



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:44 am GMT

PDB ID : 1Q15
Title : Carbapenam Synthetase
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Deposited on : 2003-07-18
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

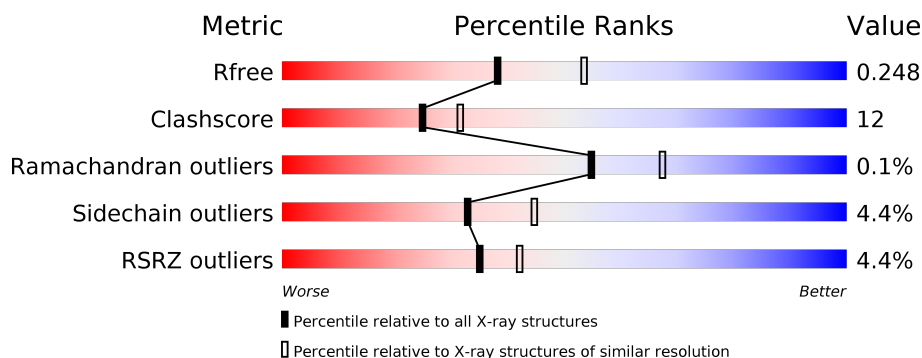
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	503	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>23%</div> <div>• •</div> </div> </div>
1	B	503	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>21%</div> <div>• •</div> </div> </div>
1	C	503	<div> <div>5%</div> <div> <div></div> <div>68%</div> <div>27%</div> <div>• •</div> </div> </div>
1	D	503	<div> <div>5%</div> <div> <div></div> <div>69%</div> <div>24%</div> <div>• 6%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15613 atoms, of which 0 are hydrogens and 0 are deuteriums.

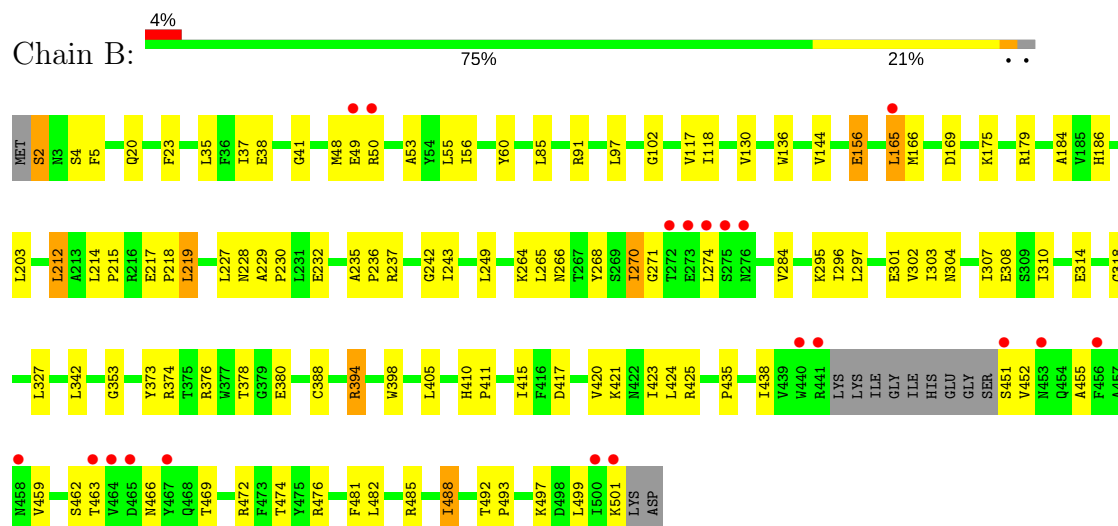
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CarA.

