Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 08:50 PM BST

PDB ID	:	5ULD
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 following versions of software and data (see references ①) were used in the production of this report:

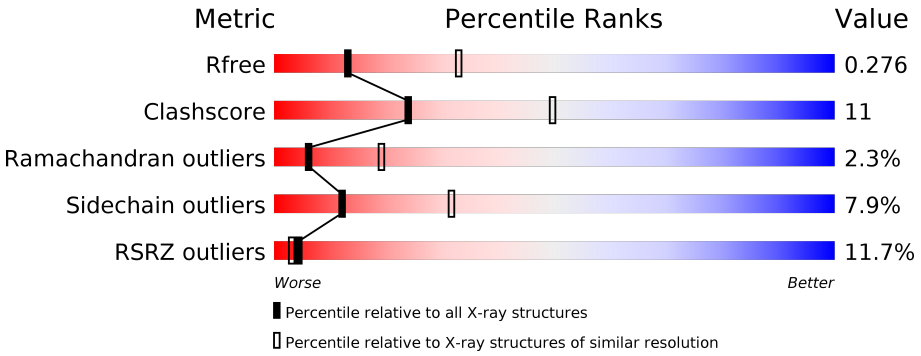
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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 on 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 <=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	13% 72% 24% ·
1	B	445	14% 72% 24% ·
1	C	445	9% 73% 23% ·
1	D	445	11% 73% 23% ·

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13456 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

Continued on next page...

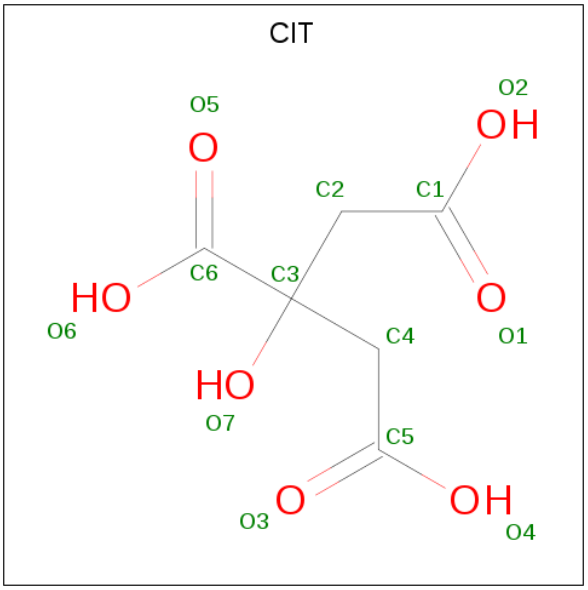
Continued from previous page...

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

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

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

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



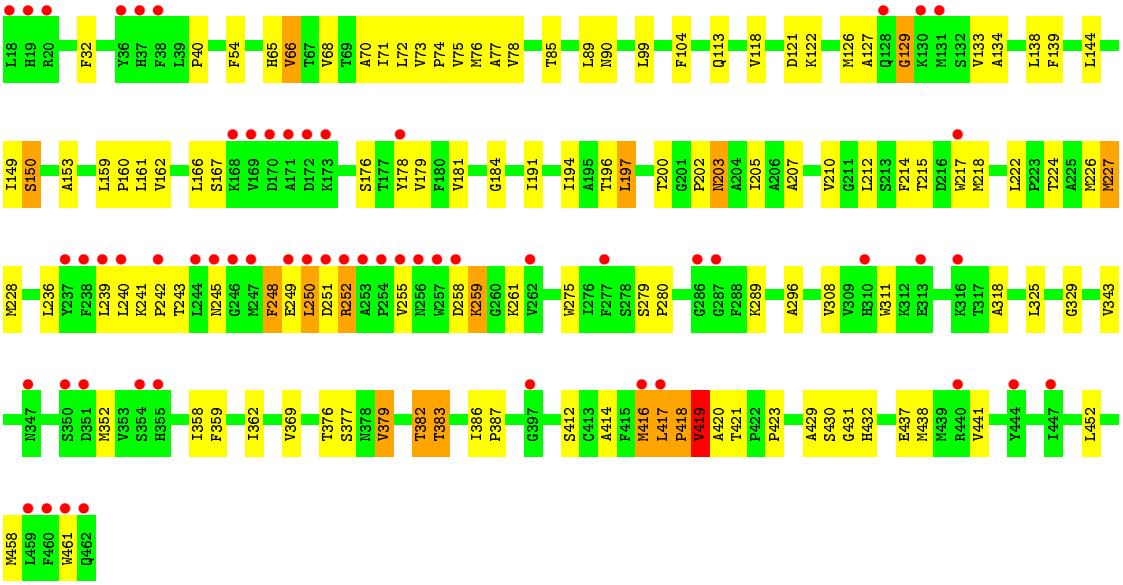
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		
3	D	1	Total	C	O	0	0
			13	6	7		

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.

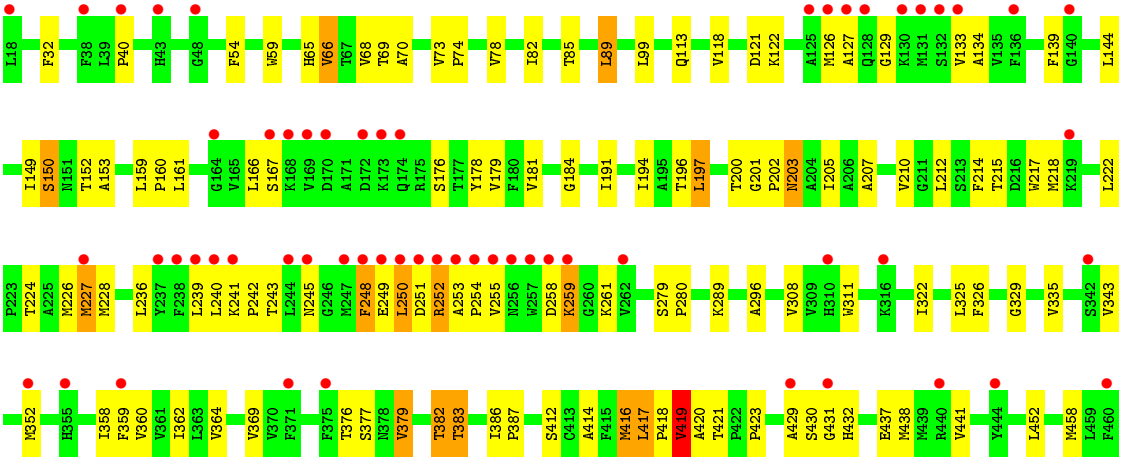
- Molecule 1: Transporter, NadC family

Chain A:



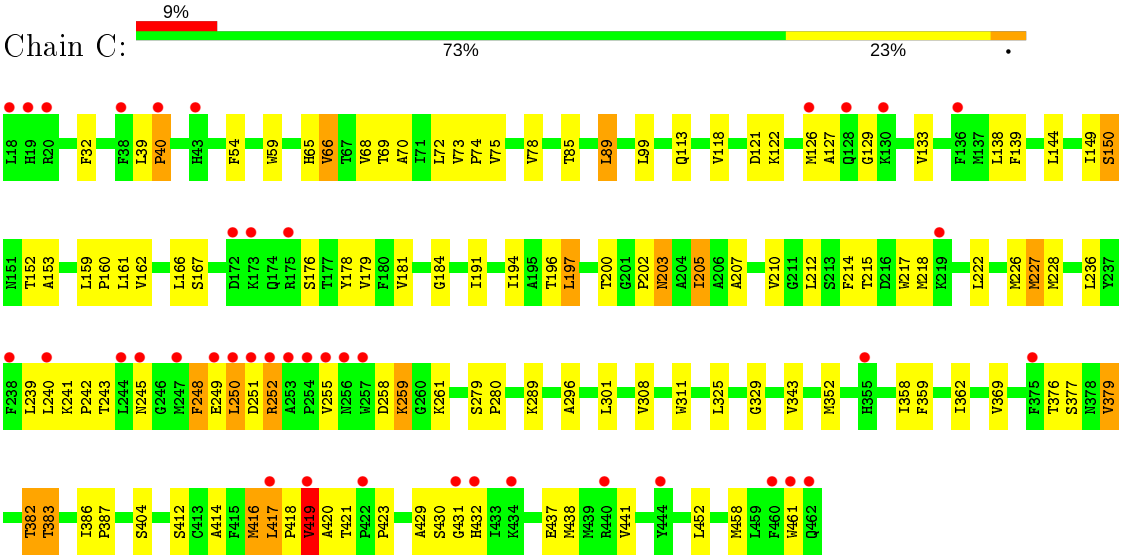
- Molecule 1: Transporter, NadC family

Chain B:



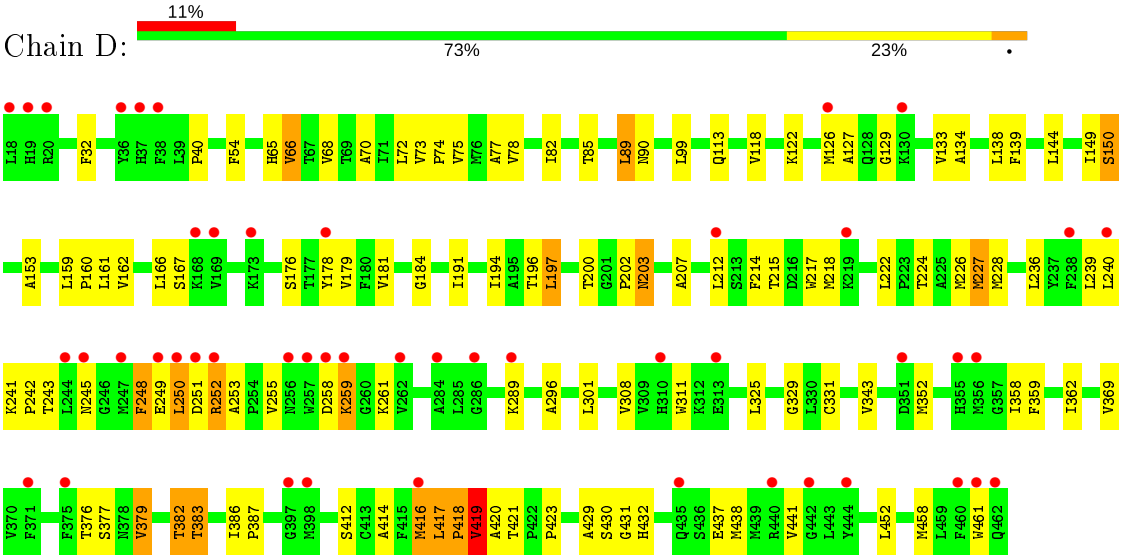
• Molecule 1: Transporter, NadC family

Chain C:



• Molecule 1: Transporter, NadC family

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	106.09Å 101.53Å 168.88Å 90.00° 99.73° 90.00°	Depositor
Resolution (Å)	15.00 – 2.78 15.00 – 2.78	Depositor EDS
% Data completeness (in resolution range)	88.9 (15.00-2.78) 89.0 (15.00-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.00 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.252 , 0.268 0.270 , 0.276	Depositor DCC
R_{free} test set	3980 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	74.3	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 53.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13456	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0/3427	0.52	0/4673
1	B	0.33	0/3427	0.52	0/4673
1	C	0.36	0/3427	0.53	0/4673
1	D	0.36	0/3427	0.54	0/4673
All	All	0.34	0/13708	0.53	0/18692

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	80	0
1	B	3349	0	3504	77	0
1	C	3349	0	3504	80	0
1	D	3349	0	3504	76	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	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	13	0	5	1	0
3	C	13	0	5	1	0
3	D	13	0	5	0	0
All	All	13456	0	14036	306	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 11.

