 (100%)	400 (90%)	32 (7%)	11 (2%)	5	17
All	All	1772/1780 (100%)	1600 (90%)	128 (7%)	44 (2%)	5	17

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	PRO
1	A	259	LYS
1	A	419	VAL
1	B	242	PRO
1	B	259	LYS
1	B	419	VAL
1	C	242	PRO

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Mol	Chain	Res	Type
1	C	259	LYS
1	C	419	VAL
1	D	242	PRO
1	D	259	LYS
1	D	419	VAL
1	A	416	MET
1	B	416	MET
1	C	416	MET
1	D	252	ARG
1	D	416	MET
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	A	40	PRO
1	A	430	SER
1	B	430	SER
1	C	66	VAL
1	C	430	SER
1	D	430	SER
1	A	431	GLY
1	B	40	PRO
1	C	40	PRO
1	C	431	GLY
1	D	40	PRO
1	D	431	GLY
1	B	66	VAL
1	B	431	GLY
1	D	66	VAL
1	A	66	VAL
1	A	129	GLY
1	C	129	GLY
1	D	129	GLY
1	B	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	351/353 (99%)	321 (92%)	30 (8%)	10	28
1	B	351/353 (99%)	322 (92%)	29 (8%)	11	29
1	C	351/353 (99%)	322 (92%)	29 (8%)	11	29
1	D	351/353 (99%)	323 (92%)	28 (8%)	12	31
All	All	1404/1412 (99%)	1288 (92%)	116 (8%)	11	29

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	LEU
1	A	121	ASP
1	A	144	LEU
1	A	158	MET
1	A	161	LEU
1	A	178	TYR
1	A	179	VAL
1	A	197	LEU
1	A	203	ASN
1	A	215	THR
1	A	227	MET
1	A	239	LEU
1	A	241	LYS
1	A	243	THR
1	A	244	LEU
1	A	248	PHE
1	A	250	LEU
1	A	259	LYS
1	A	265	LEU
1	A	289	LYS
1	A	308	VAL
1	A	343	VAL
1	A	352	MET
1	A	398	MET
1	A	412	SER
1	A	417	LEU
1	A	419	VAL
1	A	432	HIS

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Mol	Chain	Res	Type
1	A	441	VAL
1	A	461	TRP
1	B	89	LEU
1	B	121	ASP
1	B	158	MET
1	B	161	LEU
1	B	178	TYR
1	B	179	VAL
1	B	197	LEU
1	B	203	ASN
1	B	215	THR
1	B	227	MET
1	B	239	LEU
1	B	241	LYS
1	B	243	THR
1	B	244	LEU
1	B	248	PHE
1	B	250	LEU
1	B	259	LYS
1	B	265	LEU
1	B	289	LYS
1	B	308	VAL
1	B	343	VAL
1	B	352	MET
1	B	398	MET
1	B	412	SER
1	B	417	LEU
1	B	419	VAL
1	B	432	HIS
1	B	441	VAL
1	B	461	TRP
1	C	89	LEU
1	C	121	ASP
1	C	158	MET
1	C	161	LEU
1	C	178	TYR
1	C	179	VAL
1	C	197	LEU
1	C	203	ASN
1	C	215	THR
1	C	227	MET
1	C	239	LEU

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Mol	Chain	Res	Type
1	C	241	LYS
1	C	243	THR
1	C	244	LEU
1	C	248	PHE
1	C	250	LEU
1	C	259	LYS
1	C	265	LEU
1	C	289	LYS
1	C	308	VAL
1	C	343	VAL
1	C	352	MET
1	C	398	MET
1	C	412	SER
1	C	417	LEU
1	C	419	VAL
1	C	432	HIS
1	C	441	VAL
1	C	461	TRP
1	D	89	LEU
1	D	121	ASP
1	D	158	MET
1	D	161	LEU
1	D	178	TYR
1	D	179	VAL
1	D	197	LEU
1	D	203	ASN
1	D	215	THR
1	D	227	MET
1	D	239	LEU
1	D	241	LYS
1	D	244	LEU
1	D	248	PHE
1	D	250	LEU
1	D	259	LYS
1	D	265	LEU
1	D	289	LYS
1	D	308	VAL
1	D	343	VAL
1	D	352	MET
1	D	398	MET
1	D	412	SER
1	D	417	LEU

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Mol	Chain	Res	Type
1	D	419	VAL
1	D	432	HIS
1	D	441	VAL
1	D	461	TRP

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	432	HIS
1	A	462	GLN
1	B	432	HIS
1	B	462	GLN
1	C	432	HIS
1	C	462	GLN
1	D	432	HIS

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	CIT	A	503	-	12,12,12	1.00	0	17,17,17	1.36	2 (11%)
3	CIT	B	503	-	12,12,12	0.99	0	17,17,17	1.22	1 (5%)
3	CIT	D	503	-	12,12,12	0.99	0	17,17,17	1.22	1 (5%)
3	CIT	C	503	-	12,12,12	0.98	0	17,17,17	1.35	2 (11%)