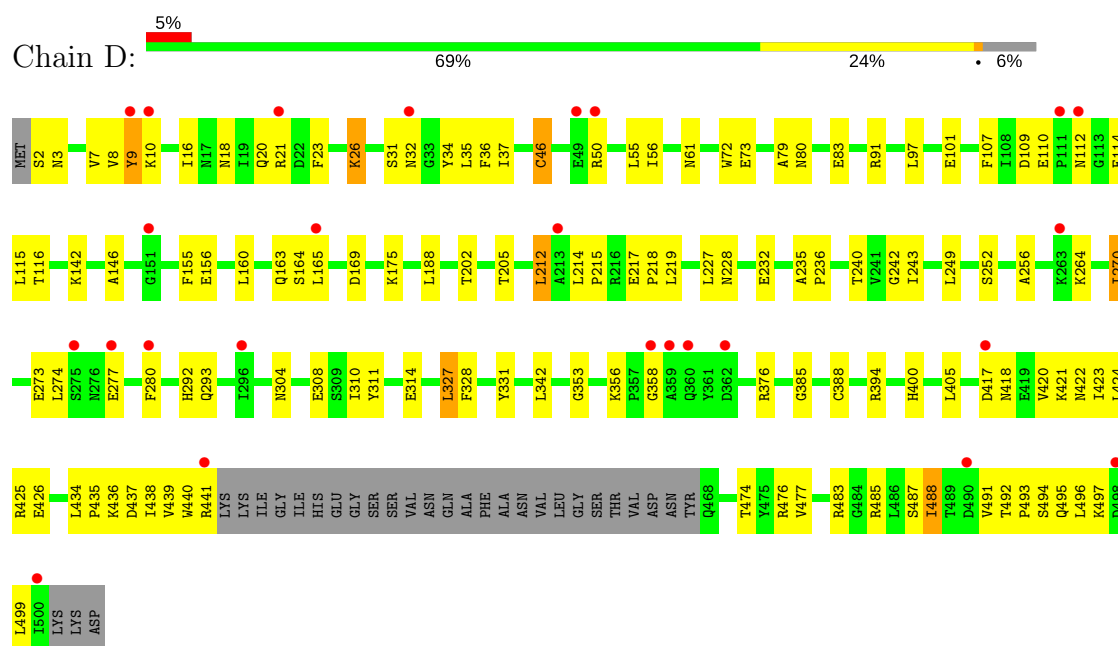
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	0	0
			3859	2456	652	739	12			
1	C	491	Total	C	N	O	S	0	0	0
			3859	2456	652	739	12			
1	B	491	Total	C	N	O	S	0	0	0
			3859	2456	652	739	12			
1	D	473	Total	C	N	O	S	0	0	0
			3724	2372	629	711	12			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	94	Total	O	0	0
			94	94		
2	B	96	Total	O	0	0
			96	96		
2	C	54	Total	O	0	0
			54	54		
2	D	68	Total	O	0	0
			68	68		



• Molecule 1: CarA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.10Å 180.39Å 96.63Å 90.00° 97.46° 90.00°	Depositor
Resolution (Å)	19.98 – 2.30 24.22 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.98-2.30) 100.0 (24.22-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	25.20 (at 2.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.203 , 0.249 0.204 , 0.248	Depositor DCC
R_{free} test set	9160 reflections (10.00%)	DCC
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15613	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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](#)

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	0.40	0/3943	0.58	0/5351
1	B	0.38	0/3943	0.57	0/5351
1	C	0.37	0/3943	0.55	0/5351
1	D	0.37	0/3805	0.55	0/5161
All	All	0.38	0/15634	0.56	0/21214

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	3859	0	3767	94	0
1	B	3859	0	3767	75	0
1	C	3859	0	3767	99	0
1	D	3724	0	3637	104	0
2	A	94	0	0	7	0
2	B	96	0	0	2	0
2	C	54	0	0	3	0
2	D	68	0	0	1	0
All	All	15613	0	14938	369	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (369) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:SER:N	1:D:388:CYS:HG	1.53	1.05
1:A:3:ASN:HB3	1:A:38:GLU:HB2	1.57	0.85
1:D:436:LYS:HD2	1:D:441:ARG:HD2	1.58	0.85
1:D:214:LEU:HD12	1:D:215:PRO:HD2	1.60	0.83
1:C:214:LEU:HD12	1:C:215:PRO:HD2	1.60	0.82
1:A:284:VAL:HG22	1:A:438:ILE:HD13	1.62	0.81
1:D:163:GLN:HG3	1:D:164:SER:H	1.46	0.80
1:D:50:ARG:HH22	1:D:112:ASN:HB3	1.48	0.79
1:C:303:ILE:HD11	1:C:459:VAL:HG21	1.65	0.79
1:C:477:VAL:HG12	1:C:499:LEU:HD13	1.65	0.78
1:A:187:VAL:CG1	1:A:199:GLU:HB2	2.14	0.78
1:A:130:VAL:HG13	1:A:136:TRP:HB2	1.62	0.78
1:A:2:SER:N	1:A:383:THR:HG1	1.82	0.77
1:A:165:LEU:HD23	1:A:165:LEU:H	1.49	0.77
1:B:117:VAL:HG13	1:B:186:HIS:HB2	1.67	0.77
1:A:277:GLU:HG3	1:A:280:PHE:HD2	1.51	0.76
1:C:187:VAL:HG13	1:C:199:GLU:HB2	1.68	0.74