All (306) 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:A:421:THR:CG2	1:A:423:PRO:HD2	1.89	1.01
1:C:421:THR:CG2	1:C:423:PRO:HD2	1.91	1.00
1:D:421:THR:CG2	1:D:423:PRO:HD2	1.91	1.00
1:B:421:THR:CG2	1:B:423:PRO:HD2	1.93	0.99
1:C:421:THR:HG22	1:C:423:PRO:HD2	0.99	0.99
1:B:421:THR:HG22	1:B:423:PRO:HD2	0.99	0.98
1:D:421:THR:HG22	1:D:423:PRO:HD2	0.99	0.98
1:A:421:THR:HG22	1:A:423:PRO:CD	1.93	0.98
1:C:421:THR:HG22	1:C:423:PRO:CD	1.95	0.96
1:A:421:THR:HG22	1:A:423:PRO:HD2	0.96	0.95
1:D:421:THR:HG22	1:D:423:PRO:CD	1.95	0.95
1:B:421:THR:HG22	1:B:423:PRO:CD	1.96	0.92
1:B:78:VAL:HG11	1:B:85:THR:HG22	1.54	0.89
1:A:78:VAL:HG11	1:A:85:THR:HG22	1.54	0.89
1:D:78:VAL:HG11	1:D:85:THR:HG22	1.55	0.88
1:C:416:MET:O	1:C:438:MET:HG2	1.74	0.88
1:A:416:MET:O	1:A:438:MET:HG2	1.73	0.88
1:C:78:VAL:HG11	1:C:85:THR:HG22	1.56	0.85
1:B:416:MET:O	1:B:438:MET:HG2	1.77	0.85
1:D:416:MET:O	1:D:438:MET:HG2	1.74	0.85
1:A:73:VAL:HB	1:A:74:PRO:HD3	1.62	0.81
1:C:73:VAL:HB	1:C:74:PRO:HD3	1.62	0.81
1:D:73:VAL:HB	1:D:74:PRO:HD3	1.63	0.81
1:A:200:THR:HG22	1:A:203:ASN:HD21	1.50	0.77
1:B:73:VAL:HB	1:B:74:PRO:HD3	1.66	0.76
1:D:200:THR:HG22	1:D:203:ASN:HD21	1.50	0.76
1:C:166:LEU:HD11	1:C:181:VAL:HB	1.67	0.76
1:D:166:LEU:HD11	1:D:181:VAL:HB	1.68	0.75
1:A:166:LEU:HD11	1:A:181:VAL:HB	1.69	0.75
1:C:200:THR:HG22	1:C:203:ASN:HD21	1.51	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:THR:HG22	1:B:203:ASN:HD21	1.53	0.74
1:B:166:LEU:HD11	1:B:181:VAL:HB	1.69	0.73
1:B:382:THR:HG22	1:B:386:ILE:HG13	1.74	0.69
1:C:222:LEU:O	1:C:226:MET:HG2	1.92	0.69
1:A:329:GLY:HA3	1:A:383:THR:HG22	1.76	0.68
1:A:227:MET:HG2	1:A:452:LEU:HD11	1.76	0.68
1:C:329:GLY:HA3	1:C:383:THR:HG22	1.75	0.68
1:A:167:SER:HB3	1:A:249:GLU:OE2	1.94	0.68
1:A:122:LYS:O	1:A:126:MET:HG2	1.94	0.67
1:A:382:THR:HG22	1:A:386:ILE:HG13	1.74	0.67
1:A:129:GLY:HA2	1:A:248:PHE:HB2	1.76	0.67
1:B:222:LEU:O	1:B:226:MET:HG2	1.95	0.66
1:D:129:GLY:HA2	1:D:248:PHE:HB2	1.77	0.66
1:C:129:GLY:HA2	1:C:248:PHE:HB2	1.77	0.66
1:B:227:MET:HG2	1:B:452:LEU:HD11	1.77	0.66
1:D:382:THR:HG22	1:D:386:ILE:HG13	1.76	0.66
1:B:122:LYS:O	1:B:126:MET:HG2	1.95	0.65
1:C:227:MET:HG2	1:C:452:LEU:HD11	1.76	0.65
1:D:167:SER:HB3	1:D:249:GLU:OE2	1.96	0.65
1:C:382:THR:HG22	1:C:386:ILE:HG13	1.78	0.65
1:B:129:GLY:HA2	1:B:248:PHE:HB2	1.77	0.65
1:D:227:MET:HG2	1:D:452:LEU:HD11	1.78	0.65
1:C:122:LYS:O	1:C:126:MET:HG2	1.96	0.65
1:D:122:LYS:O	1:D:126:MET:HG2	1.95	0.65
1:D:329:GLY:HA3	1:D:383:THR:HG22	1.79	0.65
1:D:197:LEU:HD12	1:D:214:PHE:HA	1.78	0.65
1:D:222:LEU:O	1:D:226:MET:HG2	1.98	0.64
1:B:329:GLY:HA3	1:B:383:THR:HG22	1.78	0.64
1:C:197:LEU:HD12	1:C:214:PHE:HA	1.80	0.64
1:C:167:SER:HB3	1:C:249:GLU:OE2	1.98	0.64
1:A:200:THR:HG22	1:A:203:ASN:ND2	2.13	0.63
1:B:167:SER:HB3	1:B:249:GLU:OE2	1.98	0.63
1:A:150:SER:HB3	1:A:153:ALA:HB3	1.81	0.63
1:A:78:VAL:CG1	1:A:85:THR:HG22	2.28	0.62
1:D:200:THR:HG22	1:D:203:ASN:ND2	2.14	0.62
1:D:150:SER:HB3	1:D:153:ALA:HB3	1.80	0.62
1:B:197:LEU:HD12	1:B:214:PHE:HA	1.81	0.62
1:C:200:THR:HG22	1:C:203:ASN:ND2	2.14	0.62
1:A:222:LEU:O	1:A:226:MET:HG2	1.99	0.62
1:B:113:GLN:HG3	1:B:261:LYS:HG2	1.81	0.62
1:A:197:LEU:HD12	1:A:214:PHE:HA	1.80	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:THR:HG22	1:B:203:ASN:ND2	2.15	0.61
1:C:78:VAL:CG1	1:C:85:THR:HG22	2.30	0.60
1:D:113:GLN:HG3	1:D:261:LYS:HG2	1.82	0.60
1:B:78:VAL:CG1	1:B:85:THR:HG22	2.29	0.60
1:C:113:GLN:HG3	1:C:261:LYS:HG2	1.82	0.59
1:D:418:PRO:C	1:D:420:ALA:H	2.06	0.59
1:A:113:GLN:HG3	1:A:261:LYS:HG2	1.84	0.59
1:A:418:PRO:C	1:A:420:ALA:H	2.06	0.58
1:D:362:ILE:HD11	1:D:458:MET:HE2	1.85	0.58
1:D:196:THR:HG22	1:D:218:MET:HG3	1.84	0.58
1:B:150:SER:HB3	1:B:153:ALA:HB3	1.85	0.57
1:B:418:PRO:C	1:B:420:ALA:H	2.07	0.57
1:A:196:THR:HG22	1:A:218:MET:HG3	1.86	0.57
1:C:418:PRO:C	1:C:420:ALA:H	2.08	0.57
1:D:417:LEU:HD23	1:D:417:LEU:H	1.68	0.57
1:D:78:VAL:CG1	1:D:85:THR:HG22	2.31	0.57
1:A:414:ALA:HB1	1:A:420:ALA:HB1	1.87	0.57
1:B:417:LEU:H	1:B:417:LEU:HD23	1.70	0.56
1:A:417:LEU:HD23	1:A:417:LEU:H	1.70	0.56
1:C:150:SER:HB3	1:C:153:ALA:HB3	1.85	0.56
1:C:417:LEU:H	1:C:417:LEU:HD23	1.70	0.56
1:C:159:LEU:HB3	1:C:160:PRO:HD3	1.88	0.56
1:C:196:THR:HG22	1:C:218:MET:HG3	1.88	0.56
1:C:65:HIS:HB3	1:C:68:VAL:HG23	1.88	0.56
1:D:414:ALA:HB1	1:D:420:ALA:HB1	1.89	0.55
1:D:73:VAL:HB	1:D:74:PRO:CD	2.35	0.55
1:B:196:THR:HG22	1:B:218:MET:HG3	1.89	0.55
1:C:414:ALA:HB1	1:C:420:ALA:HB1	1.88	0.55
1:D:194:ILE:O	1:D:194:ILE:HG22	2.06	0.55
1:A:362:ILE:HD11	1:A:458:MET:HE2	1.88	0.55
1:B:414:ALA:HB1	1:B:420:ALA:HB1	1.88	0.55
1:B:159:LEU:HB3	1:B:160:PRO:HD3	1.89	0.55
