



Full wwPDB X-ray Structure Validation Report ⓘ

May 10, 2017 – 07:48 PM 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029077

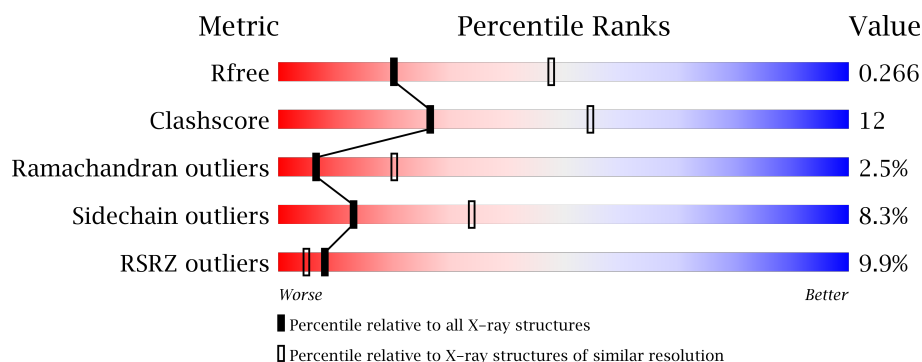
1 Overall quality at a glance

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}	100719	3276 (2.80-2.76)
Clashscore	112137	3771 (2.80-2.76)
Ramachandran outliers	110173	3707 (2.80-2.76)
Sidechain outliers	110143	3709 (2.80-2.76)
RSRZ outliers	101464	3307 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NA	A	502	-	-	-	X
2	NA	B	501	-	-	-	X
2	NA	B	502	-	-	-	X
2	NA	C	502	-	-	-	X
2	NA	D	501	-	-	-	X
3	CIT	A	503	-	-	-	X
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.

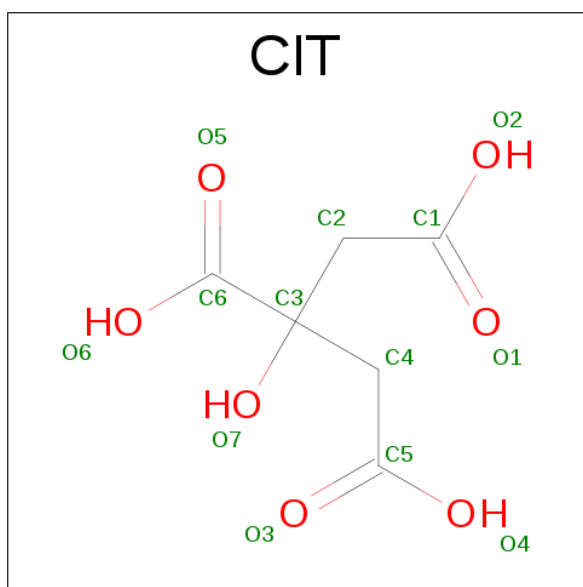
- Molecule 1 is a protein called Transporter, NadC family.

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	B	2	Total	Na	0	0
			2	2		
2	A	2	Total	Na	0	0
			2	2		
2	D	2	Total	Na	0	0
			2	2		
2	C	2	Total	Na	0	0
			2	2		

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

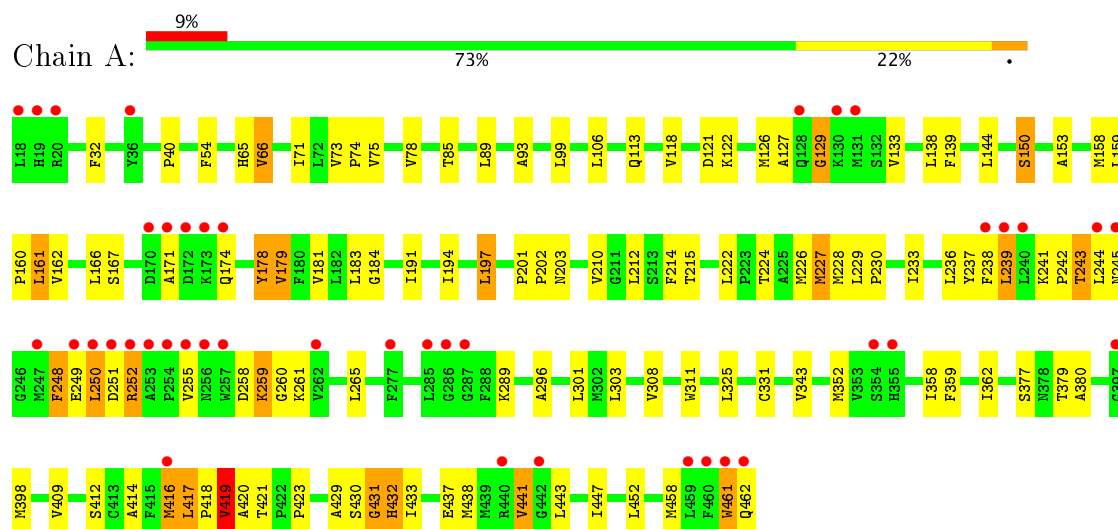


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		
3	D	1	Total	C	O	0	0
			13	6	7		