1:A:50:ARG:HH12	1:A:111:PRO:HD2	1.53	0.74
1:A:130:VAL:HG11	1:A:144:VAL:HG21	1.69	0.74
1:D:310:ILE:HG21	1:D:477:VAL:HG23	1.70	0.74
1:C:150:GLU:OE1	1:C:485:ARG:HD2	1.88	0.74
1:A:310:ILE:HG21	1:A:477:VAL:HG23	1.70	0.73
1:A:150:GLU:OE1	1:A:485:ARG:HD2	1.89	0.72
1:D:488:ILE:O	1:D:488:ILE:HD13	1.89	0.72
1:D:270:ILE:H	1:D:270:ILE:HD13	1.55	0.72
1:C:270:ILE:H	1:C:270:ILE:HD13	1.55	0.71
1:B:130:VAL:HG22	1:B:136:TRP:HB2	1.73	0.70
1:D:420:VAL:HG12	1:D:421:LYS:HG3	1.73	0.70
1:C:187:VAL:CG1	1:C:199:GLU:HB2	2.22	0.70
1:B:217:GLU:HB2	1:B:218:PRO:HD3	1.74	0.69
1:D:18:ASN:O	1:D:21:ARG:HG2	1.93	0.68
1:C:310:ILE:HG21	1:C:477:VAL:HG23	1.75	0.68
1:C:249:LEU:HD11	1:C:424:LEU:HD22	1.75	0.67
1:D:235:ALA:HB3	1:D:236:PRO:HD3	1.75	0.67
1:B:421:LYS:HB2	1:B:425:ARG:NH1	2.09	0.67
1:C:337:GLN:HG3	2:C:510:HOH:O	1.95	0.67
1:B:284:VAL:HG23	1:B:438:ILE:HD13	1.76	0.67
1:C:235:ALA:HB3	1:C:236:PRO:HD3	1.77	0.67
1:D:492:THR:HB	1:D:495:GLN:HG3	1.75	0.67
1:A:97:LEU:HD22	1:A:118:ILE:HD13	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:SER:HA	1:A:387:SER:HB2	1.76	0.67
1:B:229:ALA:HB3	1:B:230:PRO:HD3	1.77	0.66
1:A:270:ILE:H	1:A:270:ILE:HD13	1.61	0.66
1:D:115:LEU:HD23	1:D:115:LEU:H	1.60	0.66
1:A:284:VAL:CG2	1:A:438:ILE:HD13	2.26	0.65
1:C:237:ARG:HH21	1:C:394:ARG:HH22	1.45	0.64
1:A:187:VAL:HG13	1:A:199:GLU:HB2	1.79	0.64
1:A:217:GLU:HB2	1:A:218:PRO:HD3	1.79	0.64
1:C:217:GLU:HB2	1:C:218:PRO:HD3	1.78	0.64
1:D:217:GLU:HB2	1:D:218:PRO:HD3	1.80	0.64
1:C:284:VAL:HG22	1:C:438:ILE:HD13	1.79	0.64
1:A:378:THR:OG1	1:A:380:GLU:HG3	1.98	0.64
1:D:215:PRO:HG2	1:D:218:PRO:HG2	1.80	0.64
1:C:310:ILE:HD13	1:C:477:VAL:CG2	2.27	0.64
1:D:163:GLN:HG3	1:D:164:SER:N	2.12	0.63
1:A:477:VAL:HG12	1:A:499:LEU:HD13	1.82	0.62
1:B:271:GLY:O	1:B:296:ILE:HD12	2.00	0.62
1:C:353:GLY:HA2	1:C:421:LYS:HD2	1.82	0.61
1:A:488:ILE:O	1:A:488:ILE:HD13	2.01	0.61
1:B:378:THR:OG1	1:B:380:GLU:HG3	2.00	0.61
1:B:373:TYR:O	1:B:376:ARG:HG3	2.00	0.61
1:B:37:ILE:HD11	1:B:41:GLY:HA3	1.83	0.61
2:A:580:HOH:O	1:D:91:ARG:HD2	2.01	0.61
1:C:284:VAL:CG2	1:C:438:ILE:HD13	2.31	0.61
1:B:130:VAL:CG2	1:B:136:TRP:HB2	2.31	0.60
1:C:421:LYS:HB2	1:C:425:ARG:NH1	2.16	0.60
1:C:456:PHE:O	1:C:459:VAL:HG22	2.01	0.60
1:A:212:LEU:HD22	1:A:214:LEU:HB2	1.84	0.60
1:C:37:ILE:HD11	1:C:41:GLY:HA3	1.82	0.60
1:B:169:ASP:OD2	1:B:376:ARG:NH1	2.34	0.60
1:D:165:LEU:H	1:D:165:LEU:HD23	1.65	0.60