1:A:32:PHE:HB2	1:A:54:PHE:HD1	1.72	0.54
1:C:65:HIS:CD2	1:D:311:TRP:HB3	2.42	0.54
1:D:159:LEU:HB3	1:D:160:PRO:HD3	1.90	0.54
1:C:194:ILE:O	1:C:194:ILE:HG22	2.08	0.54
1:B:194:ILE:O	1:B:194:ILE:HG22	2.08	0.53
1:D:32:PHE:HB2	1:D:54:PHE:HD1	1.73	0.53
1:A:431:GLY:HA2	1:D:253:ALA:HB3	1.89	0.53
1:A:65:HIS:CD2	1:B:311:TRP:HB3	2.43	0.53
1:D:85:THR:O	1:D:89:LEU:HD22	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:PHE:HB2	1:B:54:PHE:HD1	1.71	0.53
1:C:362:ILE:HD11	1:C:458:MET:HE2	1.91	0.53
1:C:311:TRP:HB3	1:D:65:HIS:CD2	2.43	0.53
1:A:159:LEU:HB3	1:A:160:PRO:HD3	1.91	0.53
1:A:376:THR:HG22	1:A:377:SER:N	2.24	0.53
1:A:194:ILE:HG22	1:A:194:ILE:O	2.07	0.52
1:A:99:LEU:HD12	1:A:296:ALA:HB2	1.91	0.52
1:B:65:HIS:HB3	1:B:68:VAL:HG23	1.90	0.52
1:C:32:PHE:HB2	1:C:54:PHE:HD1	1.74	0.52
1:B:376:THR:HG22	1:B:377:SER:N	2.24	0.52
1:D:258:ASP:OD1	1:D:261:LYS:HG3	2.10	0.52
1:A:236:LEU:HD23	1:A:441:VAL:HG11	1.92	0.52
1:B:99:LEU:HD12	1:B:296:ALA:HB2	1.91	0.52
1:B:212:LEU:HD13	1:B:217:TRP:HD1	1.76	0.51
1:B:437:GLU:O	1:B:441:VAL:HG23	2.11	0.51
1:C:236:LEU:HD23	1:C:441:VAL:HG11	1.93	0.51
1:B:362:ILE:HD11	1:B:458:MET:HE2	1.93	0.51
1:D:437:GLU:O	1:D:441:VAL:HG23	2.10	0.51
1:C:376:THR:HG22	1:C:377:SER:N	2.26	0.51
1:D:65:HIS:HB3	1:D:68:VAL:HG23	1.92	0.51
1:B:359:PHE:CD1	1:B:458:MET:HE3	2.46	0.50
1:A:258:ASP:OD1	1:A:261:LYS:HG3	2.10	0.50
1:C:258:ASP:OD1	1:C:261:LYS:HG3	2.11	0.50
1:C:358:ILE:O	1:C:362:ILE:HG23	2.10	0.50
1:D:376:THR:HG22	1:D:377:SER:N	2.25	0.50
1:A:65:HIS:HB3	1:A:68:VAL:HG23	1.93	0.50
1:B:236:LEU:HD23	1:B:441:VAL:HG11	1.94	0.50
1:A:311:TRP:HB3	1:B:65:HIS:CD2	2.46	0.50
1:C:99:LEU:HD12	1:C:296:ALA:HB2	1.93	0.50
1:C:437:GLU:O	1:C:441:VAL:HG23	2.11	0.50
1:A:437:GLU:O	1:A:441:VAL:HG23	2.11	0.50
1:A:418:PRO:O	1:A:420:ALA:N	2.45	0.49
1:D:212:LEU:HD13	1:D:217:TRP:HD1	1.77	0.49
1:C:418:PRO:HD3	1:C:438:MET:HE3	1.94	0.49
1:B:258:ASP:OD1	1:B:261:LYS:HG3	2.12	0.49
1:C:212:LEU:HD13	1:C:217:TRP:HD1	1.77	0.49
1:D:149:ILE:O	1:D:150:SER:HB2	2.12	0.48
1:A:70:ALA:HB2	1:A:325:LEU:HD12	1.95	0.48
1:B:176:SER:HA	1:B:179:VAL:HG12	1.95	0.48
1:B:418:PRO:O	1:B:419:VAL:HG12	2.14	0.48
1:D:418:PRO:O	1:D:420:ALA:N	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:VAL:HG12	1:C:255:VAL:HB	1.95	0.48
1:B:70:ALA:HB2	1:B:325:LEU:HD12	1.96	0.48
1:A:212:LEU:HD13	1:A:217:TRP:HD1	1.78	0.48
1:C:418:PRO:O	1:C:419:VAL:HG12	2.14	0.48
1:C:429:ALA:C	1:C:431:GLY:H	2.17	0.48
1:D:99:LEU:HD12	1:D:296:ALA:HB2	1.95	0.48
1:D:118:VAL:HG12	1:D:255:VAL:HB	1.95	0.48
1:A:149:ILE:O	1:A:150:SER:HB2	2.14	0.48
1:B:191:ILE:HG12	1:B:228:MET:CE	2.42	0.48
1:C:176:SER:HA	1:C:179:VAL:HG12	1.96	0.47
1:A:118:VAL:HG12	1:A:255:VAL:HB	1.95	0.47
1:B:382:THR:HG22	1:B:386:ILE:CG1	2.43	0.47
1:B:205:ILE:HD12	1:B:382:THR:HB	1.96	0.47
1:C:251:ASP:O	1:C:252:ARG:HB3	2.15	0.47
1:C:329:GLY:HA3	1:C:383:THR:CG2	2.45	0.47
1:A:429:ALA:C	1:A:431:GLY:H	2.18	0.47
1:C:191:ILE:HG12	1:C:228:MET:CE	2.44	0.47
1:A:358:ILE:O	1:A:362:ILE:HG23	2.14	0.47
1:D:70:ALA:HB2	1:D:325:LEU:HD12	1.96	0.47
1:A:382:THR:HG22	1:A:386:ILE:CG1	2.45	0.47
1:C:75:VAL:HG11	1:D:301:LEU:HD11	1.96	0.47
1:D:386:ILE:HB	1:D:387:PRO:HD3	1.96	0.47
1:B:118:VAL:HG12	1:B:255:VAL:HB	1.97	0.47
1:B:149:ILE:O	1:B:150:SER:HB2	2.15	0.47
1:D:251:ASP:O	1:D:252:ARG:HB3	2.15	0.47
1:D:429:ALA:C	1:D:431:GLY:H	2.18	0.47
1:A:73:VAL:HB	1:A:74:PRO:CD	2.41	0.46
1:D:250:LEU:HD23	1:D:250:LEU:H	1.81	0.46
1:D:236:LEU:HD23	1:D:441:VAL:HG11	1.96	0.46
1:B:429:ALA:C	1:B:431:GLY:H	2.19	0.46
1:A:251:ASP:O	1:A:252:ARG:HB3	2.15	0.46
1:B:251:ASP:O	1:B:252:ARG:HB3	2.15	0.46
1:C:72:LEU:O	1:C:75:VAL:HG12	2.16	0.46
1:A:127:ALA:HB1	1:A:133:VAL:HG13	1.98	0.46
1:D:129:GLY:CA	1:D:248:PHE:HB2	2.44	0.46
1:B:207:ALA:HA	1:B:212:LEU:HD12	1.97	0.46
1:D:202:PRO:HD3	1:D:379:VAL:HG13	1.98	0.46
1:A:194:ILE:CG2	1:A:194:ILE:O	2.64	0.46
1:B:358:ILE:O	1:B:362:ILE:HG23	2.15	0.46
1:B:386:ILE:HB	1:B:387:PRO:HD3	1.98	0.46
1:C:418:PRO:O	1:C:420:ALA:N	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:ALA:HB2	1:C:325:LEU:HD12	1.97	0.46
1:A:210:VAL:HG23	1:A:212:LEU:HG	1.98	0.45
1:D:138:LEU:HD13	1:D:162:VAL:HG22	1.98	0.45
1:A:191:ILE:HG12	1:A:228:MET:CE	2.46	0.45
1:B:191:ILE:HG12	1:B:228:MET:HE3	1.99	0.45
1:C:418:PRO:HD3	1:C:438:MET:CE	2.46	0.45
1:D:194:ILE:O	1:D:194:ILE:CG2	2.64	0.45
1:C:127:ALA:HB1	1:C:133:VAL:HG13	1.99	0.45
1:C:205:ILE:HD12	1:C:382:THR:HB	1.97	0.45
1:D:207:ALA:HA	1:D:212:LEU:HD12	1.97	0.45
1:C:210:VAL:HG23	1:C:212:LEU:HG	1.99	0.45
1:C:129:GLY:CA	1:C:248:PHE:HB2	2.45	0.45
1:C:250:LEU:HD23	1:C:250:LEU:H	1.82	0.45