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	CIT	A	503	-	-	9/16/16/16	-
3	CIT	B	503	-	-	7/16/16/16	-
3	CIT	D	503	-	-	7/16/16/16	-
3	CIT	C	503	-	-	9/16/16/16	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	503	CIT	O6-C6-C3	3.73	119.53	113.05
3	C	503	CIT	O6-C6-C3	3.71	119.49	113.05
3	B	503	CIT	O6-C6-C3	3.34	118.84	113.05
3	D	503	CIT	O6-C6-C3	3.29	118.76	113.05
3	A	503	CIT	O5-C6-C3	-2.55	118.64	122.25
3	C	503	CIT	O5-C6-C3	-2.37	118.89	122.25

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	CIT	C2-C3-C6-O5
3	A	503	CIT	C2-C3-C6-O6
3	A	503	CIT	O7-C3-C6-O5
3	A	503	CIT	O7-C3-C6-O6
3	B	503	CIT	C2-C3-C6-O5
3	B	503	CIT	C2-C3-C6-O6
3	B	503	CIT	O7-C3-C6-O5
3	B	503	CIT	O7-C3-C6-O6

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Mol	Chain	Res	Type	Atoms
3	C	503	CIT	C2-C3-C6-O5
3	C	503	CIT	C2-C3-C6-O6
3	C	503	CIT	O7-C3-C6-O5
3	C	503	CIT	O7-C3-C6-O6
3	D	503	CIT	C2-C3-C6-O5
3	D	503	CIT	C2-C3-C6-O6
3	D	503	CIT	O7-C3-C6-O5
3	D	503	CIT	O7-C3-C6-O6
3	A	503	CIT	C1-C2-C3-O7
3	C	503	CIT	C1-C2-C3-O7
3	D	503	CIT	C1-C2-C3-O7
3	A	503	CIT	C1-C2-C3-C6
3	B	503	CIT	C1-C2-C3-O7
3	B	503	CIT	C1-C2-C3-C6
3	C	503	CIT	C1-C2-C3-C6
3	D	503	CIT	C1-C2-C3-C6
3	A	503	CIT	C1-C2-C3-C4
3	B	503	CIT	C1-C2-C3-C4
3	C	503	CIT	C1-C2-C3-C4
3	D	503	CIT	C1-C2-C3-C4
3	A	503	CIT	C4-C3-C6-O5
3	A	503	CIT	C4-C3-C6-O6
3	C	503	CIT	C4-C3-C6-O5
3	C	503	CIT	C4-C3-C6-O6

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	CIT	2	0
3	B	503	CIT	2	0
3	D	503	CIT	2	0
3	C	503	CIT	3	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%)	0.20	42 (9%) 8 6	25, 69, 127, 174	0
1	B	445/445 (100%)	0.25	48 (10%) 5 4	37, 77, 142, 179	0
1	C	445/445 (100%)	0.15	44 (9%) 7 5	23, 63, 129, 179	0
1	D	445/445 (100%)	0.12	40 (8%) 9 6	25, 65, 117, 176	0
All	All	1780/1780 (100%)	0.18	174 (9%) 7 5	23, 68, 132, 179	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	462	GLN	15.8
1	C	462	GLN	13.1
1	B	240	LEU	8.7
1	B	462	GLN	7.8
1	C	254	PRO	7.4
1	B	245	ASN	7.1
1	C	256	ASN	7.0
1	C	250	LEU	7.0
1	A	255	VAL	6.9
1	A	18	LEU	6.8
1	D	259	LYS	6.6
1	B	259	LYS	6.5
1	B	126	MET	6.4
1	A	461	TRP	6.4
1	A	247	MET	6.3
1	A	130	LYS	6.2
1	B	257	TRP	6.0
1	C	172	ASP	5.9
1	B	461	TRP	5.9
1	A	462	GLN	5.8
1	C	461	TRP	5.8