1:C:215:PRO:HG2	1:C:218:PRO:HG2	1.82	0.60
1:C:354:ILE:HD11	1:C:368:LEU:HD23	1.83	0.59
1:C:32:ASN:OD1	1:C:113:GLY:HA2	2.03	0.59
1:A:270:ILE:HD13	1:A:270:ILE:N	2.16	0.59
1:C:327:LEU:HD22	1:C:331:TYR:CE1	2.38	0.59
1:A:277:GLU:HG3	1:A:280:PHE:CD2	2.37	0.58
1:A:318:GLY:HA2	1:A:474:THR:HG21	1.84	0.58
1:A:470:LYS:O	1:A:474:THR:HG23	2.03	0.58
1:C:486:LEU:HD23	1:C:487:SER:H	1.68	0.58
1:A:235:ALA:HB3	1:A:236:PRO:HD3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:ASN:HB3	1:B:268:TYR:CE1	2.39	0.58
1:B:130:VAL:HG21	1:B:144:VAL:HG21	1.86	0.57
1:D:212:LEU:HD22	1:D:214:LEU:HB2	1.86	0.57
1:B:284:VAL:CG2	1:B:438:ILE:HD13	2.34	0.57
1:A:117:VAL:HG13	1:A:186:HIS:HB2	1.86	0.57
1:B:501:LYS:HB3	2:B:547:HOH:O	2.03	0.57
1:A:18:ASN:O	1:A:21:ARG:HG2	2.05	0.57
1:B:270:ILE:HD13	1:B:270:ILE:H	1.70	0.57
1:D:242:GLY:O	1:D:243:ILE:HD13	2.04	0.57
1:D:492:THR:O	1:D:496:LEU:HD23	2.05	0.57
1:D:214:LEU:HD23	1:D:219:LEU:HD23	1.87	0.57
1:B:48:MET:SD	1:B:53:ALA:HB2	2.45	0.56
1:C:234:LEU:HD21	1:C:394:ARG:NH1	2.20	0.56
1:D:18:ASN:HB3	1:D:146:ALA:O	2.05	0.56
1:D:310:ILE:HD13	1:D:477:VAL:CG2	2.35	0.56
1:D:9:TYR:HE1	1:D:32:ASN:HD22	1.54	0.56
1:D:421:LYS:O	1:D:425:ARG:HG3	2.05	0.56
1:D:10:LYS:NZ	1:D:32:ASN:HD21	2.04	0.56
1:A:466:ASN:O	1:A:469:THR:HG22	2.07	0.55
1:B:242:GLY:O	1:B:243:ILE:HD13	2.06	0.55
1:B:4:SER:HB2	1:B:38:GLU:OE1	2.06	0.55
1:A:472:ARG:NH1	1:A:472:ARG:HB2	2.22	0.55
1:C:199:GLU:OE2	1:D:202:THR:HG22	2.07	0.55
1:C:378:THR:OG1	1:C:380:GLU:HG3	2.07	0.55
1:D:492:THR:HB	1:D:495:GLN:CG	2.37	0.55
1:B:212:LEU:HD22	1:B:214:LEU:HB2	1.89	0.55
1:C:454:GLN:HA	1:C:464:VAL:HG12	1.89	0.55
1:D:79:ALA:HB1	1:D:83:GLU:HB2	1.89	0.55
1:D:327:LEU:HD22	1:D:331:TYR:CZ	2.42	0.54
1:C:296:ILE:HD13	1:C:297:LEU:N	2.22	0.54
1:C:303:ILE:CD1	1:C:459:VAL:HG21	2.36	0.54
1:A:229:ALA:HB3	1:A:230:PRO:HD3	1.89	0.54
1:B:420:VAL:HG12	1:B:421:LYS:HG3	1.89	0.54
1:D:491:VAL:HG13	1:D:496:LEU:HD21	1.89	0.54
1:A:295:LYS:HD3	1:A:333:GLN:OE1	2.08	0.54
1:B:421:LYS:HE3	1:B:425:ARG:HH12	1.72	0.54
1:D:492:THR:HG22	1:D:494:SER:H	1.73	0.54
1:D:155:PHE:HE2	1:D:483:ARG:HG3	1.72	0.53
1:D:7:VAL:HG22	1:D:35:LEU:HD23	1.90	0.53
1:A:243:ILE:CD1	1:A:342:LEU:HB2	2.38	0.53
1:A:310:ILE:HG21	1:A:477:VAL:CG2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:ILE:C	1:C:296:ILE:HD13	2.29	0.53
1:A:422:ASN:O	1:A:426:GLU:HG3	2.09	0.52
1:B:2:SER:OG	1:B:388:CYS:SG	2.67	0.52
