



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:51 am BST

PDB ID : 3NTJ
Title : Redox regulation of Plasmodium falciparum ornithine delta-aminotransferase
Authors : Fritz-Wolf, K.; Jortzik, E.; Stumpf, M.; Becker, K.
Deposited on : 2010-07-05
Resolution : 3.00 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 ⓘ](#)) 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 : 2.11
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) : 2.11

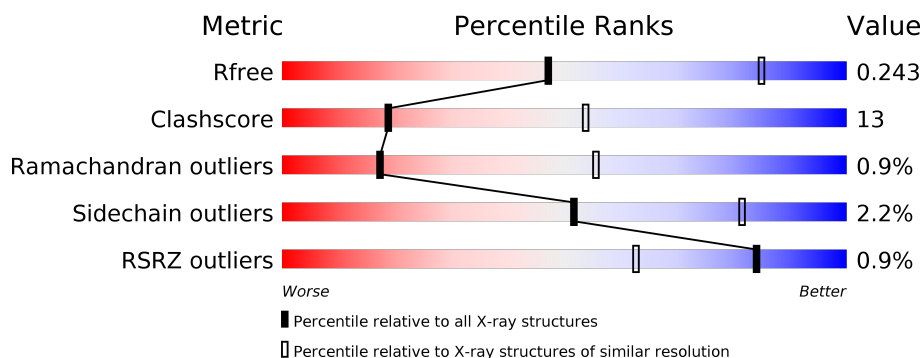
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 $\leq 5\%$. 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	422	<div> <div>%</div> <div> <div></div> <div>66%</div> <div>22%</div> <div>• 10%</div> </div> </div>
1	B	422	<div> <div>%</div> <div> <div></div> <div>65%</div> <div>27%</div> <div>• 7%</div> </div> </div>
1	C	422	<div> <div></div> <div> <div>66%</div> <div>24%</div> <div>• 9%</div> </div> </div>
1	D	422	<div> <div>%</div> <div> <div></div> <div>65%</div> <div>23%</div> <div>• 9%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12123 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 Ornithine aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	0	0
			2979	1904	497	559	19			
1	B	393	Total	C	N	O	S	0	0	0
			3078	1970	514	574	20			
1	C	386	Total	C	N	O	S	0	0	0
			3023	1936	503	565	19			
1	D	384	Total	C	N	O	S	0	0	0
			3005	1922	501	563	19			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	415	LEU	-	EXPRESSION TAG	UNP Q6LFH8
A	416	GLN	-	EXPRESSION TAG	UNP Q6LFH8
A	417	HIS	-	EXPRESSION TAG	UNP Q6LFH8
A	418	HIS	-	EXPRESSION TAG	UNP Q6LFH8
A	419	HIS	-	EXPRESSION TAG	UNP Q6LFH8
A	420	HIS	-	EXPRESSION TAG	UNP Q6LFH8
A	421	HIS	-	EXPRESSION TAG	UNP Q6LFH8
A	422	HIS	-	EXPRESSION TAG	UNP Q6LFH8
B	415	LEU	-	EXPRESSION TAG	UNP Q6LFH8
B	416	GLN	-	EXPRESSION TAG	UNP Q6LFH8
B	417	HIS	-	EXPRESSION TAG	UNP Q6LFH8
B	418	HIS	-	EXPRESSION TAG	UNP Q6LFH8
B	419	HIS	-	EXPRESSION TAG	UNP Q6LFH8
B	420	HIS	-	EXPRESSION TAG	UNP Q6LFH8
B	421	HIS	-	EXPRESSION TAG	UNP Q6LFH8
B	422	HIS	-	EXPRESSION TAG	UNP Q6LFH8
C	415	LEU	-	EXPRESSION TAG	UNP Q6LFH8
C	416	GLN	-	EXPRESSION TAG	UNP Q6LFH8
C	417	HIS	-	EXPRESSION TAG	UNP Q6LFH8
C	418	HIS	-	EXPRESSION TAG	UNP Q6LFH8
C	419	HIS	-	EXPRESSION TAG	UNP Q6LFH8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	420	HIS	-	EXPRESSION TAG	UNP Q6LFH8
C	421	HIS	-	EXPRESSION TAG	UNP Q6LFH8
C	422	HIS	-	EXPRESSION TAG	UNP Q6LFH8
D	415	LEU	-	EXPRESSION TAG	UNP Q6LFH8
D	416	GLN	-	EXPRESSION TAG	UNP Q6LFH8
D	417	HIS	-	EXPRESSION TAG	UNP Q6LFH8
D	418	HIS	-	EXPRESSION TAG	UNP Q6LFH8
D	419	HIS	-	EXPRESSION TAG	UNP Q6LFH8
D	420	HIS	-	EXPRESSION TAG	UNP Q6LFH8
D	421	HIS	-	EXPRESSION TAG	UNP Q6LFH8
D	422	HIS	-	EXPRESSION TAG	UNP Q6LFH8

