



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2021 – 02:11 PM EST

PDB ID : 7LWZ
Title : Apo Structure of Vibrio cholerae dGTPase protein VC1979
Authors : Sikkema, A.P.; Horng, J.; Klemm, B.P.; Schaaper, R.M.; Hall, T.M.T.
Deposited on : 2021-03-02
Resolution : 2.32 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
Xtriage (Phenix)	:	1.13
EDS	:	2.17.1
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)	:	2.17.1

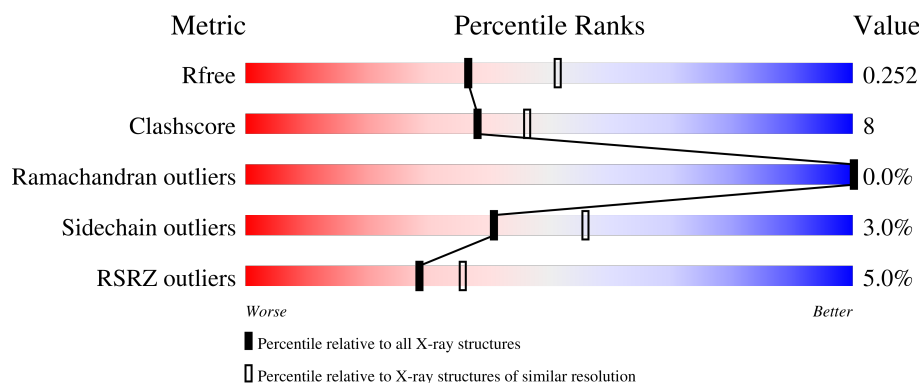
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	443	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>13%</div> <div>10%</div> </div> </div>
1	B	443	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>15%</div> <div>13%</div> </div> </div>
1	C	443	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>18%</div> <div>• 12%</div> </div> </div>
1	D	443	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>13%</div> <div>• 12%</div> </div> </div>
1	E	443	<div> <div>9%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>10%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	443	<div><div></div><div>5%</div><div>70%</div><div>13%</div><div>16%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18393 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 Deoxyguanosinetriphosphate triphosphohydrolase-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	385	Total	C	N	O	S	0	0	0
			3015	1911	537	551	16			
1	A	400	Total	C	N	O	S	0	0	0
			3103	1969	545	572	17			
1	D	392	Total	C	N	O	S	0	0	0
			3062	1941	536	568	17			
1	C	390	Total	C	N	O	S	0	0	0
			3047	1931	537	563	16			
1	F	373	Total	C	N	O	S	0	0	0
			2930	1858	520	536	16			
1	E	400	Total	C	N	O	S	0	0	0
			3098	1963	546	572	17			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	SER	-	expression tag	UNP Q9KQL9
B	0	ASN	-	expression tag	UNP Q9KQL9
B	1	ALA	-	expression tag	UNP Q9KQL9
A	-1	SER	-	expression tag	UNP Q9KQL9
A	0	ASN	-	expression tag	UNP Q9KQL9
A	1	ALA	-	expression tag	UNP Q9KQL9
D	-1	SER	-	expression tag	UNP Q9KQL9
D	0	ASN	-	expression tag	UNP Q9KQL9
D	1	ALA	-	expression tag	UNP Q9KQL9
C	-1	SER	-	expression tag	UNP Q9KQL9
C	0	ASN	-	expression tag	UNP Q9KQL9
C	1	ALA	-	expression tag	UNP Q9KQL9
F	-1	SER	-	expression tag	UNP Q9KQL9
F	0	ASN	-	expression tag	UNP Q9KQL9
F	1	ALA	-	expression tag	UNP Q9KQL9
E	-1	SER	-	expression tag	UNP Q9KQL9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	ASN	-	expression tag	UNP Q9KQL9
E	1	ALA	-	expression tag	UNP Q9KQL9

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Ni 1 1	0	0
2	A	1	Total Ni 1 1	0	0
2	D	1	Total Ni 1 1	0	0
2	C	1	Total Ni 1 1	0	0
2	F	1	Total Ni 1 1	0	0
2	E	1	Total Ni 1 1	0	0

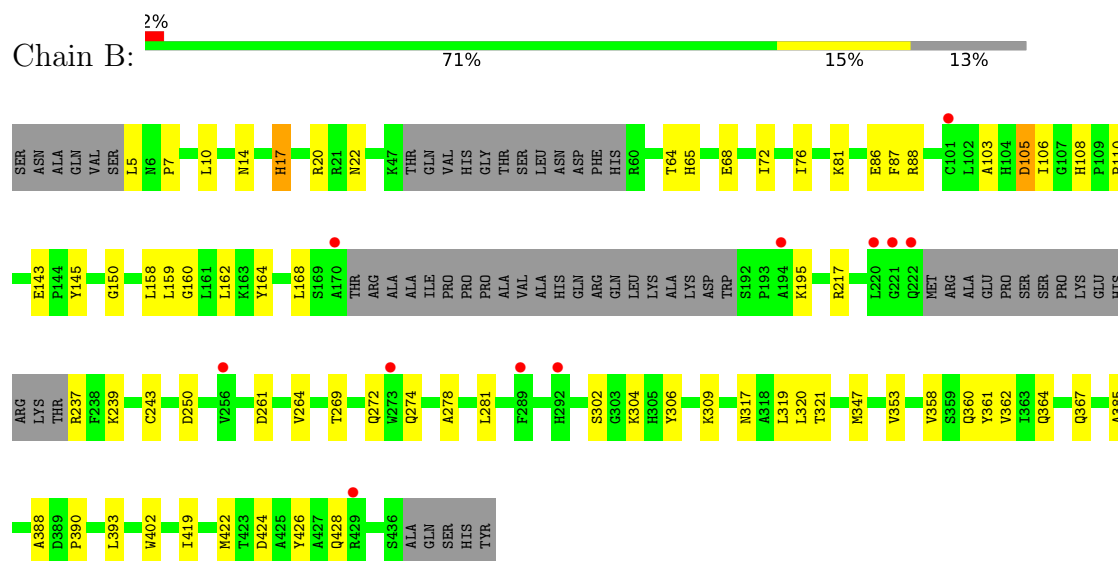
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	29	Total O 29 29	0	0
3	A	24	Total O 24 24	0	0
3	D	27	Total O 27 27	0	0
3	C	22	Total O 22 22	0	0
3	F	14	Total O 14 14	0	0
3	E	16	Total O 16 16	0	0