1:C:219:LEU:HD13	1:C:423:ILE:HG12	1.91	0.52
1:D:101:GLU:HG2	1:D:400:HIS:CD2	2.44	0.52
1:D:7:VAL:CG2	1:D:35:LEU:HD23	2.39	0.52
2:C:515:HOH:O	1:B:91:ARG:HD2	2.09	0.52
1:B:235:ALA:HB3	1:B:236:PRO:HD3	1.92	0.52
1:D:228:ASN:O	1:D:232:GLU:HG3	2.10	0.52
1:A:427:TYR:O	1:A:431:LEU:HD13	2.09	0.52
1:B:314:GLU:HG2	1:B:482:LEU:HD11	1.92	0.52
1:C:18:ASN:HB3	1:C:146:ALA:O	2.09	0.52
1:D:107:PHE:HA	1:D:116:THR:O	2.10	0.52
1:D:292:HIS:C	1:D:293:GLN:N	2.63	0.52
1:A:3:ASN:ND2	2:A:504:HOH:O	2.43	0.51
1:D:72:TRP:CE2	1:D:91:ARG:HG2	2.45	0.51
1:C:20:GLN:HA	1:C:23:PHE:O	2.11	0.51
1:C:43:TYR:HA	1:C:55:LEU:O	2.10	0.51
1:B:228:ASN:O	1:B:232:GLU:HG3	2.11	0.51
1:D:46:CYS:CB	1:D:83:GLU:HG2	2.41	0.51
1:A:169:ASP:OD2	1:A:376:ARG:NH1	2.44	0.51
1:B:307:ILE:HA	1:B:310:ILE:HD12	1.92	0.51
1:A:310:ILE:HD13	1:A:477:VAL:CG2	2.41	0.51
1:C:431:LEU:O	1:C:433:LEU:HD13	2.11	0.50
1:D:492:THR:HG23	1:D:493:PRO:HD2	1.93	0.50
1:A:228:ASN:O	1:A:232:GLU:HG3	2.11	0.50
1:C:165:LEU:N	1:C:165:LEU:HD12	2.26	0.50
1:C:6:CYS:HB2	1:C:138:THR:HB	1.93	0.50
1:D:35:LEU:HD22	1:D:36:PHE:N	2.26	0.50
1:D:252:SER:HB3	1:D:434:LEU:HD21	1.93	0.50
1:C:229:ALA:HB3	1:C:230:PRO:HD3	1.93	0.50
1:D:10:LYS:HZ3	1:D:32:ASN:HD21	1.60	0.50
1:A:157:GLU:HB2	1:A:160:LEU:HD23	1.93	0.50
1:C:129:VAL:HA	1:C:136:TRP:O	2.11	0.50
1:C:184:ALA:HA	1:C:203:LEU:HG	1.94	0.50
1:A:184:ALA:HA	1:A:203:LEU:HG	1.93	0.50
1:C:142:LYS:NZ	1:C:142:LYS:HB3	2.27	0.50
1:D:219:LEU:CD1	1:D:423:ILE:HG12	2.42	0.50
1:D:439:VAL:C	1:D:441:ARG:H	2.14	0.50
1:C:212:LEU:HD22	1:C:214:LEU:HB2	1.92	0.49
1:B:270:ILE:HD13	1:B:270:ILE:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:488:ILE:HD13	1:D:488:ILE:C	2.31	0.49
1:D:219:LEU:HD12	1:D:423:ILE:HG12	1.93	0.49
1:C:8:VAL:O	1:C:8:VAL:HG13	2.12	0.49
1:D:439:VAL:O	1:D:440:TRP:HB2	2.12	0.49
1:C:237:ARG:NH2	1:C:394:ARG:HH22	2.08	0.49
1:B:435:PRO:CG	1:B:438:ILE:HD12	2.43	0.49
1:B:476:ARG:HG2	1:B:499:LEU:HD22	1.95	0.49
1:B:184:ALA:HA	1:B:203:LEU:HG	1.93	0.49
1:A:373:TYR:HA	1:A:376:ARG:HD2	1.94	0.49
1:C:308:GLU:HG2	1:C:488:ILE:HD11	1.95	0.48
1:B:243:ILE:CD1	1:B:342:LEU:HB2	2.43	0.48
1:C:422:ASN:O	1:C:426:GLU:HG3	2.13	0.48
1:C:463:THR:HG23	1:C:466:ASN:HB2	1.95	0.48
1:C:79:ALA:HB1	1:C:83:GLU:HB2	1.95	0.48
1:D:420:VAL:CG1	1:D:421:LYS:HG3	2.41	0.48
1:A:46:CYS:HB3	1:A:83:GLU:HG3	1.95	0.48
1:C:107:PHE:HA	1:C:116:THR:O	2.14	0.48