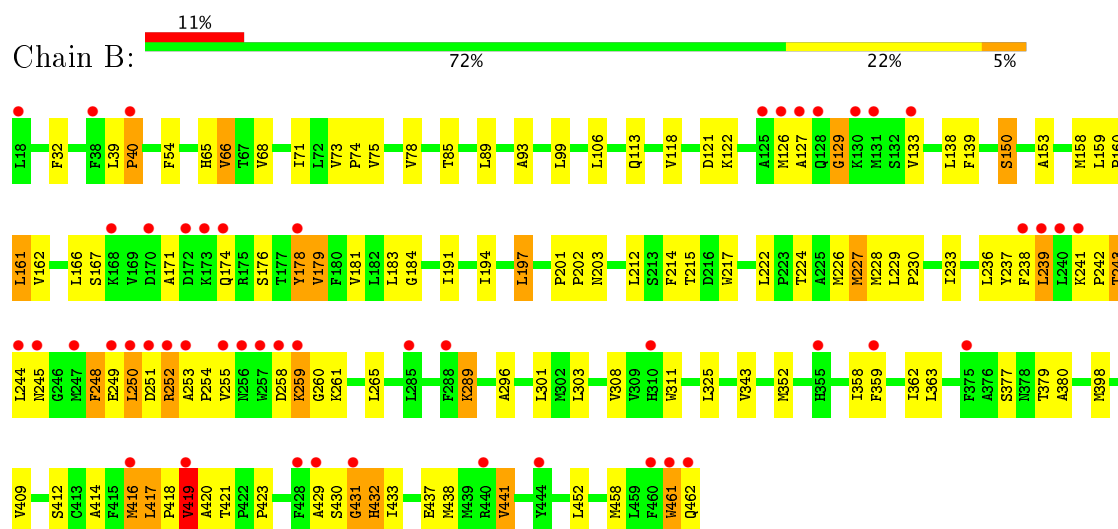
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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