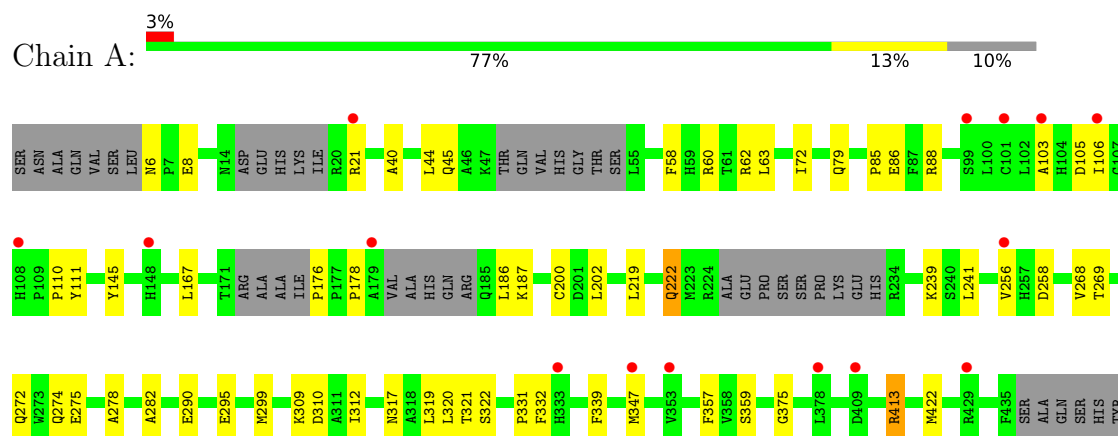
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

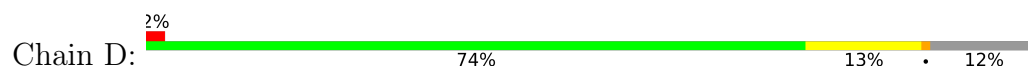
- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase-like protein 1