1:C:326:GLY:O	1:C:330:VAL:HG23	2.14	0.48
1:A:272:THR:O	1:A:275:SER:HB3	2.13	0.48
1:A:3:ASN:HB2	1:A:41:GLY:N	2.29	0.48
1:C:496:LEU:O	1:C:500:ILE:HG13	2.13	0.48
1:D:256:ALA:HB2	1:D:434:LEU:HD13	1.94	0.48
1:A:86:ALA:O	1:A:90:THR:HG23	2.14	0.48
1:D:142:LYS:HE2	1:D:311:TYR:CE1	2.49	0.48
1:C:492:THR:OG1	1:C:495:GLN:HG3	2.13	0.48
1:A:91:ARG:NH2	1:D:205:THR:H	2.11	0.48
1:C:260:ARG:HG2	1:C:260:ARG:HH11	1.79	0.47
1:B:215:PRO:HG2	1:B:218:PRO:HG2	1.96	0.47
1:B:97:LEU:HD22	1:B:118:ILE:HD13	1.96	0.47
1:D:310:ILE:O	1:D:314:GLU:HA	2.14	0.47
1:A:112:ASN:OD1	1:A:114:GLU:HB3	2.14	0.47
1:B:55:LEU:HD23	1:B:85:LEU:HD12	1.97	0.47
1:D:435:PRO:HG2	1:D:438:ILE:HD13	1.97	0.47
1:D:80:ASN:OD1	1:D:83:GLU:HG3	2.15	0.47
1:A:2:SER:N	1:A:383:THR:OG1	2.46	0.47
1:B:179:ARG:NH2	2:B:574:HOH:O	2.34	0.47
1:C:156:GLU:HG2	1:C:175:LYS:HG2	1.95	0.47
1:B:264:LYS:C	1:B:265:LEU:HD22	2.35	0.46
1:B:49:GLU:CD	1:B:49:GLU:H	2.18	0.46
1:A:456:PHE:O	1:A:459:VAL:HG22	2.14	0.46
1:B:229:ALA:HA	1:B:232:GLU:OE1	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:ARG:HG3	1:B:485:ARG:HH11	1.80	0.46
1:A:256:ALA:HB2	1:A:434:LEU:HD13	1.98	0.46
1:B:455:ALA:O	1:B:459:VAL:HG23	2.14	0.46
1:A:55:LEU:HD13	1:A:55:LEU:C	2.36	0.46
1:C:187:VAL:HG22	1:C:189:THR:HG23	1.97	0.46
1:C:329:ASN:O	1:C:333:GLN:HG2	2.15	0.46
1:C:167:ARG:HD3	1:C:171:TYR:CD1	2.51	0.46
1:C:327:LEU:HD22	1:C:331:TYR:CZ	2.51	0.46
1:C:493:PRO:O	1:C:497:LYS:HG2	2.15	0.46
1:A:472:ARG:HH11	1:A:472:ARG:HB2	1.79	0.46
1:B:249:LEU:HD13	1:B:249:LEU:C	2.36	0.46
1:C:126:PRO:O	1:C:139:ASN:HA	2.15	0.46
1:D:270:ILE:CD1	1:D:270:ILE:H	2.23	0.46
1:D:292:HIS:O	1:D:293:GLN:N	2.49	0.46
1:B:318:GLY:HA2	1:B:474:THR:HG21	1.98	0.46
1:D:35:LEU:HD22	1:D:36:PHE:H	1.79	0.46
1:D:437:ASP:OD1	1:D:438:ILE:HD12	2.16	0.46
1:A:201:ARG:NE	2:A:512:HOH:O	2.29	0.45
1:B:60:TYR:CD2	1:B:102:GLY:HA2	2.51	0.45
1:A:185:VAL:HB	1:A:203:LEU:HD21	1.98	0.45
1:A:302:VAL:HG13	1:A:452:VAL:HG13	1.97	0.45
1:C:343:THR:O	1:C:396:PRO:HD2	2.17	0.45
1:C:421:LYS:HB2	1:C:425:ARG:HH11	1.80	0.45
1:C:302:VAL:HG13	1:C:452:VAL:HG13	1.98	0.45
1:A:421:LYS:O	1:A:425:ARG:HG3	2.17	0.45
1:C:2:SER:HB3	1:C:38:GLU:OE1	2.16	0.45
1:C:310:ILE:HD13	1:C:477:VAL:HG21	1.98	0.45
1:D:16:ILE:HG13	1:D:34:TYR:CD1	2.52	0.45
1:D:2:SER:N	1:D:388:CYS:SG	2.72	0.45
1:B:415:ILE:O	1:B:415:ILE:HG23	2.17	0.45
1:B:488:ILE:HD13	1:B:488:ILE:O	2.16	0.45
1:B:462:SER:CB	1:B:469:THR:HG21	2.46	0.45