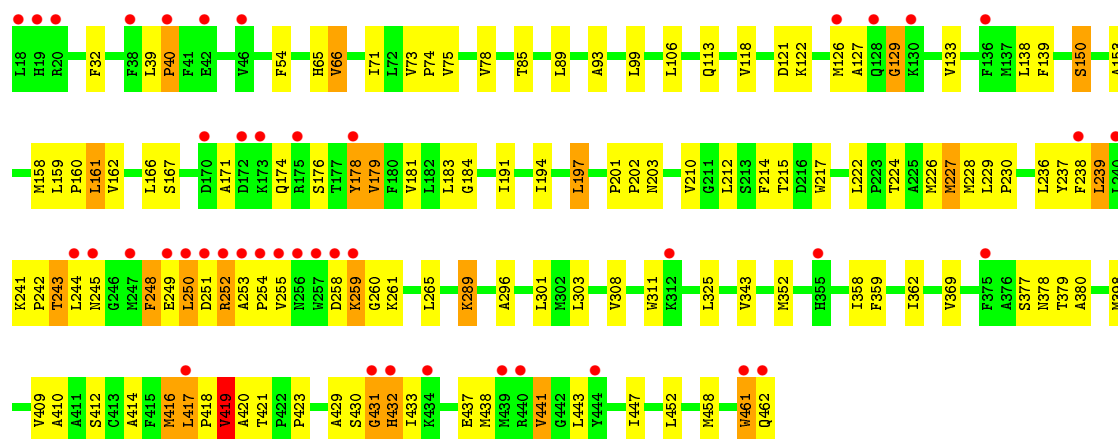


- Molecule 1: Transporter, NadC family

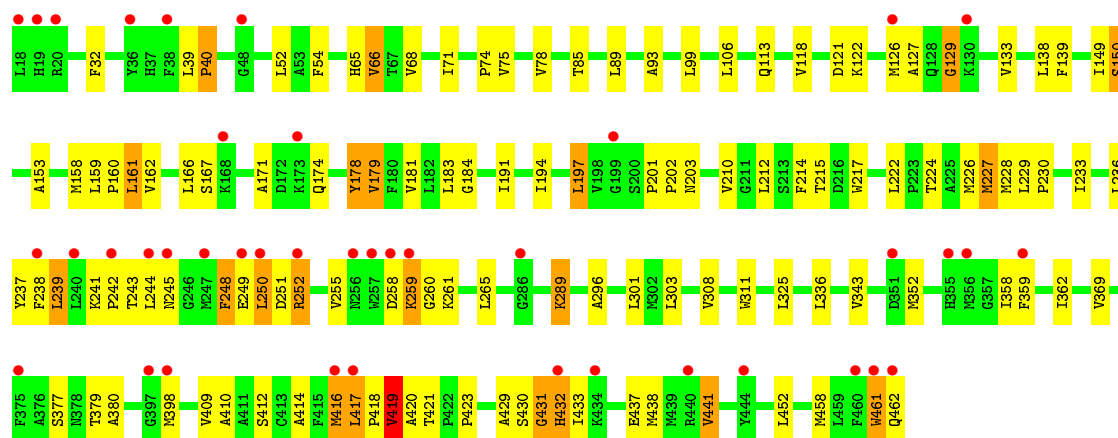


- Molecule 1: Transporter, NadC family





• 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 (5.35%)	DCC
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 , 29.1	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: NA, CIT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.34	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:D:202:PRO:HD3	1:D:379:THR:HG22	1.62	0.80
1:C:311:TRP:HB3	1:D:65:HIS:HD2	1.45	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:129:GLY:HA2	1:C:248:PHE:HB2	1.69	0.73
1:C:75:VAL:HG11	1:D:301:LEU:HD11	1.70	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:377:SER:HB3	1:B:380:ALA:HB3	1.85	0.58
1:B:66:VAL:HG12	1:B:325:LEU:HD13	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:301:LEU:HD11	1:D:75:VAL:HG11	1.85	0.57
1:C:183:LEU:HD13	1:C:433:ILE:CD1	2.35	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:167:SER:HB3	1:D:249:GLU:OE2	2.06	0.56
1:D:71:ILE:O	1:D:74:PRO:HD2	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:O	1:D:194:ILE:HG22	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:HG22	1:A:194:ILE:O	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:O	1:B:194:ILE:HG22	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:H	1:B:417:LEU:HD23	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:H	1:C:417:LEU:HD23	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:D:183:LEU:HD13	1:D:433:ILE:CD1	2.43	0.49
1:C:93:ALA:HB2	1:D:93:ALA:HB2	1.94	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:CG2	1:A:194:ILE:O	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:C:461:TRP:HE3	1:C:462:GLN:HG3	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: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:243:THR:C	1:D:245:ASN:H	2.18	0.46
1:D:74:PRO:O	1:D:78:VAL:HG23	2.15	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:359:PHE:CD1	1:D:458:MET:HE3	2.50	0.46
1:D:178:TYR:HE2	1:D:432:HIS:CG	2.34	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:CG2	1:C:194:ILE:O	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:161:LEU:HD11	1:C:252:ARG:NH2	2.33	0.43
1:C:138:LEU:HD13	1:C:162:VAL:HG22	2.01	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:179:VAL:HG23	1:B:432:HIS:CE1	2.55	0.42
1:B:166:LEU:HD11	1:B:181:VAL:CB	2.49	0.42
1:B:289:LYS:HD2	1:B:289:LYS:HA	1.81	0.42
1:D:250:LEU:HD23	1:D:250:LEU:H	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:179:VAL:HG23	1:D:432:HIS:CE1	2.55	0.42
1:D:166:LEU:HD11	1:D:181:VAL:CB	2.49	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:201:PRO:HG2	1:D:379:THR:HG21	2.02	0.42
1:D:129:GLY:CA	1:D:248:PHE:HB2	2.43	0.42
1:D:258:ASP:OD1	1:D:261:LYS:HG3	2.20	0.42
1:A:250:LEU:HD23	1:A:250:LEU:H	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:D:210:VAL:HG23	1:D:212:LEU:HG	2.02	0.41
1:C:311:TRP:CB	1:D:65:HIS:CD2	3.00	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:201:PRO:HB2	1:B:379:THR:HG21	2.02	0.40
1:B:74:PRO:O	1:B:78:VAL:HG23	2.21	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:233:ILE:O	1:A:237:TYR:HB2	2.22	0.40
1:A:178:TYR:CE2	1:A:432:HIS:CG	3.10	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 [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%)	401 (90%)	31 (7%)	11 (2%)	6	20
1	B	443/445 (100%)	400 (90%)	32 (7%)	11 (2%)	6	20
1	C	443/445 (100%)	399 (90%)	33 (7%)	11 (2%)	6	20
1	D	443/445 (100%)	400 (90%)	32 (7%)	11 (2%)	6	20
All	All	1772/1780 (100%)	1600 (90%)	128 (7%)	44 (2%)	6	20