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

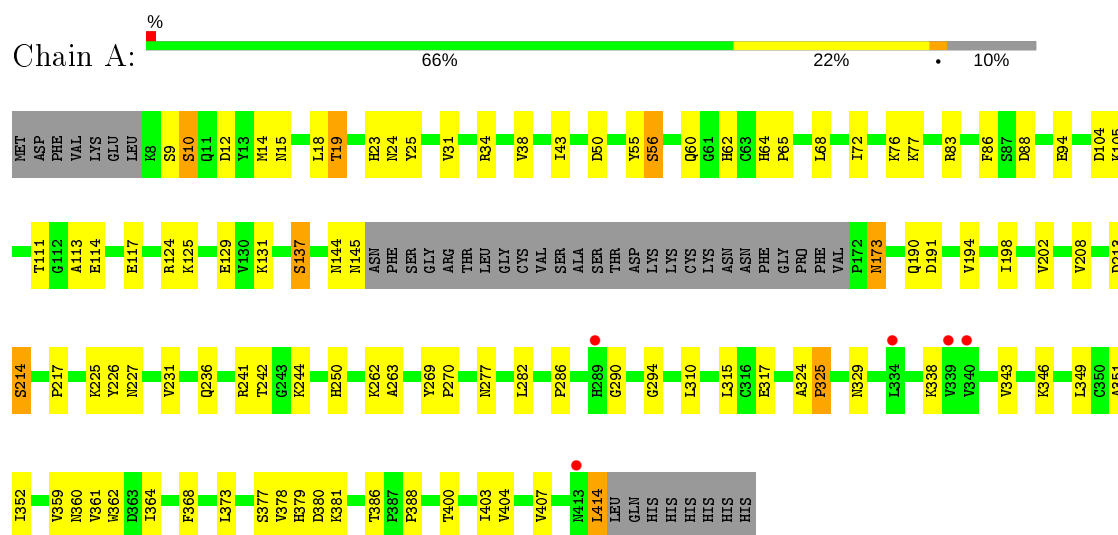
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total 5	O 5	0	0
3	B	4	Total 4	O 4	0	0
3	C	4	Total 4	O 4	0	0
3	D	5	Total 5	O 5	0	0

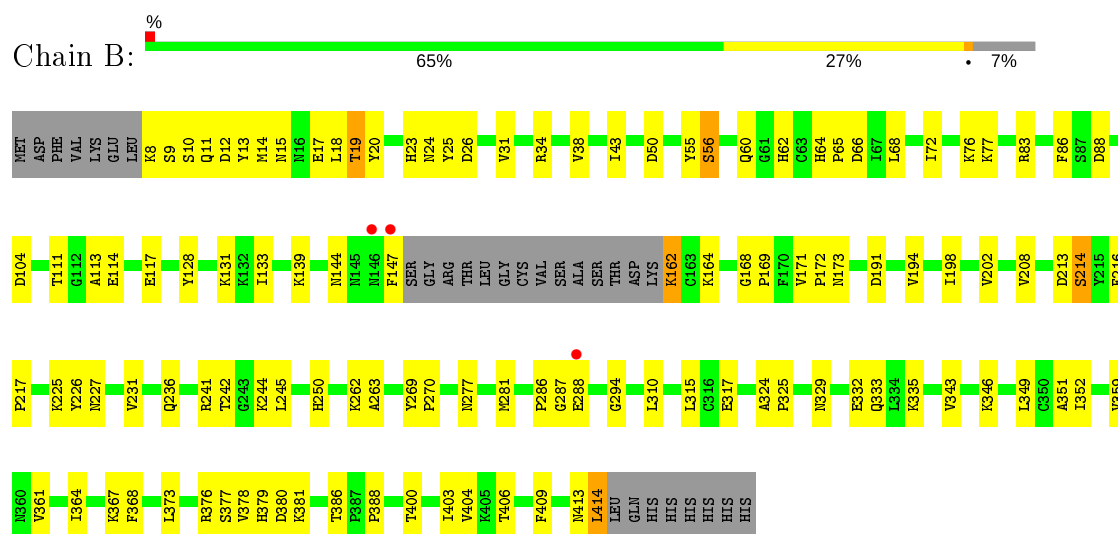
3 Residue-property plots

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: Ornithine aminotransferase