1:D:9:TYR:OH	1:D:114:GLU:HA	2.17	0.45
1:A:435:PRO:CG	1:A:438:ILE:HD12	2.47	0.44
1:D:26:LYS:HB2	1:D:26:LYS:NZ	2.32	0.44
1:D:425:ARG:HE	1:D:440:TRP:HB2	1.82	0.44
1:C:306:ILE:HG23	1:C:321:ALA:HB1	2.00	0.44
1:D:61:ASN:ND2	1:D:101:GLU:HG3	2.33	0.44
1:D:277:GLU:HG3	1:D:280:PHE:CD2	2.53	0.44
1:D:243:ILE:HD12	1:D:342:LEU:HB2	1.98	0.44
1:A:3:ASN:HB3	1:A:38:GLU:CB	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:454:GLN:HA	1:C:464:VAL:CG1	2.47	0.44
1:C:454:GLN:NE2	1:C:458:ASN:OD1	2.50	0.44
1:D:35:LEU:HD11	1:D:37:ILE:HD11	2.00	0.44
1:D:485:ARG:HH21	1:D:499:LEU:HD21	1.83	0.44
1:A:2:SER:N	1:A:103:ASP:OD2	2.51	0.44
1:D:115:LEU:HD23	1:D:115:LEU:N	2.26	0.44
1:D:115:LEU:CD2	1:D:188:LEU:HB2	2.48	0.44
1:B:274:LEU:HB2	1:B:451:SER:HB2	1.99	0.44
1:C:242:GLY:O	1:C:341:MET:HA	2.18	0.44
1:D:8:VAL:O	1:D:8:VAL:HG13	2.18	0.44
1:D:97:LEU:HD12	1:D:97:LEU:N	2.33	0.43
1:A:115:LEU:HD23	2:A:563:HOH:O	2.16	0.43
1:B:156:GLU:HG2	1:B:175:LYS:CG	2.48	0.43
1:B:5:PHE:CD1	1:B:56:ILE:HG21	2.54	0.43
1:C:256:ALA:HB2	1:C:434:LEU:CD1	2.48	0.43
1:A:285:ALA:HB1	1:A:292:HIS:HB2	2.00	0.43
1:C:58:SER:HB2	2:C:551:HOH:O	2.19	0.43
1:D:304:ASN:O	1:D:308:GLU:HG3	2.19	0.43
1:D:169:ASP:OD2	1:D:376:ARG:NH1	2.51	0.43
1:D:46:CYS:HB3	1:D:83:GLU:HG2	2.00	0.43
1:A:110:GLU:HG3	1:A:114:GLU:O	2.18	0.43
1:A:216:ARG:HD2	2:A:557:HOH:O	2.19	0.43
1:B:410:HIS:HA	1:B:411:PRO:HD3	1.87	0.43
1:B:60:TYR:CE2	1:B:102:GLY:HA2	2.53	0.43
1:C:274:LEU:HD22	1:C:274:LEU:N	2.33	0.43
1:A:21:ARG:NH2	2:A:524:HOH:O	2.49	0.43
1:B:215:PRO:O	1:B:218:PRO:HD2	2.18	0.43
1:B:353:GLY:HA2	1:B:420:VAL:HG11	2.01	0.43
1:C:328:PHE:HA	1:C:331:TYR:CD2	2.53	0.43
1:C:253:LEU:CD2	1:C:424:LEU:HD21	2.48	0.43
1:A:165:LEU:N	1:A:165:LEU:HD23	2.27	0.43
1:B:295:LYS:HD2	1:B:297:LEU:HD23	2.01	0.43
1:B:295:LYS:HE3	1:B:301:GLU:OE1	2.18	0.43
1:B:462:SER:HB3	1:B:469:THR:HG21	2.00	0.43
1:C:318:GLY:HA2	1:C:474:THR:HG21	2.01	0.43
1:C:86:ALA:O	1:C:90:THR:HG23	2.17	0.43
1:C:243:ILE:HD13	1:C:255:THR:HA	2.01	0.43
1:D:20:GLN:HA	1:D:23:PHE:O	2.19	0.43
1:C:19:ILE:CG1	1:C:147:ALA:HB2	2.48	0.43
1:C:167:ARG:HG2	1:C:167:ARG:NH1	2.33	0.43
1:A:425:ARG:HB3	1:A:441:ARG:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:ASN:O	1:B:469:THR:HG22	2.19	0.43
1:A:242:GLY:O	1:A:243:ILE:HD13	2.19	0.42
1:B:421:LYS:HB2	1:B:425:ARG:HH11	1.83	0.42
1:C:110:GLU:HA	1:C:111:PRO:HD3	1.88	0.42