1:D:418:PRO:HD3	1:D:438:MET:HE3	1.98	0.45
1:A:207:ALA:HA	1:A:212:LEU:HD12	1.98	0.45
1:A:205:ILE:HD12	1:A:382:THR:HB	1.98	0.45
1:C:139:PHE:CE2	1:C:184:GLY:HA3	2.52	0.45
1:C:73:VAL:HB	1:C:74:PRO:CD	2.40	0.45
1:A:129:GLY:CA	1:A:248:PHE:HB2	2.44	0.45
1:A:202:PRO:HD3	1:A:379:VAL:HG13	1.99	0.45
1:B:418:PRO:O	1:B:420:ALA:N	2.50	0.45
1:C:152:THR:OG1	3:C:503:CIT:O4	2.27	0.45
1:D:358:ILE:O	1:D:362:ILE:HG23	2.17	0.45
1:A:250:LEU:HD23	1:A:250:LEU:H	1.82	0.45
1:D:191:ILE:HG12	1:D:228:MET:CE	2.46	0.44
1:B:127:ALA:HB1	1:B:133:VAL:HG13	1.99	0.44
1:D:418:PRO:O	1:D:419:VAL:HG12	2.17	0.44
1:A:417:LEU:HB2	1:A:418:PRO:HD2	2.00	0.44
1:A:176:SER:HA	1:A:179:VAL:HG12	2.00	0.44
1:A:329:GLY:HA3	1:A:383:THR:CG2	2.46	0.44
1:C:301:LEU:HD11	1:D:75:VAL:HG11	2.00	0.44
1:D:127:ALA:HB1	1:D:133:VAL:HG13	1.99	0.44
1:D:224:THR:O	1:D:228:MET:HB2	2.17	0.44
1:C:194:ILE:CG2	1:C:194:ILE:O	2.65	0.44
1:D:176:SER:HA	1:D:179:VAL:HG12	2.00	0.44
1:B:250:LEU:HD23	1:B:250:LEU:H	1.82	0.44
1:C:191:ILE:HG12	1:C:228:MET:HE3	1.99	0.44
1:B:176:SER:HB2	1:B:240:LEU:O	2.18	0.43
1:B:129:GLY:CA	1:B:248:PHE:HB2	2.45	0.43
1:C:386:ILE:HB	1:C:387:PRO:HD3	2.00	0.43
1:D:176:SER:HB2	1:D:240:LEU:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LEU:HD13	1:A:162:VAL:HG22	2.01	0.43
1:A:139:PHE:CE2	1:A:184:GLY:HA3	2.53	0.43
1:C:176:SER:HB2	1:C:240:LEU:O	2.18	0.43
1:D:418:PRO:HD3	1:D:438:MET:CE	2.48	0.43
1:A:118:VAL:HA	1:A:255:VAL:HG21	2.00	0.43
1:A:176:SER:HB2	1:A:240:LEU:O	2.17	0.43
1:B:194:ILE:CG2	1:B:194:ILE:O	2.66	0.43
1:C:118:VAL:HA	1:C:255:VAL:HG21	2.00	0.43
1:D:73:VAL:HG12	1:D:331:CYS:SG	2.58	0.43
1:D:382:THR:HG22	1:D:386:ILE:CG1	2.44	0.43
1:B:417:LEU:HB2	1:B:418:PRO:HD2	2.00	0.43
1:C:417:LEU:HB2	1:C:418:PRO:HD2	2.01	0.43
1:C:359:PHE:CD1	1:C:458:MET:HE3	2.53	0.43
1:D:118:VAL:HA	1:D:255:VAL:HG21	2.01	0.43
1:B:85:THR:O	1:B:89:LEU:HD22	2.19	0.43
1:C:200:THR:CG2	1:C:203:ASN:ND2	2.81	0.43
1:C:149:ILE:O	1:C:150:SER:HB2	2.19	0.43
1:D:139:PHE:CE2	1:D:184:GLY:HA3	2.54	0.43
1:A:418:PRO:HD3	1:A:438:MET:CE	2.49	0.42
1:A:279:SER:HB3	1:A:280:PRO:HD3	2.01	0.42
1:B:139:PHE:CE2	1:B:184:GLY:HA3	2.54	0.42
1:C:207:ALA:HA	1:C:212:LEU:HD12	2.01	0.42
1:C:359:PHE:HA	1:C:458:MET:HE1	2.01	0.42
1:D:243:THR:C	1:D:245:ASN:H	2.22	0.42
1:A:71:ILE:O	1:A:74:PRO:HD2	2.20	0.42
1:A:386:ILE:HB	1:A:387:PRO:HD3	2.01	0.42
1:A:418:PRO:O	1:A:419:VAL:HG12	2.19	0.42
1:B:59:TRP:NE1	1:B:69:THR:HB	2.35	0.42
1:D:77:ALA:HA	1:D:82:ILE:HD12	2.02	0.42
1:B:202:PRO:HD3	1:B:379:VAL:HG13	2.01	0.42
1:D:72:LEU:O	1:D:75:VAL:HG12	2.19	0.42
1:A:416:MET:O	1:A:438:MET:CG	2.58	0.42
1:D:418:PRO:C	1:D:420:ALA:N	2.72	0.42
1:D:417:LEU:HB2	1:D:418:PRO:HD2	2.02	0.42
1:A:418:PRO:HD3	1:A:438:MET:HE3	2.00	0.42
1:A:359:PHE:CD1	1:A:458:MET:HE3	2.55	0.42
1:B:418:PRO:HD3	1:B:438:MET:CE	2.50	0.42
1:A:418:PRO:C	1:A:420:ALA:N	2.72	0.41
1:B:224:THR:O	1:B:228:MET:HB2	2.20	0.41
1:D:200:THR:CG2	1:D:203:ASN:ND2	2.82	0.41
1:D:359:PHE:HA	1:D:458:MET:HE1	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:THR:O	1:A:228:MET:HB2	2.19	0.41
1:B:118:VAL:HA	1:B:255:VAL:HG21	2.01	0.41
1:B:82:ILE:HD13	1:B:335:VAL:HG13	2.01	0.41
1:C:59:TRP:NE1	1:C:69:THR:HB	2.36	0.41
1:B:152:THR:OG1	3:B:503:CIT:O3	2.26	0.41
1:C:85:THR:O	1:C:89:LEU:HD22	2.21	0.41
1:B:253:ALA:HA	1:B:254:PRO:HD3	1.97	0.41
1:A:243:THR:C	1:A:245:ASN:H	2.24	0.41
1:B:134:ALA:HB2	1:B:248:PHE:CE1	2.56	0.41
1:B:359:PHE:HA	1:B:458:MET:HE1	2.02	0.41
1:A:134:ALA:HB2	1:A:248:PHE:CE1	2.56	0.41
1:B:243:THR:C	1:B:245:ASN:H	2.23	0.41
1:C:243:THR:C	1:C:245:ASN:H	2.24	0.41
1:D:134:ALA:HB2	1:D:248:PHE:CE1	2.56	0.41
1:A:72:LEU:O	1:A:75:VAL:HG12	2.21	0.41
1:C:202:PRO:HD3	1:C:379:VAL:HG13	2.03	0.41
1:C:418:PRO:C	1:C:420:ALA:N	2.74	0.41
1:A:200:THR:CG2	1:A:203:ASN:ND2	2.82	0.40
1:A:214:PHE:CD2	1:A:275:TRP:HB3	2.56	0.40
1:A:104:PHE:CG	1:A:318:ALA:HA	2.57	0.40
1:B:210:VAL:HG23	1:B:212:LEU:HG	2.02	0.40
1:B:279:SER:HB3	1:B:280:PRO:HD3	2.02	0.40
1:B:360:VAL:O	1:B:364:VAL:HG23	2.22	0.40
1:C:138:LEU:HD13	1:C:162:VAL:HG22	2.03	0.40
1:B:322:ILE:HG22	1:B:326:PHE:CZ	2.56	0.40
1:C:386:ILE:HD13	1:C:404:SER:HA	2.04	0.40
1:C:39:LEU:HA	1:C:40:PRO:HD3	1.89	0.40
1:A:76:MET:O	1:A:77:ALA:C	2.60	0.40
1:B:201:GLY:HA3	1:B:379:VAL:CG1	2.51	0.40
1:C:279:SER:HB3	1:C:280:PRO:HD3	2.02	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%)	400 (90%)	31 (7%)	12 (3%)	5	15
1	B	443/445 (100%)	401 (90%)	33 (7%)	9 (2%)	7	22
1	C	443/445 (100%)	399 (90%)	35 (8%)	9 (2%)	7	22
1	D	443/445 (100%)	400 (90%)	32 (7%)	11 (2%)	5	17
All	All	1772/1780 (100%)	1600 (90%)	131 (7%)	41 (2%)	6	19