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%)	12	33
1	B	351/353 (99%)	322 (92%)	29 (8%)	13	34
1	C	351/353 (99%)	322 (92%)	29 (8%)	13	34
1	D	351/353 (99%)	323 (92%)	28 (8%)	14	36
All	All	1404/1412 (99%)	1288 (92%)	116 (8%)	13	34

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

Some 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 carbohydrates 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	-	3,12,12	0.72	0	3,17,17	1.37	1 (33%)
3	CIT	B	503	-	3,12,12	0.75	0	3,17,17	1.47	1 (33%)
3	CIT	C	503	-	3,12,12	0.65	0	3,17,17	1.37	1 (33%)
3	CIT	D	503	-	3,12,12	0.66	0	3,17,17	1.35	1 (33%)

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	-	-	0/6/16/16	0/0/0/0
3	CIT	B	503	-	-	0/6/16/16	0/0/0/0
3	CIT	C	503	-	-	0/6/16/16	0/0/0/0
3	CIT	D	503	-	-	0/6/16/16	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	503	CIT	C3-C4-C5	-2.54	110.98	114.95
3	C	503	CIT	C3-C4-C5	-2.36	111.26	114.95
3	A	503	CIT	C3-C4-C5	-2.35	111.27	114.95
3	D	503	CIT	C3-C4-C5	-2.32	111.32	114.95

There are no chirality outliers.

There are no torsion outliers.