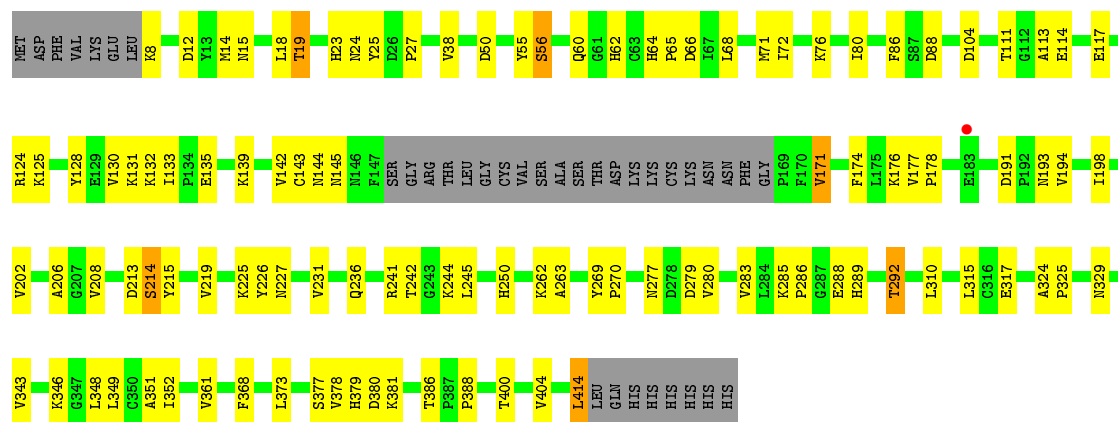


• Molecule 1: Ornithine aminotransferase

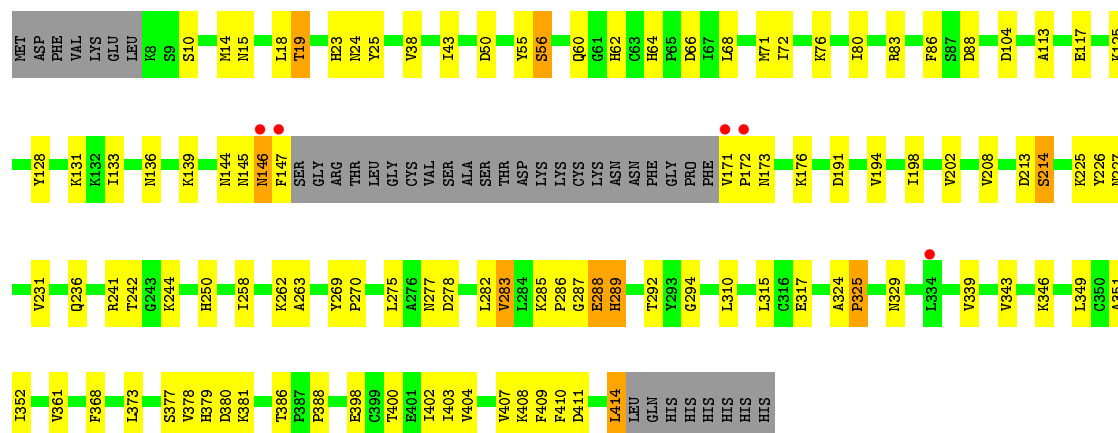


• Molecule 1: Ornithine aminotransferase





● Molecule 1: Ornithine aminotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.39Å 104.97Å 181.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.83 – 3.00 48.83 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.83-3.00) 99.5 (48.83-3.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.86 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.191 , 0.242 0.194 , 0.243	Depositor DCC
R_{free} test set	2358 reflections (6.00%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12123	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.78% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.46	0/3037	0.57	0/4110
1	B	0.48	0/3140	0.58	0/4249
1	C	0.48	0/3084	0.57	0/4175
1	D	0.47	0/3064	0.58	0/4148
All	All	0.47	0/12325	0.58	0/16682

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2979	0	3002	85	0
1	B	3078	0	3096	88	0
1	C	3023	0	3042	80	0
1	D	3005	0	3025	93	0
2	A	10	0	0	2	0
2	C	10	0	0	0	0
3	A	5	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	5	0	0	0	0
All	All	12123	0	12165	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 13.