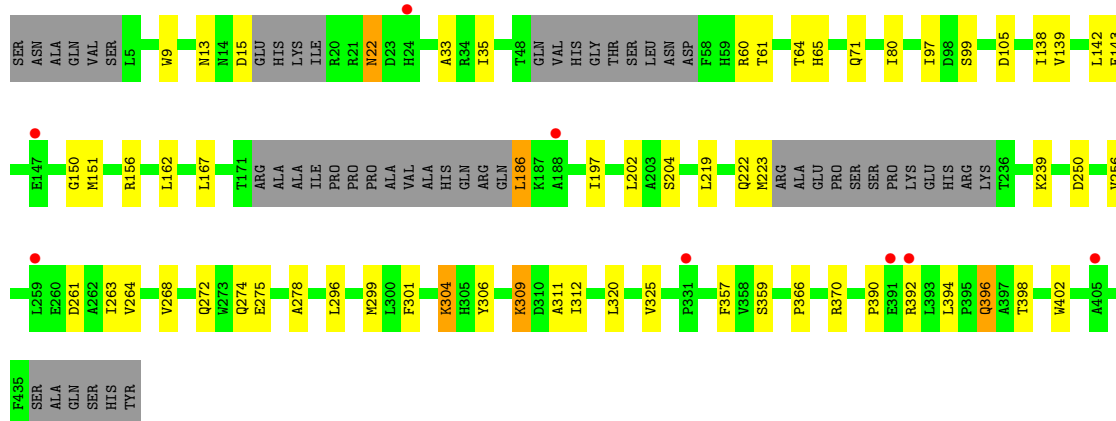


- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase-like protein 1

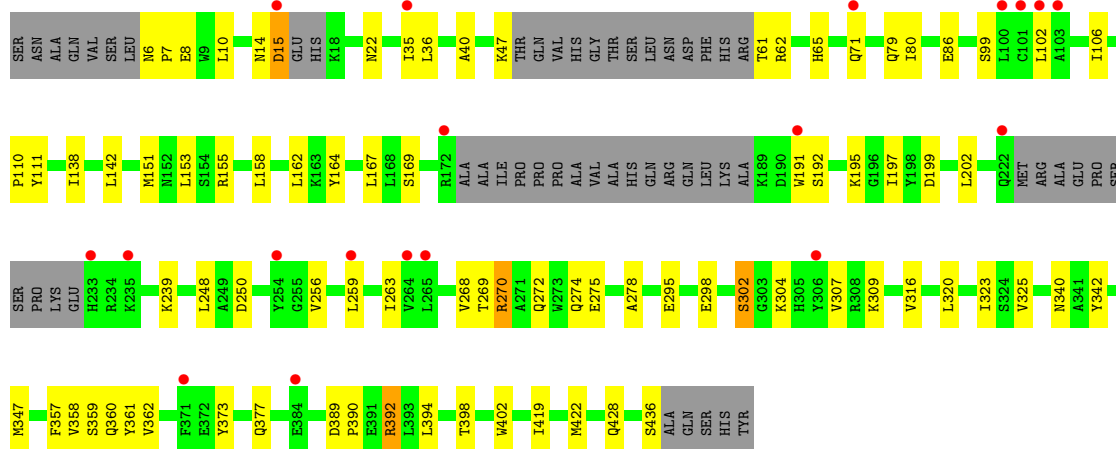


- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase-like protein 1

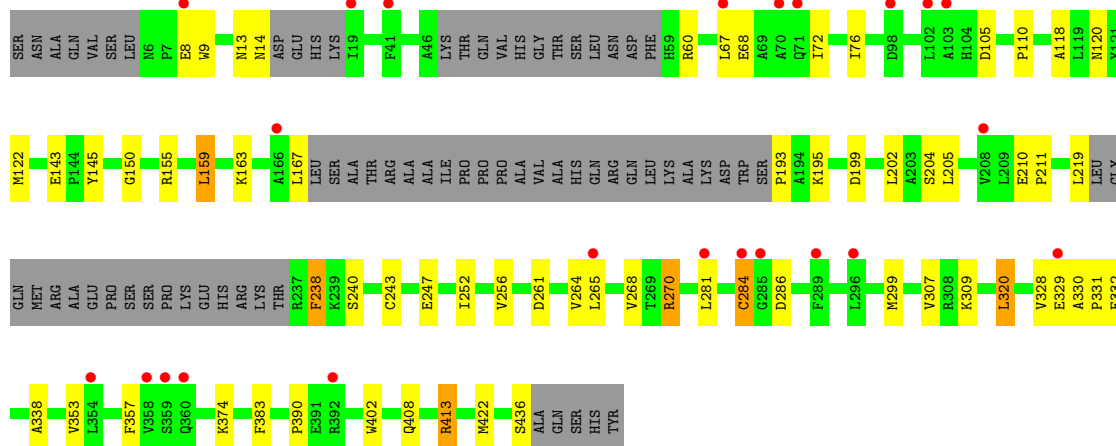




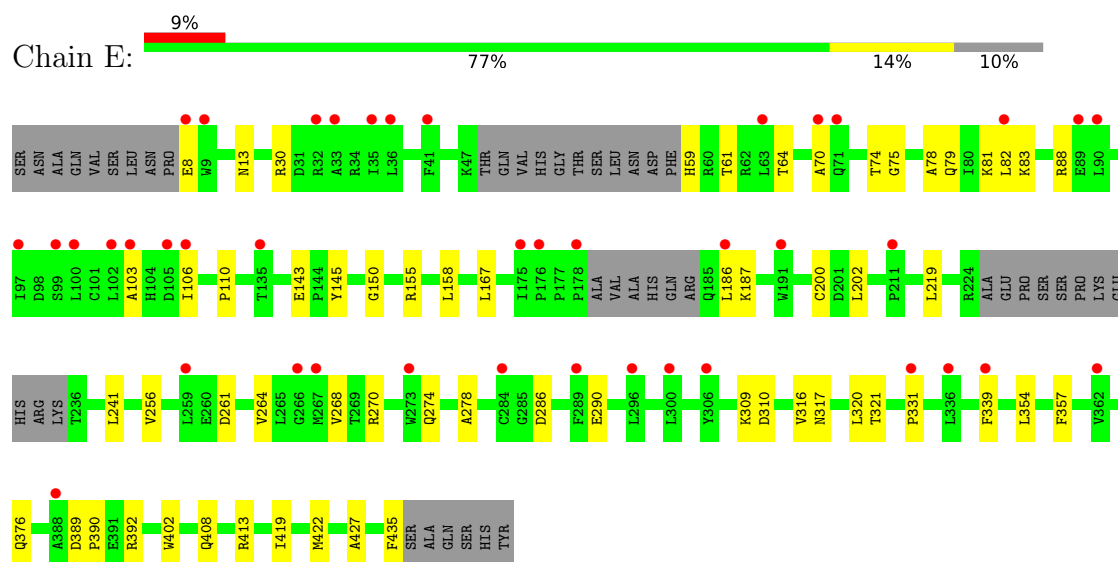
- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase-like protein 1



- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase-like protein 1



- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase-like protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.00Å 161.87Å 184.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.86 – 2.32 39.53 – 2.32	Depositor EDS
% Data completeness (in resolution range)	98.6 (37.86-2.32) 89.1 (39.53-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.52 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.218 , 0.252 0.218 , 0.252	Depositor DCC
R_{free} test set	6148 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å ²)	56.5	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18393	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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: NI

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	0.44	0/3170	0.63	0/4297
1	B	0.47	0/3081	0.65	0/4173
1	C	0.50	0/3114	0.64	0/4220
1	D	0.46	0/3129	0.63	0/4242
1	E	0.49	0/3165	0.66	0/4292
1	F	0.45	0/2995	0.62	0/4056
All	All	0.47	0/18654	0.64	0/25280