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	C	503	CIT	3	0
3	D	503	CIT	2	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, 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%)	0.21	42 (9%) 9 6	25, 69, 127, 174	0
1	B	445/445 (100%)	0.25	49 (11%) 6 4	37, 77, 142, 179	0
1	C	445/445 (100%)	0.16	44 (9%) 8 5	23, 63, 129, 179	0
1	D	445/445 (100%)	0.13	41 (9%) 10 6	25, 65, 117, 176	0
All	All	1780/1780 (100%)	0.19	176 (9%) 8 5	23, 68, 132, 179	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	462	GLN	15.9
1	C	462	GLN	13.1
1	B	240	LEU	8.9
1	B	462	GLN	7.9
1	C	254	PRO	7.5
1	B	245	ASN	7.3
1	C	256	ASN	7.0
1	A	18	LEU	6.9
1	A	255	VAL	6.8
1	C	250	LEU	6.8
1	D	259	LYS	6.6
1	B	259	LYS	6.6
1	B	126	MET	6.4
1	A	247	MET	6.4
1	A	130	LYS	6.3
1	A	461	TRP	6.2
1	C	172	ASP	6.0
1	B	257	TRP	6.0
1	C	253	ALA	5.8
1	C	461	TRP	5.8
1	A	462	GLN	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	461	TRP	5.7
1	B	247	MET	5.6
1	A	240	LEU	5.6
1	B	258	ASP	5.6
1	C	245	ASN	5.1
1	C	38	PHE	5.0
1	A	245	ASN	5.0
1	C	247	MET	4.9
1	B	355	HIS	4.7
1	C	251	ASP	4.7
1	A	128	GLN	4.7
1	C	355	HIS	4.7
1	C	249	GLU	4.6
1	B	173	LYS	4.6
1	D	130	LYS	4.5
1	B	249	GLU	4.5
1	A	252	ARG	4.5
1	D	258	ASP	4.5
1	A	256	ASN	4.4
1	B	172	ASP	4.4
1	D	245	ASN	4.3
1	D	461	TRP	4.3
1	B	256	ASN	4.3
1	B	170	ASP	4.2
1	C	128	GLN	4.2
1	C	18	LEU	4.2
1	C	19	HIS	4.1
1	B	18	LEU	4.0
1	A	355	HIS	4.0
1	A	173	LYS	4.0
1	A	253	ALA	4.0
1	B	40	PRO	4.0
1	B	133	VAL	4.0
1	A	286	GLY	3.9
1	B	127	ALA	3.9
1	B	128	GLN	3.8
1	C	255	VAL	3.8
1	A	460	PHE	3.8
1	D	168	LYS	3.7
1	C	431	GLY	3.7
1	D	375	PHE	3.7
1	D	355	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	398	MET	3.6
1	B	429	ALA	3.6
1	B	239	LEU	3.5
1	C	130	LYS	3.5
1	C	240	LEU	3.4
1	A	19	HIS	3.4
1	B	125	ALA	3.4
1	A	251	ASP	3.4
1	B	168	LYS	3.4
1	B	375	PHE	3.4
1	A	170	ASP	3.3
1	D	249	GLU	3.3
1	B	255	VAL	3.3
1	A	171	ALA	3.3
1	D	252	ARG	3.3
1	B	130	LYS	3.3
1	A	239	LEU	3.3
1	C	20	ARG	3.3
1	C	252	ARG	3.3
1	C	444	TYR	3.2
1	B	252	ARG	3.2
1	D	444	TYR	3.2
1	B	285	LEU	3.2
1	A	249	GLU	3.2
1	D	173	LYS	3.2
1	C	173	LYS	3.2
1	B	251	ASP	3.1
1	D	244	LEU	3.1
1	D	242	PRO	3.0
1	B	38	PHE	3.0
1	B	431	GLY	3.0
1	D	18	LEU	3.0
1	C	46	VAL	2.9
1	B	250	LEU	2.9
1	C	259	LYS	2.9
1	A	257	TRP	2.8
1	C	432	HIS	2.8
1	D	247	MET	2.8
1	D	256	ASN	2.8
1	D	460	PHE	2.8
1	C	170	ASP	2.8
1	C	258	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	440	ARG	2.8
1	A	277	PHE	2.8
1	C	257	TRP	2.8
1	C	126	MET	2.7
1	D	38	PHE	2.7
1	D	240	LEU	2.7
1	D	19	HIS	2.7
1	A	254	PRO	2.7
1	D	416	MET	2.7
1	A	440	ARG	2.6
1	A	20	ARG	2.6
1	C	375	PHE	2.6
1	A	250	LEU	2.6
1	A	285	LEU	2.6
1	B	444	TYR	2.6
1	D	434	LYS	2.5
1	A	459	LEU	2.5
1	D	250	LEU	2.5
1	B	460	PHE	2.5
1	C	238	PHE	2.5
1	A	174	GLN	2.5
1	C	440	ARG	2.4
1	A	442	GLY	2.4
1	D	432	HIS	2.4
1	B	244	LEU	2.4
1	A	238	PHE	2.4
1	B	131	MET	2.4
1	A	244	LEU	2.4
1	B	416	MET	2.4
1	B	241	LYS	2.4
1	C	178	TYR	2.3
1	B	253	ALA	2.3
1	D	126	MET	2.3
1	C	417	LEU	2.3
1	D	397	GLY	2.3
1	C	136	PHE	2.3
1	C	40	PRO	2.3
1	D	36	TYR	2.3
1	A	262	VAL	2.3
1	D	257	TRP	2.3
1	A	354	SER	2.3
1	C	244	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	310	HIS	2.2
1	B	178	TYR	2.2
1	D	351	ASP	2.2
1	A	287	GLY	2.2
1	B	419	VAL	2.2
1	D	417	LEU	2.2
1	B	288	PHE	2.2
1	C	439	MET	2.2
1	C	312	LYS	2.2
1	B	428	PHE	2.2
1	D	359	PHE	2.2
1	A	131	MET	2.2
1	D	356	MET	2.1
1	D	48	GLY	2.1
1	D	20	ARG	2.1
1	D	238	PHE	2.1
1	A	36	TYR	2.1
1	A	172	ASP	2.1
1	B	238	PHE	2.1
1	C	42	GLU	2.1
1	B	440	ARG	2.1
1	D	286	GLY	2.1
1	A	397	GLY	2.1
1	A	416	MET	2.1
1	C	434	LYS	2.0
1	B	359	PHE	2.0
1	B	174	GLN	2.0
1	C	175	ARG	2.0
1	D	199	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
3	CIT	B	503	13/13	0.67	0.66	16.16	92,129,141,146	0
3	CIT	C	503	13/13	0.67	0.88	12.73	100,132,144,153	0
3	CIT	D	503	13/13	0.76	0.56	7.96	92,123,145,162	0
2	NA	D	501	1/1	0.99	0.56	5.93	98,98,98,98	0
3	CIT	A	503	13/13	0.87	0.37	5.82	86,124,140,148	0
2	NA	C	502	1/1	0.69	0.30	5.16	89,89,89,89	0
2	NA	B	502	1/1	0.87	0.27	3.82	87,87,87,87	0
2	NA	A	502	1/1	0.82	0.25	2.36	68,68,68,68	0
2	NA	B	501	1/1	0.88	0.24	2.06	90,90,90,90	0
2	NA	D	502	1/1	0.63	0.20	1.19	75,75,75,75	0
2	NA	A	501	1/1	0.99	0.13	-0.22	72,72,72,72	0
2	NA	C	501	1/1	0.95	0.12	-1.13	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.