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:C:414:LEU:N	1:C:414:LEU:HD12	1.82	0.94
1:C:414:LEU:H	1:C:414:LEU:HD12	1.36	0.90
1:A:403:ILE:O	1:A:407:VAL:HG23	1.74	0.88
1:D:213:ASP:O	1:D:214:SER:HB3	1.74	0.87
1:A:213:ASP:O	1:A:214:SER:HB3	1.74	0.86
1:C:378:VAL:O	1:C:379:HIS:HB2	1.76	0.86
1:A:378:VAL:O	1:A:379:HIS:HB2	1.74	0.85
1:D:131:LYS:HE3	1:D:227:ASN:O	1.75	0.85
1:B:213:ASP:O	1:B:214:SER:HB3	1.74	0.85
1:C:213:ASP:O	1:C:214:SER:HB3	1.77	0.83
1:D:378:VAL:O	1:D:379:HIS:HB2	1.76	0.83
1:A:225:LYS:HD2	1:D:23:HIS:CD2	2.14	0.83
1:B:378:VAL:O	1:B:379:HIS:HB2	1.75	0.83
1:A:225:LYS:NZ	1:D:23:HIS:CE1	2.47	0.82
1:D:171:VAL:C	1:D:173:ASN:H	1.82	0.81
1:A:225:LYS:HZ2	1:D:23:HIS:CE1	1.99	0.79
1:B:172:PRO:O	1:B:173:ASN:HB2	1.86	0.74
1:A:225:LYS:NZ	1:D:18:LEU:HD22	2.03	0.73
1:A:125:LYS:HE2	1:A:129:GLU:OE2	1.90	0.72
1:B:367:LYS:HE2	1:B:409:PHE:CD1	2.24	0.72
1:A:262:LYS:NZ	2:A:441:SO4:O4	2.23	0.72
1:A:68:LEU:O	1:A:72:ILE:HG13	1.91	0.70
1:D:139:LYS:HE2	1:D:172:PRO:HD3	1.74	0.69
1:B:171:VAL:HG13	1:B:172:PRO:HD2	1.76	0.67
1:C:131:LYS:HG3	1:C:227:ASN:HD22	1.58	0.67
1:D:68:LEU:O	1:D:72:ILE:HG13	1.94	0.67
1:B:68:LEU:O	1:B:72:ILE:HG13	1.95	0.67
1:D:38:VAL:HG23	1:D:388:PRO:HD2	1.77	0.66
1:B:38:VAL:HG23	1:B:388:PRO:HD2	1.76	0.66
1:A:104:ASP:HB2	1:A:277:ASN:HA	1.79	0.65
1:D:136:ASN:O	1:D:171:VAL:HG11	1.96	0.65
1:B:413:ASN:C	1:B:414:LEU:HD23	2.18	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:VAL:HG23	1:A:388:PRO:HD2	1.79	0.64
1:C:414:LEU:CD1	1:C:414:LEU:H	2.09	0.64
1:D:104:ASP:HB2	1:D:277:ASN:HA	1.80	0.64
1:D:400:THR:O	1:D:404:VAL:HG23	1.97	0.64
1:C:68:LEU:O	1:C:72:ILE:HG13	1.98	0.63
1:A:225:LYS:HZ3	1:D:18:LEU:HB3	1.61	0.63
1:A:9:SER:H	1:A:12:ASP:HB2	1.65	0.62
1:B:379:HIS:HB3	1:B:381:LYS:HG2	1.80	0.62
1:C:379:HIS:HB3	1:C:381:LYS:HG2	1.80	0.62
1:C:38:VAL:HG23	1:C:388:PRO:HD2	1.80	0.62
1:A:286:PRO:HB3	1:B:26:ASP:HB2	1.82	0.61
1:A:400:THR:O	1:A:404:VAL:HG23	2.00	0.61
1:B:104:ASP:HB2	1:B:277:ASN:HA	1.80	0.61
1:C:131:LYS:HG3	1:C:227:ASN:ND2	2.15	0.61
1:D:379:HIS:HB3	1:D:381:LYS:HG2	1.82	0.61
1:A:379:HIS:HB3	1:A:381:LYS:HG2	1.83	0.61
1:D:15:ASN:O	1:D:19:THR:HG23	2.01	0.60
1:C:343:VAL:HG22	1:C:352:ILE:HG12	1.83	0.60
1:B:14:MET:O	1:B:18:LEU:HG	2.03	0.59
1:C:400:THR:O	1:C:404:VAL:HG23	2.03	0.59
1:B:8:LYS:HA	1:B:12:ASP:OD2	2.02	0.58
1:D:411:ASP:O	1:D:414:LEU:HD12	2.03	0.58
1:C:113:ALA:O	1:C:117:GLU:HG2	2.02	0.58
1:C:50:ASP:OD2	1:C:62:HIS:HE1	1.85	0.58
1:B:162:LYS:HG2	1:B:164:LYS:HE2	1.86	0.58
1:B:131:LYS:HE3	1:B:227:ASN:O	2.03	0.58
1:B:128:TYR:HA	1:B:133:ILE:O	2.04	0.58
1:B:131:LYS:HD3	1:B:133:ILE:HD11	1.86	0.58
1:A:225:LYS:HZ1	1:D:23:HIS:CE1	2.19	0.57
1:B:15:ASN:O	1:B:19:THR:HG23	2.03	0.57
1:C:280:VAL:O	1:C:283:VAL:HG23	2.04	0.57
1:B:139:LYS:HE3	1:B:171:VAL:CG2	2.35	0.57
1:C:104:ASP:HB2	1:C:277:ASN:HA	1.86	0.57
1:C:171:VAL:HG22	1:C:174:PHE:HD1	1.69	0.57
1:A:310:LEU:HA	1:A:315:LEU:HD12	1.86	0.56
1:B:400:THR:O	1:B:404:VAL:HG23	2.06	0.56
1:D:343:VAL:HG22	1:D:352:ILE:HG12	1.87	0.56
1:B:11:GLN:HA	1:B:14:MET:HE3	1.88	0.56
1:D:171:VAL:CG2	1:D:173:ASN:HA	2.36	0.56
1:A:343:VAL:HG22	1:A:352:ILE:HG12	1.87	0.56
1:C:15:ASN:O	1:C:19:THR:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:LYS:HE3	1:B:171:VAL:HG21	1.88	0.55
1:A:225:LYS:CE	1:D:18:LEU:HD22	2.36	0.55
1:C:286:PRO:C	1:C:288:GLU:H	2.10	0.55
1:D:113:ALA:O	1:D:117:GLU:HG2	2.06	0.55
1:A:9:SER:O	1:A:10:SER:C	2.44	0.55
1:B:171:VAL:HG13	1:B:172:PRO:CD	2.37	0.55
1:B:18:LEU:O	1:B:23:HIS:HE1	1.89	0.55