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	PRO
1	A	419	VAL
1	B	242	PRO
1	B	419	VAL
1	C	242	PRO
1	C	419	VAL
1	D	242	PRO
1	D	419	VAL
1	A	150	SER
1	A	252	ARG
1	A	259	LYS
1	A	416	MET
1	B	150	SER
1	B	252	ARG
1	B	259	LYS
1	B	416	MET
1	C	150	SER
1	C	252	ARG
1	C	259	LYS
1	C	416	MET
1	D	150	SER
1	D	252	ARG
1	D	259	LYS
1	D	416	MET
1	C	66	VAL
1	D	90	ASN
1	A	430	SER
1	B	430	SER
1	C	430	SER
1	D	430	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	40	PRO
1	A	90	ASN
1	B	66	VAL
1	B	40	PRO
1	D	40	PRO
1	D	66	VAL
1	C	40	PRO
1	A	66	VAL
1	A	418	PRO
1	D	418	PRO
1	A	129	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	355/355 (100%)	327 (92%)	28 (8%)	12	31
1	B	355/355 (100%)	327 (92%)	28 (8%)	12	31
1	C	355/355 (100%)	326 (92%)	29 (8%)	11	30
1	D	355/355 (100%)	328 (92%)	27 (8%)	13	33
All	All	1420/1420 (100%)	1308 (92%)	112 (8%)	12	31