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	3103	0	2970	38	0
1	B	3015	0	2932	53	0
1	C	3047	0	2939	61	0
1	D	3062	0	2952	42	0
1	E	3098	0	2967	39	0
1	F	2930	0	2841	52	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	24	0	0	1	0
3	B	29	0	0	1	0
3	C	22	0	0	3	0
3	D	27	0	0	4	0
3	E	16	0	0	3	0
3	F	14	0	0	3	0
All	All	18393	0	17601	271	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (271) 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:269:THR:HG22	3:C:616:HOH:O	1.74	0.87
1:B:72:ILE:HG23	1:B:320:LEU:HD21	1.56	0.87
1:A:72:ILE:HG23	1:A:320:LEU:HD11	1.64	0.80
1:F:219:LEU:C	3:F:610:HOH:O	2.22	0.78
1:C:268:VAL:HG21	1:C:357:PHE:HZ	1.47	0.78
1:E:167:LEU:HD11	1:E:202:LEU:HD13	1.67	0.76
1:C:65:HIS:CE1	1:C:250:ASP:OD1	2.40	0.75
1:B:86:GLU:HG2	1:B:87:PHE:CD1	2.22	0.74
1:C:6:ASN:OD1	1:C:7:PRO:HD2	1.88	0.74
1:D:186:LEU:CD2	3:D:622:HOH:O	2.36	0.74
1:D:65:HIS:CE1	1:D:250:ASP:OD1	2.41	0.73
1:C:47:LYS:HB2	1:C:62:ARG:HD2	1.71	0.73
1:B:424:ASP:O	1:B:428:GLN:HG3	1.88	0.73
1:C:35:ILE:HA	1:C:151:MET:HE3	1.70	0.73
1:D:186:LEU:N	1:D:186:LEU:HD12	2.05	0.72
1:A:256:VAL:HG12	1:A:312:ILE:HG23	1.71	0.71
1:B:261:ASP:HA	1:B:264:VAL:HG12	1.73	0.71
1:F:238:PHE:HD1	1:F:332:PHE:CE2	2.08	0.70
1:D:22:ASN:ND2	1:D:22:ASN:H	1.89	0.70
1:C:302:SER:OG	1:C:307:VAL:HG21	1.90	0.70
1:F:268:VAL:HG21	1:F:357:PHE:HZ	1.56	0.70
1:F:264:VAL:HG13	1:F:265:LEU:HD12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:59:HIS:N	3:E:601:HOH:O	2.25	0.69
1:C:167:LEU:HD21	1:C:202:LEU:HD13	1.74	0.68
1:D:186:LEU:HD23	3:D:622:HOH:O	1.92	0.68
1:C:6:ASN:N	3:C:601:HOH:O	2.25	0.68
1:F:238:PHE:CD1	1:F:332:PHE:HE2	2.11	0.68
1:B:76:ILE:HG13	1:B:320:LEU:HD22	1.75	0.67
1:D:162:LEU:HD22	1:D:197:ILE:HD11	1.75	0.67
1:A:176:PRO:N	3:A:601:HOH:O	2.28	0.67
1:E:219:LEU:HD11	1:E:331:PRO:HD2	1.77	0.67
1:D:60:ARG:NE	1:D:261:ASP:OD2	2.28	0.66
1:C:47:LYS:CB	1:C:62:ARG:HD2	2.26	0.66
1:F:238:PHE:CD1	1:F:332:PHE:CE2	2.83	0.66
1:C:256:VAL:HG21	1:C:316:VAL:HG22	1.78	0.65
1:B:164:TYR:CD2	1:B:195:LYS:HB3	2.31	0.64
1:B:76:ILE:CG1	1:B:320:LEU:HD22	2.28	0.64
1:C:304:LYS:HB3	1:C:307:VAL:HG22	1.81	0.63
1:B:237:ARG:N	3:B:602:HOH:O	2.31	0.63
1:F:72:ILE:HG23	1:F:320:LEU:HD11	1.82	0.62
1:D:33:ALA:HB1	1:C:71:GLN:NE2	2.15	0.61
1:C:61:THR:N	3:C:602:HOH:O	2.33	0.61
1:C:138:ILE:HA	1:C:142:LEU:HB2	1.83	0.61
1:C:268:VAL:HG21	1:C:357:PHE:CZ	2.32	0.61
1:B:422:MET:HE2	1:B:426:TYR:HD1	1.65	0.61
1:C:304:LYS:CB	1:C:307:VAL:HG22	2.30	0.61
1:E:422:MET:HE3	1:E:427:ALA:HB2	1.81	0.60
1:B:367:GLN:OE1	1:B:367:GLN:N	2.19	0.60
1:E:309:LYS:NZ	1:E:310:ASP:OD1	2.33	0.60
1:C:274:GLN:HA	1:C:278:ALA:HB3	1.83	0.60
1:A:40:ALA:HB1	1:A:106:ILE:HG23	1.84	0.60
1:D:268:VAL:HG11	1:D:357:PHE:HZ	1.66	0.60
1:C:158:LEU:O	1:C:162:LEU:HD22	2.02	0.59
1:F:60:ARG:NH1	1:F:68:GLU:OE1	2.35	0.59
1:A:167:LEU:HD11	1:A:202:LEU:HD13	1.84	0.59
1:C:304:LYS:HB2	1:C:307:VAL:CG2	2.33	0.59
1:A:219:LEU:HD22	1:A:332:PHE:CZ	2.38	0.59
1:E:286:ASP:O	1:E:290:GLU:HG3	2.03	0.59
1:B:304:LYS:HD3	1:B:306:TYR:OH	2.03	0.58
1:E:79:GLN:HG3	1:E:83:LYS:NZ	2.19	0.58
1:B:103:ALA:O	1:B:106:ILE:HG12	2.04	0.58
1:C:295:GLU:HA	1:C:295:GLU:OE2	2.04	0.58
1:B:269:THR:HG22	1:B:272:GLN:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:394:LEU:HD13	1:D:398:THR:HG22	1.85	0.57
1:C:272:GLN:HA	1:C:275:GLU:HG2	1.85	0.57
1:F:270:ARG:HG3	1:F:270:ARG:HH11	1.69	0.57
1:B:158:LEU:O	1:B:162:LEU:HD22	2.04	0.57
1:B:309:LYS:HE3	1:A:145:TYR:CE1	2.40	0.57
1:E:186:LEU:HD13	1:E:187:LYS:N	2.20	0.57
1:A:58:PHE:CZ	1:A:60:ARG:HB2	2.40	0.56
1:F:238:PHE:HD2	1:F:238:PHE:N	2.03	0.56
1:B:145:TYR:O	1:A:309:LYS:HE3	2.06	0.56
1:F:329:GLU:HA	1:F:329:GLU:OE1	2.06	0.56
1:B:422:MET:HE2	1:B:426:TYR:CD1	2.41	0.56
1:C:80:ILE:HD13	1:C:325:VAL:HG23	1.88	0.56
1:B:360:GLN:HA	1:B:364:GLN:HB2	1.87	0.56
1:D:390:PRO:HG2	1:D:402:TRP:CZ2	2.42	0.55
1:E:268:VAL:HG21	1:E:357:PHE:HZ	1.71	0.55
1:B:86:GLU:HG2	1:B:87:PHE:HD1	1.67	0.55
1:E:389:ASP:CG	1:E:392:ARG:HB2	2.26	0.55
1:B:17:HIS:HE1	1:A:310:ASP:OD2	1.90	0.55
1:B:309:LYS:HE3	1:A:145:TYR:CZ	2.41	0.55
1:F:219:LEU:HD13	1:F:330:ALA:HB1	1.88	0.55
1:E:256:VAL:HG21	1:E:316:VAL:CG1	2.35	0.55
1:E:268:VAL:HG21	1:E:357:PHE:CZ	2.41	0.55
1:B:20:ARG:NH1	1:B:20:ARG:HG3	2.21	0.55
1:D:22:ASN:CB	1:C:79:GLN:HE22	2.20	0.55
1:C:40:ALA:HB1	1:C:106:ILE:HG23	1.87	0.55
1:A:186:LEU:HD23	1:A:187:LYS:N	2.21	0.55