1:C:18:LEU:O	1:C:23:HIS:HE1	1.90	0.55
1:A:113:ALA:O	1:A:117:GLU:HG2	2.07	0.55
1:B:244:LYS:HG2	1:B:250:HIS:CE1	2.42	0.55
1:D:368:PHE:HB3	1:D:373:LEU:O	2.06	0.55
1:B:378:VAL:O	1:B:379:HIS:CB	2.50	0.55
1:A:38:VAL:HA	1:A:388:PRO:HG2	1.88	0.54
1:B:242:THR:HB	1:B:346:LYS:HG2	1.89	0.54
1:D:361:VAL:HG21	1:D:381:LYS:HA	1.90	0.54
1:A:50:ASP:OD2	1:A:62:HIS:HE1	1.90	0.54
1:D:50:ASP:OD2	1:D:62:HIS:HE1	1.90	0.54
1:A:131:LYS:NZ	1:A:227:ASN:O	2.39	0.54
1:D:278:ASP:HB3	1:D:282:LEU:HD12	1.89	0.54
1:B:38:VAL:HA	1:B:388:PRO:HG2	1.89	0.54
1:B:50:ASP:OD2	1:B:62:HIS:HE1	1.90	0.53
1:D:310:LEU:HA	1:D:315:LEU:HD12	1.89	0.53
1:A:378:VAL:O	1:A:379:HIS:CB	2.51	0.53
1:B:310:LEU:HA	1:B:315:LEU:HD12	1.90	0.53
1:B:378:VAL:O	1:B:378:VAL:HG12	2.07	0.53
1:C:368:PHE:HB3	1:C:373:LEU:O	2.08	0.53
1:C:361:VAL:HG21	1:C:381:LYS:HA	1.91	0.53
1:B:113:ALA:O	1:B:117:GLU:HG2	2.07	0.53
1:B:361:VAL:HG21	1:B:381:LYS:HA	1.91	0.53
1:B:343:VAL:HG22	1:B:352:ILE:HG12	1.90	0.53
1:C:225:LYS:HD3	1:C:226:TYR:CE2	2.44	0.53
1:C:310:LEU:HA	1:C:315:LEU:HD12	1.91	0.53
1:C:378:VAL:O	1:C:379:HIS:CB	2.52	0.53
1:C:55:TYR:O	1:C:56:SER:HB2	2.09	0.53
1:D:18:LEU:O	1:D:23:HIS:HE1	1.92	0.53
1:A:338:LYS:HD2	1:A:414:LEU:HD11	1.90	0.53
1:D:324:ALA:HB3	1:D:325:PRO:HD3	1.91	0.53
1:C:324:ALA:HB3	1:C:325:PRO:HD3	1.91	0.52
1:A:18:LEU:O	1:A:23:HIS:HE1	1.93	0.52
1:D:244:LYS:HG2	1:D:250:HIS:CE1	2.45	0.52
1:D:242:THR:HB	1:D:346:LYS:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:PHE:HB3	1:B:373:LEU:O	2.09	0.52
1:A:361:VAL:HG21	1:A:381:LYS:HA	1.92	0.52
1:C:8:LYS:HA	1:C:12:ASP:OD2	2.10	0.52
1:C:270:PRO:HD3	1:D:269:TYR:CZ	2.44	0.52
1:A:241:ARG:HG3	1:A:349:LEU:HB2	1.92	0.52
1:A:225:LYS:HZ3	1:D:18:LEU:HD22	1.74	0.52
1:D:171:VAL:HG22	1:D:173:ASN:H	1.74	0.51
1:B:225:LYS:HD3	1:B:226:TYR:CE2	2.46	0.51
1:B:208:VAL:HG21	1:B:351:ALA:HB2	1.93	0.51
1:C:27:PRO:HG2	1:D:86:PHE:CZ	2.45	0.51
1:A:83:ARG:HD3	1:A:294:GLY:O	2.11	0.51
2:A:423:SO4:O4	1:B:262:LYS:NZ	2.42	0.51
1:C:111:THR:OG1	1:C:114:GLU:HG3	2.11	0.51
1:C:236:GLN:OE1	1:C:262:LYS:HE2	2.11	0.51
1:A:214:SER:HA	1:C:130:VAL:HG22	1.93	0.51
1:D:171:VAL:C	1:D:173:ASN:N	2.52	0.50
1:A:144:ASN:O	1:A:145:ASN:HB2	2.11	0.50
1:A:244:LYS:HG2	1:A:250:HIS:CE1	2.46	0.50
1:C:125:LYS:HG2	1:C:283:VAL:HG12	1.93	0.50
1:C:241:ARG:HG3	1:C:349:LEU:HB2	1.92	0.50
1:D:72:ILE:O	1:D:76:LYS:HG3	2.11	0.50
1:C:144:ASN:HD22	1:C:178:PRO:HA	1.75	0.50
1:C:56:SER:O	1:C:263:ALA:HB2	2.12	0.50
1:D:236:GLN:OE1	1:D:262:LYS:HE2	2.12	0.50
1:A:15:ASN:O	1:A:19:THR:HG23	2.11	0.50
1:C:130:VAL:HG12	1:C:131:LYS:N	2.27	0.50
1:B:13:TYR:CD2	1:B:43:ILE:HG13	2.47	0.50
1:B:241:ARG:HG3	1:B:349:LEU:HB2	1.93	0.50
1:B:111:THR:OG1	1:B:114:GLU:HG3	2.12	0.50
1:B:367:LYS:HB3	1:B:406:THR:HG23	1.93	0.50
1:C:64:HIS:CE1	1:C:66:ASP:HB2	2.48	0.49
1:D:144:ASN:O	1:D:146:ASN:N	2.45	0.49
1:A:242:THR:HB	1:A:346:LYS:HG2	1.94	0.49
1:C:14:MET:O	1:C:18:LEU:HG	2.13	0.49
1:B:379:HIS:O	1:B:380:ASP:HB2	2.11	0.49
1:A:236:GLN:OE1	1:A:262:LYS:HE2	2.13	0.49
1:A:14:MET:O	1:A:18:LEU:HG	2.12	0.49
1:B:236:GLN:OE1	1:B:262:LYS:HE2	2.12	0.49
1:D:125:LYS:HG2	1:D:283:VAL:HG13	1.93	0.49
1:B:139:LYS:HG2	1:B:171:VAL:CG1	2.43	0.49
1:D:407:VAL:O	1:D:408:LYS:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:VAL:HG21	1:A:351:ALA:HB2	1.94	0.48
1:A:56:SER:O	1:A:263:ALA:HB2	2.14	0.48
1:D:144:ASN:C	1:D:146:ASN:N	2.66	0.48
1:A:214:SER:HB2	1:C:279:ASP:HB2	1.96	0.48
1:C:242:THR:HB	1:C:346:LYS:HG2	1.94	0.48
1:C:244:LYS:HG2	1:C:250:HIS:CE1	2.48	0.48