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	VAL
1	A	89	LEU
1	A	121	ASP
1	A	144	LEU
1	A	161	LEU
1	A	178	TYR
1	A	197	LEU
1	A	203	ASN
1	A	215	THR
1	A	227	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	239	LEU
1	A	241	LYS
1	A	248	PHE
1	A	250	LEU
1	A	259	LYS
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	383	THR
1	A	412	SER
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	121	ASP
1	B	144	LEU
1	B	161	LEU
1	B	178	TYR
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	248	PHE
1	B	250	LEU
1	B	259	LYS
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	383	THR
1	B	412	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	121	ASP
1	C	144	LEU
1	C	161	LEU
1	C	178	TYR
1	C	197	LEU
1	C	203	ASN
1	C	205	ILE
1	C	215	THR
1	C	227	MET
1	C	239	LEU
1	C	241	LYS
1	C	248	PHE
1	C	250	LEU
1	C	259	LYS
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	383	THR
1	C	412	SER
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	144	LEU
1	D	161	LEU
1	D	178	TYR
1	D	197	LEU
1	D	203	ASN
1	D	215	THR
1	D	227	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	239	LEU
1	D	241	LYS
1	D	248	PHE
1	D	250	LEU
1	D	259	LYS
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	383	THR
1	D	412	SER
1	D	417	LEU
1	D	419	VAL
1	D	432	HIS
1	D	461	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	432	HIS
1	B	43	HIS
1	B	203	ASN
1	C	43	HIS
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 (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	-	3,12,12	0.70	0	3,17,17	1.58	1 (33%)
3	CIT	B	503	-	3,12,12	0.74	0	3,17,17	1.96	2 (66%)
3	CIT	C	503	-	3,12,12	0.94	0	3,17,17	1.72	1 (33%)
3	CIT	D	503	-	3,12,12	0.83	0	3,17,17	1.65	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	-	-	3/6/16/16	-
3	CIT	B	503	-	-	3/6/16/16	-
3	CIT	C	503	-	-	3/6/16/16	-
3	CIT	D	503	-	-	3/6/16/16	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	503	CIT	C3-C4-C5	-2.59	110.84	114.98
3	C	503	CIT	C3-C4-C5	-2.49	111.00	114.98
3	D	503	CIT	C3-C4-C5	-2.35	111.23	114.98
3	A	503	CIT	C3-C4-C5	-2.15	111.54	114.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	503	CIT	C4-C3-C2	2.00	114.68	109.33