1:A:269:THR:OG1	1:A:272:GLN:HG3	2.07	0.55
1:C:111:TYR:OH	1:C:428:GLN:HG3	2.05	0.55
1:D:304:LYS:HG2	1:D:306:TYR:CZ	2.41	0.55
1:C:358:VAL:O	1:C:362:VAL:HB	2.06	0.55
1:E:143:GLU:O	1:E:150:GLY:HA2	2.07	0.55
1:C:164:TYR:CZ	1:C:195:LYS:HD2	2.42	0.55
1:F:238:PHE:N	1:F:238:PHE:CD2	2.75	0.55
1:C:390:PRO:HG2	1:C:402:TRP:CZ2	2.42	0.54
1:F:261:ASP:O	1:F:265:LEU:HB2	2.07	0.54
1:D:366:PRO:O	1:D:370:ARG:HG3	2.07	0.54
1:F:76:ILE:HG13	1:F:320:LEU:HD11	1.90	0.54
1:B:159:LEU:HA	1:B:162:LEU:HD23	1.89	0.54
1:A:268:VAL:HG21	1:A:357:PHE:HZ	1.73	0.54
1:F:145:TYR:O	1:E:309:LYS:HE3	2.07	0.53
1:F:328:VAL:HG12	1:F:338:ALA:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:390:PRO:HG2	1:C:402:TRP:CE2	2.43	0.53
1:B:164:TYR:CE2	1:B:195:LYS:HB3	2.44	0.53
1:C:35:ILE:HD12	1:C:99:SER:HB3	1.90	0.53
1:D:296:LEU:HD23	1:D:299:MET:HE1	1.91	0.53
1:F:252:ILE:O	1:F:256:VAL:HG12	2.09	0.53
1:E:274:GLN:HA	1:E:278:ALA:HB3	1.91	0.53
1:D:299:MET:HE3	1:D:311:ALA:HA	1.92	0.52
1:F:122:MET:HE2	1:F:383:PHE:HB3	1.92	0.52
1:C:151:MET:HE1	1:C:153:LEU:HD21	1.92	0.51
1:B:22:ASN:HB2	1:A:79:GLN:HE22	1.75	0.51
1:F:9:TRP:CE3	1:F:155:ARG:HG2	2.45	0.51
1:F:163:LYS:HG2	1:F:243:CYS:SG	2.49	0.51
1:E:435:PHE:C	3:E:607:HOH:O	2.48	0.51
1:B:64:THR:O	1:B:68:GLU:HG3	2.11	0.51
1:A:44:LEU:HD11	1:A:106:ILE:HD13	1.91	0.51
1:C:259:LEU:O	1:C:263:ILE:HG13	2.11	0.51
1:F:167:LEU:HD21	1:F:205:LEU:HD23	1.93	0.51
1:C:22:ASN:OD1	1:C:22:ASN:N	2.25	0.51
1:B:269:THR:CG2	1:B:272:GLN:HG3	2.40	0.51
1:F:76:ILE:HG13	1:F:320:LEU:CD1	2.41	0.51
1:B:17:HIS:CE1	1:A:310:ASP:OD2	2.64	0.51
1:D:256:VAL:HG12	1:D:312:ILE:HG23	1.93	0.50
1:C:6:ASN:OD1	1:C:7:PRO:CD	2.56	0.50
1:A:110:PRO:HG3	1:A:422:MET:O	2.11	0.50
1:B:110:PRO:HG3	1:B:422:MET:O	2.11	0.50
1:D:33:ALA:HB1	1:C:71:GLN:HE22	1.75	0.50
1:F:14:ASN:C	3:F:611:HOH:O	2.49	0.50
1:E:70:ALA:O	1:E:74:THR:HG23	2.12	0.50
1:E:256:VAL:HG21	1:E:316:VAL:HG12	1.94	0.49
1:E:110:PRO:HG3	1:E:422:MET:O	2.11	0.49
1:A:219:LEU:HD11	1:A:331:PRO:HD2	1.94	0.49
1:D:274:GLN:HA	1:D:278:ALA:HB3	1.94	0.49
1:F:163:LYS:HD2	1:F:247:GLU:HG2	1.94	0.49
1:A:200:CYS:SG	1:A:413:ARG:HD2	2.52	0.49
1:C:373:TYR:O	1:C:377:GLN:HG2	2.13	0.49
1:A:6:ASN:ND2	1:A:8:GLU:HB2	2.28	0.49
1:F:238:PHE:HD1	1:F:332:PHE:CZ	2.31	0.49
1:D:61:THR:H	1:D:64:THR:HB	1.78	0.49
1:D:186:LEU:HD21	3:D:622:HOH:O	2.07	0.49
1:D:263:ILE:HD12	1:D:301:PHE:CZ	2.48	0.49
1:A:85:PRO:HA	1:A:88:ARG:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LEU:O	1:A:222:GLN:HB2	2.13	0.49
1:E:390:PRO:HG2	1:E:402:TRP:CZ2	2.48	0.49
1:B:274:GLN:HA	1:B:278:ALA:HB3	1.95	0.48
1:C:389:ASP:OD2	1:C:392:ARG:HD2	2.14	0.48
1:E:81:LYS:HG2	1:E:88:ARG:HG2	1.96	0.48
1:B:160:GLY:O	1:B:243:CYS:HB2	2.13	0.48
1:F:328:VAL:HG11	1:F:338:ALA:HA	1.96	0.48
1:A:103:ALA:HA	1:A:106:ILE:HG12	1.96	0.48
1:B:358:VAL:O	1:B:362:VAL:HB	2.13	0.48
1:F:72:ILE:HG23	1:F:320:LEU:CD1	2.43	0.47
1:B:419:ILE:HA	1:B:422:MET:SD	2.54	0.47
1:C:304:LYS:CB	1:C:307:VAL:CG2	2.92	0.47
1:A:274:GLN:HA	1:A:278:ALA:HB3	1.97	0.47
1:D:320:LEU:HD23	1:D:320:LEU:C	2.35	0.47
1:F:110:PRO:HG3	1:F:422:MET:O	2.14	0.47
1:F:167:LEU:HD23	1:F:167:LEU:N	2.30	0.47
1:F:390:PRO:HG2	1:F:402:TRP:CZ2	2.49	0.47
1:C:248:LEU:HD13	1:C:323:ILE:HG12	1.96	0.47
1:B:65:HIS:CE1	1:B:250:ASP:OD1	2.68	0.47
1:B:360:GLN:HG3	1:B:361:TYR:CD2	2.49	0.47
1:A:45:GLN:HG3	1:A:63:LEU:HD13	1.97	0.47
1:F:120:ASN:CG	1:F:193:PRO:HB3	2.34	0.47
1:B:20:ARG:HG3	1:B:20:ARG:HH11	1.79	0.47
1:B:319:LEU:HD23	1:B:347:MET:HG3	1.97	0.46
1:E:317:ASN:O	1:E:321:THR:HG23	2.16	0.46
1:C:302:SER:OG	1:C:307:VAL:CG2	2.61	0.46
1:C:304:LYS:HB2	1:C:307:VAL:HG21	1.97	0.46
1:E:8:GLU:HG3	1:E:155:ARG:NH1	2.30	0.46
1:D:296:LEU:HD23	1:D:299:MET:CE	2.45	0.46
1:D:299:MET:HB2	1:D:299:MET:HE2	1.83	0.46
1:F:219:LEU:HA	1:F:219:LEU:HD23	1.79	0.46
1:A:317:ASN:O	1:A:321:THR:HG23	2.16	0.46
1:D:219:LEU:HD23	1:D:222:GLN:NE2	2.31	0.46
1:B:304:LYS:HD3	1:B:306:TYR:CZ	2.52	0.45
1:C:8:GLU:O	1:C:155:ARG:NH1	2.49	0.45
1:C:191:TRP:O	1:C:192:SER:C	2.55	0.45
1:A:219:LEU:O	1:A:219:LEU:HD23	2.17	0.45
1:C:14:ASN:OD1	1:C:15:ASP:N	2.50	0.45
1:F:167:LEU:HD11	1:F:202:LEU:HG	1.99	0.45
1:B:7:PRO:HA	1:B:10:LEU:HD23	1.99	0.45
1:A:111:TYR:CG	1:A:375:GLY:HA3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LEU:HD23	1:A:186:LEU:C	2.37	0.45
1:F:390:PRO:HG2	1:F:402:TRP:CE2	2.51	0.45
1:C:256:VAL:HG21	1:C:316:VAL:CG2	2.45	0.45