1:D:379:HIS:O	1:D:380:ASP:HB2	2.13	0.48
1:A:144:ASN:O	1:A:145:ASN:CB	2.61	0.48
1:B:15:ASN:O	1:B:19:THR:CG2	2.62	0.48
1:A:124:ARG:HH21	1:A:173:ASN:HB2	1.79	0.48
1:A:368:PHE:HB3	1:A:373:LEU:O	2.13	0.48
1:D:378:VAL:O	1:D:379:HIS:CB	2.53	0.48
1:D:55:TYR:O	1:D:56:SER:HB2	2.13	0.48
1:D:339:VAL:HG22	1:D:411:ASP:OD1	2.13	0.48
1:C:208:VAL:HG21	1:C:351:ALA:HB2	1.95	0.47
1:D:213:ASP:O	1:D:214:SER:CB	2.52	0.47
1:A:190:GLN:OE1	1:D:15:ASN:HB3	2.13	0.47
1:C:145:ASN:HB2	1:C:206:ALA:HB2	1.96	0.47
1:C:128:TYR:HA	1:C:133:ILE:O	2.14	0.47
1:C:142:VAL:O	1:C:176:LYS:HA	2.14	0.47
1:C:198:ILE:HG12	1:C:231:VAL:HB	1.95	0.47
1:A:60:GLN:OE1	1:A:60:GLN:N	2.42	0.47
1:D:15:ASN:O	1:D:19:THR:CG2	2.61	0.47
1:D:56:SER:O	1:D:263:ALA:HB2	2.15	0.47
1:A:379:HIS:O	1:A:380:ASP:HB2	2.15	0.47
1:C:139:LYS:NZ	1:C:193:ASN:HB2	2.29	0.47
1:D:125:LYS:HB3	1:D:283:VAL:CG1	2.45	0.47
1:A:15:ASN:O	1:A:19:THR:CG2	2.63	0.47
1:A:213:ASP:O	1:A:214:SER:CB	2.52	0.47
1:A:269:TYR:CZ	1:B:270:PRO:HD3	2.49	0.47
1:A:88:ASP:N	1:A:88:ASP:OD1	2.48	0.47
1:D:55:TYR:O	1:D:262:LYS:HD3	2.15	0.47
1:D:208:VAL:HG21	1:D:351:ALA:HB2	1.96	0.47
1:B:139:LYS:HG2	1:B:171:VAL:HG11	1.96	0.47
1:C:379:HIS:O	1:C:380:ASP:HB2	2.14	0.47
1:A:64:HIS:HA	1:A:65:PRO:HD3	1.72	0.46
1:B:245:LEU:HA	1:B:245:LEU:HD23	1.82	0.46
1:C:215:TYR:O	1:C:219:VAL:HG23	2.15	0.46
1:C:378:VAL:HG12	1:C:378:VAL:O	2.14	0.46
1:C:191:ASP:HB3	1:C:194:VAL:HG23	1.98	0.46
1:D:171:VAL:HG23	1:D:173:ASN:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:MET:HE3	1:D:71:MET:HG2	1.97	0.46
1:A:378:VAL:HG12	1:A:378:VAL:O	2.16	0.46
1:C:25:TYR:CZ	1:D:83:ARG:HG3	2.51	0.46
1:C:245:LEU:HD23	1:C:245:LEU:HA	1.77	0.46
1:A:217:PRO:HG2	1:C:130:VAL:HG22	1.98	0.46
1:C:15:ASN:O	1:C:19:THR:CG2	2.64	0.46
1:C:125:LYS:HG2	1:C:283:VAL:CG1	2.46	0.46
1:D:171:VAL:CG2	1:D:173:ASN:H	2.29	0.46
1:D:191:ASP:HB3	1:D:194:VAL:HG23	1.97	0.46
1:D:317:GLU:OE1	1:D:317:GLU:N	2.38	0.46
1:D:38:VAL:HA	1:D:388:PRO:HG2	1.97	0.46
1:A:324:ALA:HB3	1:A:325:PRO:HD3	1.98	0.46
1:D:146:ASN:ND2	1:D:379:HIS:NE2	2.64	0.46
1:D:241:ARG:HG3	1:D:349:LEU:HB2	1.97	0.46
1:C:139:LYS:HZ2	1:C:193:ASN:HB2	1.81	0.45
1:A:368:PHE:HE1	1:A:403:ILE:HA	1.81	0.45
1:B:55:TYR:O	1:B:56:SER:HB2	2.17	0.45
1:D:408:LYS:O	1:D:409:PHE:C	2.54	0.45
1:D:60:GLN:N	1:D:60:GLN:OE1	2.46	0.45
1:A:225:LYS:HD3	1:A:226:TYR:CE2	2.51	0.45
1:B:191:ASP:HB3	1:B:194:VAL:HG23	1.98	0.45
1:B:8:LYS:HE3	1:B:8:LYS:HB3	1.80	0.45
1:D:128:TYR:HA	1:D:133:ILE:O	2.16	0.45
1:B:368:PHE:HE1	1:B:403:ILE:HA	1.81	0.45
1:B:88:ASP:OD1	1:B:88:ASP:N	2.50	0.45
1:A:225:LYS:CD	1:D:23:HIS:CD2	2.95	0.45
1:A:14:MET:HG2	1:B:86:PHE:CZ	2.52	0.45
1:C:171:VAL:HG22	1:C:174:PHE:CD1	2.49	0.45
1:C:38:VAL:HA	1:C:388:PRO:HG2	1.98	0.45
1:C:72:ILE:O	1:C:76:LYS:HG3	2.17	0.45
1:A:72:ILE:O	1:A:76:LYS:HG3	2.17	0.44
1:B:286:PRO:C	1:B:288:GLU:H	2.19	0.44
1:D:361:VAL:HG12	1:D:377:SER:HB3	1.99	0.44
1:A:31:VAL:HA	1:B:86:PHE:HB2	2.00	0.44
1:D:378:VAL:HG12	1:D:378:VAL:O	2.17	0.44
1:B:349:LEU:HA	1:B:386:THR:HG22	1.99	0.44
1:C:361:VAL:HG12	1:C:377:SER:HB3	1.98	0.44
1:D:144:ASN:OD1	1:D:176:LYS:HB3	2.18	0.44
1:D:14:MET:O	1:D:18:LEU:HG	2.17	0.44
1:D:361:VAL:HG21	1:D:381:LYS:CA	2.47	0.44
1:D:368:PHE:HE1	1:D:403:ILE:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:ASP:N	1:D:88:ASP:OD1	2.51	0.44
1:A:349:LEU:HA	1:A:386:THR:HG22	2.00	0.44
1:A:86:PHE:HB2	1:B:31:VAL:HA	2.00	0.44
1:D:171:VAL:HG22	1:D:173:ASN:N	2.33	0.44
1:D:198:ILE:HG12	1:D:231:VAL:HB	2.00	0.44