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Mol	Chain	Res	Type	RSRZ
1	C	253	ALA	5.7
1	B	247	MET	5.6
1	A	240	LEU	5.6
1	B	258	ASP	5.4
1	C	245	ASN	5.0
1	A	245	ASN	5.0
1	A	128	GLN	4.9
1	C	38	PHE	4.9
1	C	247	MET	4.9
1	B	355	HIS	4.8
1	C	355	HIS	4.8
1	C	251	ASP	4.7
1	B	173	LYS	4.6
1	C	249	GLU	4.6
1	A	252	ARG	4.5
1	B	172	ASP	4.5
1	D	258	ASP	4.5
1	A	256	ASN	4.5
1	D	130	LYS	4.5
1	B	249	GLU	4.4
1	D	461	TRP	4.4
1	D	245	ASN	4.3
1	B	256	ASN	4.3
1	C	128	GLN	4.3
1	B	170	ASP	4.3
1	C	18	LEU	4.2
1	C	19	HIS	4.0
1	A	355	HIS	4.0
1	A	253	ALA	4.0
1	B	40	PRO	4.0
1	A	173	LYS	3.9
1	B	18	LEU	3.9
1	B	128	GLN	3.9
1	B	133	VAL	3.9
1	A	286	GLY	3.9
1	B	127	ALA	3.8
1	D	355	HIS	3.8
1	C	255	VAL	3.8
1	D	168	LYS	3.7
1	A	460	PHE	3.7
1	D	375	PHE	3.7
1	C	431	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	398	MET	3.6
1	B	429	ALA	3.6
1	C	240	LEU	3.5
1	B	239	LEU	3.5
1	C	130	LYS	3.5
1	D	249	GLU	3.4
1	B	255	VAL	3.4
1	B	375	PHE	3.4
1	A	170	ASP	3.4
1	A	251	ASP	3.4
1	B	125	ALA	3.4
1	A	19	HIS	3.3
1	D	252	ARG	3.3
1	A	239	LEU	3.3
1	A	171	ALA	3.3
1	B	130	LYS	3.3
1	D	444	TYR	3.2
1	C	444	TYR	3.2
1	C	252	ARG	3.2
1	C	20	ARG	3.2
1	B	168	LYS	3.2
1	C	173	LYS	3.2
1	D	173	LYS	3.1
1	B	285	LEU	3.1
1	B	252	ARG	3.1
1	B	251	ASP	3.1
1	A	249	GLU	3.1
1	D	244	LEU	3.1
1	D	242	PRO	3.0
1	B	38	PHE	3.0
1	C	46	VAL	2.9
1	A	257	TRP	2.9
1	B	431	GLY	2.9
1	D	18	LEU	2.9
1	B	250	LEU	2.9
1	D	247	MET	2.9
1	D	256	ASN	2.9
1	C	432	HIS	2.9
1	D	460	PHE	2.8
1	C	257	TRP	2.8
1	D	440	ARG	2.8
1	C	170	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	277	PHE	2.7
1	C	259	LYS	2.7
1	C	126	MET	2.7
1	A	250	LEU	2.7
1	C	258	ASP	2.7
1	D	38	PHE	2.7
1	A	254	PRO	2.7
1	D	240	LEU	2.7
1	D	416	MET	2.6
1	D	250	LEU	2.6
1	A	20	ARG	2.6
1	B	444	TYR	2.6
1	D	19	HIS	2.6
1	C	375	PHE	2.6
1	A	440	ARG	2.6
1	C	238	PHE	2.5
1	C	440	ARG	2.5
1	A	285	LEU	2.5
1	A	459	LEU	2.5
1	A	238	PHE	2.5
1	B	460	PHE	2.5
1	D	434	LYS	2.4
1	A	174	GLN	2.4
1	D	432	HIS	2.4
1	A	442	GLY	2.4
1	B	241	LYS	2.4
1	B	131	MET	2.3
1	B	244	LEU	2.3
1	B	253	ALA	2.3
1	B	416	MET	2.3
1	A	244	LEU	2.3
1	C	178	TYR	2.3
1	C	417	LEU	2.3
1	A	262	VAL	2.3
1	C	136	PHE	2.3
1	C	40	PRO	2.3
1	D	397	GLY	2.3
1	D	257	TRP	2.3
1	A	354	SER	2.3
1	D	126	MET	2.2
1	D	36	TYR	2.2
1	B	419	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	310	HIS	2.2
1	A	287	GLY	2.2
1	C	42	GLU	2.2
1	C	244	LEU	2.2
1	D	417	LEU	2.2
1	C	439	MET	2.2
1	D	359	PHE	2.2
1	B	178	TYR	2.2
1	C	312	LYS	2.2
1	D	351	ASP	2.2
1	D	20	ARG	2.2
1	B	288	PHE	2.2
1	C	434	LYS	2.1
1	B	238	PHE	2.1
1	D	238	PHE	2.1
1	A	131	MET	2.1
1	D	48	GLY	2.1
1	B	428	PHE	2.1
1	C	175	ARG	2.1
1	D	356	MET	2.1
1	A	172	ASP	2.1
1	B	440	ARG	2.1
1	A	397	GLY	2.0
1	B	338	GLN	2.0
1	A	36	TYR	2.0
1	D	286	GLY	2.0
1	A	416	MET	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, 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(Å ²)	Q<0.9
2	NA	D	502	1/1	0.64	0.19	75,75,75,75	0
3	CIT	B	503	13/13	0.67	0.66	92,129,141,146	0
3	CIT	C	503	13/13	0.68	0.89	100,132,144,153	0
2	NA	C	502	1/1	0.70	0.30	89,89,89,89	0
3	CIT	D	503	13/13	0.76	0.56	92,123,145,162	0
2	NA	A	502	1/1	0.83	0.25	68,68,68,68	0
3	CIT	A	503	13/13	0.86	0.37	86,124,140,148	0
2	NA	B	502	1/1	0.87	0.28	87,87,87,87	0
2	NA	B	501	1/1	0.88	0.24	90,90,90,90	0
2	NA	C	501	1/1	0.95	0.12	69,69,69,69	0
2	NA	D	501	1/1	0.99	0.56	98,98,98,98	0
2	NA	A	501	1/1	0.99	0.12	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.