1:F:8:GLU:OE2	1:F:155:ARG:NH2	2.49	0.45
1:D:309:LYS:HE3	1:D:309:LYS:HB3	1.80	0.45
1:E:158:LEU:HD23	1:E:158:LEU:HA	1.77	0.45
1:C:162:LEU:HD12	1:C:197:ILE:HD11	1.98	0.45
1:B:81:LYS:HE2	1:B:88:ARG:HG3	1.99	0.45
1:A:21:ARG:HD2	1:A:21:ARG:HA	1.62	0.44
1:F:219:LEU:HD11	1:F:331:PRO:HD2	1.98	0.44
1:C:86:GLU:CD	1:C:86:GLU:H	2.20	0.44
1:F:261:ASP:HA	1:F:264:VAL:HG12	1.99	0.44
1:D:22:ASN:ND2	1:D:22:ASN:N	2.61	0.44
1:D:22:ASN:HB2	1:C:79:GLN:OE1	2.16	0.44
1:E:419:ILE:HG23	1:E:422:MET:CE	2.47	0.44
1:C:302:SER:OG	1:C:304:LYS:HB2	2.17	0.44
1:C:169:SER:OG	1:C:199:ASP:OD2	2.36	0.44
1:E:103:ALA:O	1:E:106:ILE:HG12	2.18	0.44
1:F:299:MET:HB3	1:F:307:VAL:HG12	2.00	0.43
1:F:328:VAL:CG1	1:F:338:ALA:HA	2.48	0.43
1:F:413:ARG:NH1	3:F:602:HOH:O	2.48	0.43
1:E:200:CYS:SG	1:E:413:ARG:HD2	2.57	0.43
1:E:261:ASP:HA	1:E:264:VAL:HG12	1.99	0.43
1:D:80:ILE:HD13	1:D:325:VAL:HG23	2.01	0.43
1:A:295:GLU:O	1:A:299:MET:HG3	2.18	0.43
1:A:322:SER:CB	1:A:347:MET:HG2	2.48	0.43
1:F:243:CYS:O	1:F:247:GLU:HG3	2.19	0.43
1:E:408:GLN:NE2	1:E:408:GLN:HA	2.34	0.43
1:E:61:THR:H	1:E:64:THR:HB	1.83	0.43
1:B:5:LEU:HA	1:B:5:LEU:HD23	1.74	0.43
1:E:75:GLY:O	1:E:320:LEU:HD21	2.19	0.43
1:B:81:LYS:HE3	1:B:81:LYS:HB3	1.66	0.43
1:B:217:ARG:HE	1:B:217:ARG:HB3	1.71	0.43
1:F:159:LEU:HD23	1:F:240:SER:HB3	2.01	0.43
1:F:261:ASP:HB3	1:F:265:LEU:HD13	2.01	0.43
1:F:210:GLU:N	1:F:211:PRO:HD2	2.34	0.43
1:E:30:ARG:NH1	3:E:603:HOH:O	2.52	0.42
1:E:78:ALA:O	1:E:82:LEU:HG	2.19	0.42
1:E:354:LEU:HD12	1:E:354:LEU:HA	1.83	0.42
1:D:167:LEU:HD21	1:D:202:LEU:HG	2.01	0.42
1:C:36:LEU:HD21	1:C:102:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ASN:O	1:B:321:THR:HG23	2.19	0.42
1:B:390:PRO:HG2	1:B:402:TRP:CZ2	2.53	0.42
1:B:393:LEU:HD22	1:D:370:ARG:HG2	2.02	0.42
1:C:47:LYS:HB3	1:C:62:ARG:HD2	2.00	0.42
1:C:340:ASN:HB2	1:C:342:TYR:CZ	2.55	0.42
1:E:270:ARG:HA	1:E:270:ARG:HD3	1.84	0.42
1:C:106:ILE:HD13	1:C:106:ILE:HA	1.78	0.42
1:D:9:TRP:HB3	1:D:156:ARG:HB2	2.01	0.42
1:A:106:ILE:HD13	1:A:106:ILE:HA	1.75	0.42
1:F:281:LEU:HA	1:F:284:CYS:HB3	2.02	0.42
1:D:261:ASP:HA	1:D:264:VAL:HG22	2.00	0.42
1:D:272:GLN:HA	1:D:275:GLU:HG2	2.01	0.42
1:E:79:GLN:HG3	1:E:83:LYS:HZ3	1.84	0.42
1:A:282:ALA:O	1:A:290:GLU:HG2	2.20	0.41
1:D:143:GLU:O	1:D:150:GLY:HA2	2.20	0.41
1:C:270:ARG:HH22	1:C:298:GLU:HA	1.85	0.41
1:B:281:LEU:HG	1:B:353:VAL:HG11	2.03	0.41
1:B:145:TYR:CE1	1:A:309:LYS:HD3	2.56	0.41
1:F:219:LEU:CD1	1:F:330:ALA:HB1	2.50	0.41
1:B:390:PRO:HG2	1:B:402:TRP:CE2	2.56	0.41
1:C:110:PRO:HB2	1:C:111:TYR:CD2	2.56	0.41
1:C:419:ILE:HA	1:C:422:MET:HE3	2.02	0.41
1:F:67:LEU:HD23	1:F:67:LEU:HA	1.92	0.41
1:F:309:LYS:HE3	1:E:145:TYR:O	2.20	0.41
1:F:281:LEU:HG	1:F:353:VAL:HG11	2.03	0.41
1:C:7:PRO:O	1:C:10:LEU:N	2.53	0.41
1:F:143:GLU:O	1:F:150:GLY:HA2	2.21	0.41
1:B:105:ASP:OD1	1:B:108:HIS:CE1	2.74	0.41
1:A:241:LEU:HB2	1:A:339:PHE:O	2.21	0.41
1:D:139:VAL:HB	1:D:151:MET:HE2	2.02	0.41
1:C:394:LEU:HD13	1:C:398:THR:HG22	2.02	0.41
1:F:118:ALA:O	1:F:122:MET:HG2	2.21	0.41
1:B:143:GLU:O	1:B:150:GLY:HA2	2.21	0.41
1:D:35:ILE:HD12	1:D:99:SER:HB3	2.03	0.41
1:E:241:LEU:HB2	1:E:339:PHE:O	2.21	0.41
1:D:22:ASN:H	1:D:22:ASN:HD22	1.66	0.40
1:D:97:ILE:HD12	1:D:97:ILE:HA	1.90	0.40
1:D:138:ILE:HA	1:D:142:LEU:HB2	2.03	0.40
1:E:79:GLN:HG3	1:E:83:LYS:HZ1	1.82	0.40
1:A:319:LEU:HD23	1:A:347:MET:HG3	2.02	0.40
1:D:396:GLN:HG2	3:D:616:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:GLN:C	1:C:361:TYR:HD2	2.25	0.40
1:B:76:ILE:HG12	1:B:320:LEU:HD22	2.02	0.40
1:B:385:ALA:O	1:B:388:ALA:HB3	2.20	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	388/443 (88%)	379 (98%)	8 (2%)	1 (0%)	41	50
1	B	377/443 (85%)	369 (98%)	8 (2%)	0	100	100
1	C	380/443 (86%)	372 (98%)	8 (2%)	0	100	100
1	D	382/443 (86%)	375 (98%)	7 (2%)	0	100	100
1	E	392/443 (88%)	386 (98%)	6 (2%)	0	100	100
1	F	363/443 (82%)	353 (97%)	10 (3%)	0	100	100
All	All	2282/2658 (86%)	2234 (98%)	47 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	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	314/372 (84%)	305 (97%)	9 (3%)	42	57
1	B	310/372 (83%)	304 (98%)	6 (2%)	57	73
1	C	313/372 (84%)	303 (97%)	10 (3%)	39	53
1	D	315/372 (85%)	301 (96%)	14 (4%)	28	39
1	E	312/372 (84%)	310 (99%)	2 (1%)	86	93
1	F	302/372 (81%)	287 (95%)	15 (5%)	24	34
All	All	1866/2232 (84%)	1810 (97%)	56 (3%)	41	56