1:A:43:ILE:HD13	1:A:43:ILE:HA	1.82	0.44
1:B:332:GLU:O	1:B:335:LYS:HG2	2.18	0.43
1:D:146:ASN:HB3	1:D:147:PHE:H	1.61	0.43
1:A:361:VAL:HG21	1:A:381:LYS:CA	2.48	0.43
1:C:124:ARG:HB3	1:C:135:GLU:HG3	2.00	0.43
1:C:349:LEU:HA	1:C:386:THR:HG22	2.01	0.43
1:D:225:LYS:HD3	1:D:226:TYR:CE2	2.53	0.43
1:B:317:GLU:OE1	1:B:317:GLU:N	2.42	0.43
1:B:198:ILE:HG12	1:B:231:VAL:HB	2.00	0.43
1:D:287:GLY:O	1:D:289:HIS:N	2.52	0.43
1:A:34:ARG:HA	1:B:77:LYS:O	2.19	0.43
1:C:269:TYR:CZ	1:D:270:PRO:HD3	2.54	0.43
1:B:72:ILE:O	1:B:76:LYS:HG3	2.19	0.42
1:A:24:ASN:ND2	1:A:25:TYR:CE2	2.87	0.42
1:B:144:ASN:HB3	1:B:147:PHE:HA	1.99	0.42
1:B:324:ALA:HB3	1:B:325:PRO:HD3	2.00	0.42
1:C:145:ASN:HB2	1:C:206:ALA:CB	2.49	0.42
1:C:24:ASN:ND2	1:C:25:TYR:CE2	2.86	0.42
1:C:317:GLU:N	1:C:317:GLU:OE1	2.43	0.42
1:A:105:LYS:HA	1:B:20:TYR:O	2.19	0.42
1:B:24:ASN:ND2	1:B:25:TYR:CE2	2.87	0.42
1:B:9:SER:O	1:B:10:SER:C	2.57	0.42
1:D:43:ILE:HA	1:D:43:ILE:HD13	1.75	0.42
1:B:139:LYS:CG	1:B:171:VAL:HG11	2.48	0.42
1:A:111:THR:OG1	1:A:114:GLU:HG3	2.19	0.42
1:A:361:VAL:HG12	1:A:377:SER:HB3	2.01	0.42
1:A:282:LEU:HD23	1:A:282:LEU:HA	1.81	0.42
1:A:55:TYR:O	1:A:262:LYS:HD3	2.19	0.42
1:C:361:VAL:HG21	1:C:381:LYS:CA	2.49	0.42
1:D:64:HIS:CE1	1:D:66:ASP:HB2	2.54	0.42
1:D:83:ARG:HD3	1:D:294:GLY:O	2.20	0.42
1:C:88:ASP:OD1	1:C:88:ASP:N	2.52	0.42
1:D:398:GLU:O	1:D:402:ILE:HG13	2.20	0.42
1:A:191:ASP:HB3	1:A:194:VAL:HG23	2.01	0.42
1:A:270:PRO:HD3	1:B:269:TYR:CZ	2.54	0.42
1:D:407:VAL:O	1:D:410:PHE:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:GLY:HA3	1:B:169:PRO:HD3	1.88	0.42
1:C:60:GLN:N	1:C:60:GLN:OE1	2.42	0.42
1:D:146:ASN:HD22	1:D:146:ASN:HA	1.59	0.42
1:A:359:VAL:HG21	1:A:364:ILE:HD11	2.02	0.41
1:B:56:SER:O	1:B:263:ALA:HB2	2.20	0.41
1:A:77:LYS:O	1:B:34:ARG:HA	2.20	0.41
1:B:376:ARG:HG3	1:B:377:SER:N	2.35	0.41
1:C:64:HIS:HA	1:C:65:PRO:HD3	1.75	0.41
1:B:139:LYS:NZ	1:B:191:ASP:OD2	2.37	0.41
1:D:80:ILE:HD11	1:D:292:THR:HG22	2.02	0.41
1:B:216:PHE:N	1:B:217:PRO:CD	2.83	0.41
1:B:359:VAL:HG21	1:B:364:ILE:HD11	2.02	0.41
1:D:285:LYS:O	1:D:288:GLU:HG3	2.19	0.41
1:A:360:ASN:OD1	1:A:362:TRP:HB3	2.21	0.41
1:B:43:ILE:HA	1:B:43:ILE:HD13	1.78	0.41
1:D:408:LYS:O	1:D:411:ASP:N	2.53	0.41
1:B:60:GLN:OE1	1:B:60:GLN:N	2.43	0.41
1:A:324:ALA:N	1:A:325:PRO:CD	2.84	0.41
1:B:361:VAL:HG21	1:B:381:LYS:CA	2.50	0.41
1:C:143:CYS:HA	1:C:177:VAL:O	2.21	0.41
1:D:349:LEU:HA	1:D:386:THR:HG22	2.03	0.41
1:A:198:ILE:HG12	1:A:231:VAL:HB	2.02	0.41
1:C:80:ILE:HD11	1:C:292:THR:HG22	2.03	0.41
1:D:24:ASN:ND2	1:D:25:TYR:CE2	2.89	0.41
1:A:241:ARG:CG	1:A:349:LEU:HB2	2.50	0.41
1:B:281:MET:O	1:B:281:MET:HG3	2.21	0.41
1:A:317:GLU:OE1	1:A:317:GLU:N	2.40	0.40
1:B:64:HIS:CE1	1:B:66:ASP:HB2	2.55	0.40
1:C:213:ASP:O	1:C:214:SER:CB	2.56	0.40
1:C:348:LEU:HA	1:C:348:LEU:HD23	1.88	0.40
1:C:86:PHE:CZ	1:D:14:MET:HG2	2.57	0.40
1:B:83:ARG:HD3	1:B:294:GLY:O	2.22	0.40
1:B:333:GLN:HE21	1:B:333:GLN:HB3	1.74	0.40
1:C:285:LYS:HA	1:C:286:PRO:HD3	1.96	0.40
1:D:258:ILE:HB	1:D:275:LEU:HB2	2.03	0.40
1:B:139:LYS:HE3	1:B:171:VAL:CG1	2.50	0.40
1:A:338:LYS:HB3	1:A:414:LEU:HD21	2.03	0.40
1:A:94:GLU:OE1	1:B:17:GLU:HG2	2.22	0.40
1:B:64:HIS:HA	1:B:65:PRO:HD3	1.73	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	377/422 (89%)	347 (92%)	25 (7%)	5 (1%)	12	45
1	B	389/422 (92%)	357 (92%)	30 (8%)	2 (0%)	29	68
1	C	382/422 (90%)	354 (93%)	26 (7%)	2 (0%)	29	68
1	D	380/422 (90%)	344 (90%)	31 (8%)	5 (1%)	12	45
All	All	1528/1688 (90%)	1402 (92%)	112 (7%)	14 (1%)	17	55