There are no chirality outliers.

All (12) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	503	CIT	1	0
3	C	503	CIT	1	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, 95^{th} 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%)	0.48	58 (13%) 3 2	33, 77, 130, 173	0
1	B	445/445 (100%)	0.53	61 (13%) 3 2	45, 85, 142, 186	0
1	C	445/445 (100%)	0.37	41 (9%) 9 6	26, 70, 136, 190	0
1	D	445/445 (100%)	0.24	48 (10%) 5 4	6, 56, 101, 165	0
All	All	1780/1780 (100%)	0.40	208 (11%) 4 3	6, 73, 133, 190	0

All (208) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	462	GLN	14.5
1	C	250	LEU	10.5
1	A	130	LYS	9.0
1	C	254	PRO	8.3
1	C	462	GLN	8.1
1	B	462	GLN	8.0
1	C	355	HIS	7.6
1	B	247	MET	7.6
1	B	132	SER	7.0
1	B	133	VAL	6.9
1	A	240	LEU	6.8
1	B	258	ASP	6.2
1	B	240	LEU	6.1
1	B	259	LYS	6.1
1	A	247	MET	6.0
1	C	247	MET	6.0
1	B	128	GLN	5.9
1	A	128	GLN	5.9
1	C	128	GLN	5.9
1	B	245	ASN	5.7
1	C	253	ALA	5.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	245	ASN	5.5
1	A	252	ARG	5.5
1	D	130	LYS	5.4
1	B	173	LYS	5.4
1	A	462	GLN	5.3
1	A	249	GLU	5.3
1	A	19	HIS	5.3
1	C	251	ASP	5.3
1	A	168	LYS	5.2
1	C	461	TRP	5.2
1	D	168	LYS	5.1
1	A	245	ASN	5.1
1	A	255	VAL	5.1
1	B	257	TRP	5.1
1	A	251	ASP	5.1
1	B	255	VAL	5.0
1	A	18	LEU	5.0
1	D	245	ASN	4.9
1	A	173	LYS	4.9
1	C	130	LYS	4.9
1	B	355	HIS	4.9
1	B	238	PHE	4.9
1	C	256	ASN	4.8
1	A	355	HIS	4.8
1	A	461	TRP	4.7
1	B	168	LYS	4.7
1	B	18	LEU	4.7
1	B	126	MET	4.6
1	B	127	ALA	4.6
1	B	256	ASN	4.5
1	B	40	PRO	4.5
1	D	247	MET	4.5
1	C	38	PHE	4.5
1	C	172	ASP	4.5
1	C	18	LEU	4.4
1	A	257	TRP	4.3
1	D	19	HIS	4.3
1	D	440	ARG	4.3
1	A	354	SER	4.2
1	D	461	TRP	4.2
1	A	256	ASN	4.2
1	A	250	LEU	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	431	GLY	4.2
1	D	460	PHE	4.1
1	C	444	TYR	4.1
1	B	125	ALA	4.0
1	D	256	ASN	4.0
1	C	19	HIS	4.0
1	B	169	VAL	4.0
1	D	259	LYS	4.0
1	D	398	MET	3.9
1	D	444	TYR	3.9
1	D	356	MET	3.9
1	A	254	PRO	3.8
1	D	257	TRP	3.8
1	A	253	ALA	3.8
1	D	355	HIS	3.8
1	B	461	TRP	3.8
1	D	38	PHE	3.8
1	A	310	HIS	3.7
1	D	310	HIS	3.7
1	C	175	ARG	3.7
1	A	460	PHE	3.6
1	B	170	ASP	3.6
1	D	250	LEU	3.6
1	A	171	ALA	3.6
1	C	238	PHE	3.5
1	C	252	ARG	3.5
1	B	167	SER	3.5
1	B	248	PHE	3.5
1	D	126	MET	3.5
1	D	249	GLU	3.5
1	B	172	ASP	3.5
1	B	444	TYR	3.4
1	C	240	LEU	3.4
1	C	375	PHE	3.4
1	A	239	LEU	3.4
1	B	38	PHE	3.4
1	C	249	GLU	3.3
1	D	258	ASP	3.3
1	C	173	LYS	3.2
1	A	286	GLY	3.2
1	B	253	ALA	3.2
1	A	172	ASP	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	460	PHE	3.2
1	B	174	GLN	3.2
1	B	244	LEU	3.2
1	A	397	GLY	3.2
1	B	375	PHE	3.2
1	B	431	GLY	3.2
1	D	416	MET	3.1
1	D	18	LEU	3.1
1	D	238	PHE	3.1
1	A	277	PHE	3.1
1	D	375	PHE	3.1
1	B	219	LYS	3.1
1	A	417	LEU	3.0
1	B	131	MET	3.0
1	C	20	ARG	3.0
1	C	257	TRP	3.0
1	B	251	ASP	3.0
1	B	262	VAL	2.9
1	D	435	GLN	2.8
1	D	173	LYS	2.8
1	C	434	LYS	2.8
1	A	258	ASP	2.8
1	C	126	MET	2.8
1	B	239	LEU	2.7
1	D	397	GLY	2.7
1	B	130	LYS	2.7
1	B	164	GLY	2.7
1	B	252	ARG	2.7
1	D	240	LEU	2.7
1	C	440	ARG	2.7
1	A	217	TRP	2.7
1	C	244	LEU	2.7
1	A	246	GLY	2.6
1	C	255	VAL	2.6
1	B	250	LEU	2.6
1	A	347	ASN	2.6
1	A	416	MET	2.6
1	C	422	PRO	2.6
1	A	170	ASP	2.6
1	C	40	PRO	2.6
1	D	289	LYS	2.6
1	B	249	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	38	PHE	2.6
1	A	440	ARG	2.5
1	A	459	LEU	2.5
1	B	440	ARG	2.5
1	A	20	ARG	2.5
1	B	316	LYS	2.5
1	A	37	HIS	2.5
1	C	432	HIS	2.5
1	D	219	LYS	2.4
1	C	136	PHE	2.4
1	A	444	TYR	2.4
1	A	287	GLY	2.4
1	B	254	PRO	2.4
1	B	429	ALA	2.4
1	B	48	GLY	2.4
1	A	316	LYS	2.4
1	D	351	ASP	2.4
1	C	219	LYS	2.4
1	D	262	VAL	2.3
1	A	131	MET	2.3
1	C	43	HIS	2.3
1	D	36	TYR	2.3
1	D	284	ALA	2.3
1	B	310	HIS	2.3
1	A	351	ASP	2.3
1	D	442	GLY	2.3
1	B	352	MET	2.3
1	B	342	SER	2.2
1	D	313	GLU	2.2
1	D	252	ARG	2.2
1	B	140	GLY	2.2
1	A	242	PRO	2.2
1	A	350	SER	2.2
1	A	36	TYR	2.2
1	A	238	PHE	2.2
1	A	262	VAL	2.2
1	B	43	HIS	2.2
1	A	447	ILE	2.2
1	D	169	VAL	2.2
1	D	251	ASP	2.2
1	B	227	MET	2.2
1	D	371	PHE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	417	LEU	2.1
1	D	244	LEU	2.1
1	D	20	ARG	2.1
1	A	313	GLU	2.1
1	C	419	VAL	2.1
1	B	371	PHE	2.1
1	A	169	VAL	2.1
1	D	37	HIS	2.1
1	B	241	LYS	2.1
1	D	212	LEU	2.1
1	B	136	PHE	2.1
1	B	359	PHE	2.1
1	B	237	TYR	2.0
1	D	178	TYR	2.0
1	D	286	GLY	2.0
1	A	178	TYR	2.0
1	A	237	TYR	2.0
1	C	460	PHE	2.0
1	A	244	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	0.73	0.21	57,57,57,57	0
2	NA	A	502	1/1	0.80	0.27	70,70,70,70	0
3	CIT	B	503	13/13	0.84	0.32	53,77,87,89	0
3	CIT	C	503	13/13	0.84	0.35	50,67,73,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CIT	D	503	13/13	0.86	0.21	58,78,86,91	0
3	CIT	A	503	13/13	0.88	0.21	49,68,72,73	0
2	NA	C	502	1/1	0.92	0.21	69,69,69,69	0
2	NA	B	501	1/1	0.93	0.18	95,95,95,95	0
2	NA	B	502	1/1	0.93	0.24	104,104,104,104	0
2	NA	C	501	1/1	0.95	0.14	72,72,72,72	0
2	NA	D	501	1/1	0.96	0.45	72,72,72,72	0
2	NA	A	501	1/1	0.98	0.17	63,63,63,63	0

6.5 Other polymers

There are no such residues in this entry.