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	14	ASN
1	B	17	HIS
1	B	105	ASP
1	B	168	LEU
1	B	239	LYS
1	B	302	SER
1	A	62	ARG
1	A	86	GLU
1	A	105	ASP
1	A	222	GLN
1	A	239	LYS
1	A	258	ASP
1	A	275	GLU
1	A	359	SER
1	A	413	ARG
1	D	13	ASN
1	D	15	ASP
1	D	22	ASN
1	D	71	GLN
1	D	105	ASP
1	D	186	LEU
1	D	204	SER
1	D	223	MET
1	D	239	LYS
1	D	304	LYS
1	D	309	LYS
1	D	359	SER
1	D	392	ARG
1	D	396	GLN
1	C	15	ASP

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Mol	Chain	Res	Type
1	C	239	LYS
1	C	270	ARG
1	C	302	SER
1	C	309	LYS
1	C	320	LEU
1	C	347	MET
1	C	359	SER
1	C	392	ARG
1	C	436	SER
1	F	13	ASN
1	F	105	ASP
1	F	159	LEU
1	F	195	LYS
1	F	199	ASP
1	F	204	SER
1	F	238	PHE
1	F	270	ARG
1	F	284	CYS
1	F	286	ASP
1	F	320	LEU
1	F	374	LYS
1	F	408	GLN
1	F	413	ARG
1	F	436	SER
1	E	13	ASN
1	E	376	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	13	ASN
1	B	17	HIS
1	B	356	HIS
1	A	14	ASN
1	D	22	ASN
1	D	149	HIS
1	D	222	GLN
1	D	396	GLN
1	C	13	ASN
1	C	432	GLN
1	F	13	ASN
1	F	108	HIS