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	SER
1	B	214	SER
1	C	214	SER
1	C	292	THR
1	D	145	ASN
1	D	214	SER
1	D	288	GLU
1	A	137	SER
1	D	286	PRO
1	A	10	SER
1	A	290	GLY
1	B	287	GLY
1	A	325	PRO
1	D	325	PRO

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	331/368 (90%)	324 (98%)	7 (2%)	53	82
1	B	342/368 (93%)	336 (98%)	6 (2%)	59	85
1	C	336/368 (91%)	328 (98%)	8 (2%)	49	79
1	D	334/368 (91%)	325 (97%)	9 (3%)	44	77
All	All	1343/1472 (91%)	1313 (98%)	30 (2%)	52	81

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	A	56	SER
1	A	137	SER
1	A	173	ASN
1	A	202	VAL
1	A	329	ASN
1	A	414	LEU
1	B	19	THR
1	B	56	SER
1	B	162	LYS
1	B	202	VAL
1	B	329	ASN
1	B	414	LEU
1	C	19	THR
1	C	56	SER
1	C	132	LYS
1	C	171	VAL
1	C	202	VAL
1	C	289	HIS
1	C	329	ASN
1	C	414	LEU
1	D	10	SER
1	D	19	THR
1	D	56	SER
1	D	146	ASN
1	D	202	VAL
1	D	283	VAL
1	D	289	HIS
1	D	329	ASN
1	D	414	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	62	HIS
1	A	110	ASN
1	A	193	ASN
1	A	227	ASN
1	A	333	GLN
1	A	371	ASN
1	B	23	HIS
1	B	62	HIS
1	B	227	ASN
1	B	333	GLN
1	B	371	ASN
1	C	23	HIS
1	C	62	HIS
1	C	144	ASN
1	C	146	ASN
1	C	227	ASN
1	C	333	GLN
1	C	371	ASN
1	D	23	HIS
1	D	62	HIS
1	D	146	ASN
1	D	333	GLN
1	D	371	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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	$\# Z > 2$
2	SO4	A	423	-	4,4,4	0.30	0	6,6,6	0.27	0
2	SO4	C	441	-	4,4,4	0.24	0	6,6,6	0.27	0
2	SO4	A	441	-	4,4,4	0.21	0	6,6,6	0.33	0
2	SO4	C	423	-	4,4,4	0.24	0	6,6,6	0.37	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	423	SO4	1	0
2	A	441	SO4	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, 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	381/422 (90%)	-0.23	5 (1%) 77 51	16, 32, 66, 110	0
1	B	393/422 (93%)	-0.38	3 (0%) 86 65	15, 32, 64, 125	0
1	C	386/422 (91%)	-0.36	1 (0%) 94 84	16, 32, 69, 113	0
1	D	384/422 (90%)	-0.29	5 (1%) 77 51	16, 32, 72, 121	0
All	All	1544/1688 (91%)	-0.32	14 (0%) 84 63	15, 32, 69, 125	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	147	PHE	6.6
1	D	146	ASN	4.0
1	D	147	PHE	2.9
1	A	339	VAL	2.9
1	D	171	VAL	2.9
1	B	288	GLU	2.7
1	A	413	ASN	2.6
1	B	146	ASN	2.6
1	A	340	VAL	2.6
1	A	334	LEU	2.5
1	C	183	GLU	2.4
1	D	172	PRO	2.4
1	A	289	HIS	2.0
1	D	334	LEU	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 [i](#)

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. 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(\AA^2)	Q<0.9
2	SO4	A	423	5/5	0.94	0.18	32,35,54,65	0
2	SO4	C	423	5/5	0.95	0.14	35,41,61,67	0
2	SO4	A	441	5/5	0.96	0.14	21,34,68,80	0
2	SO4	C	441	5/5	0.96	0.13	32,36,65,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.