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Mol	Chain	Res	Type
1	F	349	ASN
1	E	408	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	400/443 (90%)	0.39	15 (3%) 40 47	58, 75, 105, 142	0
1	B	385/443 (86%)	0.31	11 (2%) 51 59	51, 73, 105, 129	0
1	C	390/443 (88%)	0.40	19 (4%) 29 37	57, 74, 111, 160	0
1	D	392/443 (88%)	0.28	8 (2%) 65 72	55, 71, 104, 122	0
1	E	400/443 (90%)	0.63	41 (10%) 6 9	56, 79, 113, 142	0
1	F	373/443 (84%)	0.63	23 (6%) 20 26	59, 82, 117, 150	0
All	All	2340/2658 (88%)	0.44	117 (5%) 28 36	51, 76, 111, 160	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	284	CYS	4.6
1	D	188	ALA	4.6
1	C	233	HIS	4.6
1	F	265	LEU	4.6
1	A	21	ARG	4.0
1	C	264	VAL	4.0
1	E	306	TYR	3.9
1	C	254	TYR	3.8
1	F	284	CYS	3.8
1	C	235	LYS	3.8
1	E	33	ALA	3.6
1	F	166	ALA	3.5
1	A	103	ALA	3.5
1	E	273	TRP	3.5
1	B	222	GLN	3.5
1	D	259	LEU	3.5
1	F	103	ALA	3.5
1	F	354	LEU	3.4
1	F	358	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	103	ALA	3.3
1	E	36	LEU	3.2
1	E	90	LEU	3.2
1	E	100	LEU	3.2
1	E	388	ALA	3.1
1	E	8	GLU	3.0
1	E	331	PRO	3.0
1	A	256	VAL	2.9
1	E	362	VAL	2.9
1	A	148	HIS	2.9
1	B	289	PHE	2.9
1	E	102	LEU	2.9
1	A	333	HIS	2.8
1	A	429	ARG	2.8
1	C	222	GLN	2.8
1	A	106	ILE	2.8
1	E	191	TRP	2.8
1	E	300	LEU	2.7
1	D	331	PRO	2.7
1	F	67	LEU	2.7
1	F	281	LEU	2.7
1	C	101	CYS	2.7
1	E	336	LEU	2.7
1	E	32	ARG	2.7
1	F	329	GLU	2.7
1	F	41	PHE	2.7
1	B	273	TRP	2.6
1	E	175	ILE	2.6
1	E	70	ALA	2.6
1	C	15	ASP	2.6
1	E	103	ALA	2.6
1	E	35	ILE	2.6
1	E	41	PHE	2.6
1	B	220	LEU	2.6
1	E	186	LEU	2.6
1	A	108	HIS	2.6
1	E	82	LEU	2.5
1	B	221	GLY	2.5
1	E	289	PHE	2.5
1	E	339	PHE	2.5
1	D	147	GLU	2.5
1	C	384	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	347	MET	2.4
1	F	102	LEU	2.4
1	E	259	LEU	2.4
1	E	296	LEU	2.4
1	E	176	PRO	2.4
1	D	391	GLU	2.4
1	F	296	LEU	2.4
1	E	266	GLY	2.4
1	F	208	VAL	2.4
1	D	405	ALA	2.4
1	E	99	SER	2.4
1	A	409	ASP	2.3
1	E	211	PRO	2.3
1	B	194	ALA	2.3
1	C	100	LEU	2.3
1	F	71	GLN	2.3
1	E	178	PRO	2.3
1	C	191	TRP	2.3
1	F	19	ILE	2.3
1	F	70	ALA	2.3
1	C	102	LEU	2.3
1	F	8	GLU	2.3
1	A	179	ALA	2.3
1	D	392	ARG	2.3
1	B	101	CYS	2.2
1	C	71	GLN	2.2
1	F	360	GLN	2.2
1	E	63	LEU	2.2
1	D	24	HIS	2.2
1	A	353	VAL	2.2
1	E	89	GLU	2.2
1	C	371	PHE	2.2
1	E	105	ASP	2.2
1	E	71	GLN	2.2
1	B	292	HIS	2.1
1	C	259	LEU	2.1
1	F	392	ARG	2.1
1	B	170	ALA	2.1
1	F	98	ASP	2.1
1	C	35	ILE	2.1
1	F	359	SER	2.1
1	A	101	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	256	VAL	2.1
1	B	429	ARG	2.1
1	F	289	PHE	2.1
1	E	9	TRP	2.1
1	C	306	TYR	2.1
1	E	267	MET	2.1
1	C	172	ARG	2.0
1	A	378	LEU	2.0
1	C	265	LEU	2.0
1	F	285	GLY	2.0
1	E	97	ILE	2.0
1	E	106	ILE	2.0
1	A	99	SER	2.0
1	E	135	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NI	E	501	1/1	0.57	0.12	87,87,87,87	0
2	NI	C	501	1/1	0.78	0.27	109,109,109,109	0
2	NI	F	501	1/1	0.79	0.12	92,92,92,92	0
2	NI	B	501	1/1	0.82	0.14	84,84,84,84	0
2	NI	A	501	1/1	0.94	0.18	81,81,81,81	0
2	NI	D	501	1/1	0.95	0.17	80,80,80,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.