1:A:187:VAL:HG12	1:A:199:GLU:HB2	1.95	0.42
1:D:487:SER:O	1:D:491:VAL:HG23	2.19	0.42
1:D:492:THR:HG22	1:D:494:SER:N	2.35	0.42
1:A:256:ALA:HB2	1:A:434:LEU:CD1	2.49	0.42
1:C:466:ASN:OD1	1:C:469:THR:HG22	2.18	0.42
1:A:353:GLY:HA2	1:A:420:VAL:HG11	2.02	0.42
1:B:227:LEU:HA	1:B:227:LEU:HD23	1.91	0.42
1:C:8:VAL:HG22	1:C:11:GLY:HA3	2.01	0.42
1:D:31:SER:HB3	1:D:109:ASP:OD2	2.19	0.42
1:D:328:PHE:CE1	1:D:385:GLY:HA3	2.54	0.42
1:A:234:LEU:HD11	1:A:394:ARG:HG2	2.01	0.42
1:D:491:VAL:CG1	1:D:496:LEU:HD21	2.50	0.42
1:C:204:THR:HG22	1:B:91:ARG:NH1	2.34	0.42
1:C:266:ASN:OD1	1:C:291:HIS:HB3	2.20	0.42
1:A:364:PRO:O	1:A:368:LEU:HG	2.20	0.42
1:A:46:CYS:CB	1:A:83:GLU:HG3	2.49	0.42
1:B:304:ASN:O	1:B:308:GLU:HG3	2.19	0.42
1:C:120:GLU:CD	1:C:123:GLY:H	2.23	0.42
1:C:283:GLN:HB3	1:C:438:ILE:HD11	2.01	0.42
1:D:353:GLY:HA2	1:D:421:LYS:HD2	2.00	0.42
1:D:156:GLU:HG2	1:D:175:LYS:HG2	2.01	0.42
1:C:56:ILE:N	1:C:56:ILE:HD12	2.35	0.42
1:D:240:THR:OG1	1:D:264:LYS:HD2	2.20	0.42
1:D:311:TYR:CE2	1:D:488:ILE:HB	2.55	0.42
1:A:3:ASN:OD1	1:A:40:ASN:N	2.36	0.41
1:A:219:LEU:CD2	1:A:423:ILE:HG12	2.50	0.41
1:B:302:VAL:HG13	1:B:452:VAL:HG13	2.01	0.41
1:B:492:THR:HB	1:B:493:PRO:HD2	2.01	0.41
1:C:270:ILE:HA	1:C:295:LYS:O	2.19	0.41
1:D:256:ALA:HB2	1:D:434:LEU:CD1	2.49	0.41
1:D:3:ASN:HB2	2:D:534:HOH:O	2.20	0.41
1:A:424:LEU:HA	1:A:424:LEU:HD23	1.89	0.41
1:B:117:VAL:CG1	1:B:186:HIS:HB2	2.45	0.41
1:A:156:GLU:HG2	1:A:175:LYS:CG	2.50	0.41
1:B:303:ILE:CD1	1:B:459:VAL:HG21	2.50	0.41
1:C:486:LEU:HD23	1:C:487:SER:N	2.34	0.41
1:D:160:LEU:O	1:D:163:GLN:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:ALA:HA	1:C:34:TYR:CD2	2.55	0.41
1:A:101:GLU:HG2	1:A:400:HIS:CD2	2.56	0.41
1:B:20:GLN:HA	1:B:23:PHE:O	2.21	0.41
1:C:463:THR:CG2	1:C:466:ASN:HB2	2.49	0.41
1:A:272:THR:HG23	1:A:451:SER:HB2	2.03	0.41
1:A:472:ARG:O	1:A:476:ARG:HD3	2.20	0.41
1:B:56:ILE:HD12	1:B:56:ILE:N	2.35	0.41
1:D:243:ILE:CD1	1:D:342:LEU:HB2	2.50	0.41
1:D:422:ASN:O	1:D:426:GLU:HG3	2.21	0.41
1:A:55:LEU:HD23	1:A:85:LEU:HD12	2.03	0.41
1:C:72:TRP:CE2	1:C:91:ARG:HG2	2.56	0.41
1:D:249:LEU:C	1:D:249:LEU:HD13	2.41	0.41
1:B:165:LEU:CD1	1:B:166:MET:HG2	2.51	0.41
1:B:237:ARG:NH1	1:B:394:ARG:HH22	2.18	0.41
1:A:50:ARG:NH1	1:A:111:PRO:HD2	2.29	0.41
1:A:35:LEU:C	1:A:35:LEU:HD13	2.42	0.41
1:B:374:ARG:O	1:B:378:THR:HG23	2.21	0.41
1:A:302:VAL:CG1	1:A:452:VAL:HG13	2.50	0.41
1:A:454:GLN:HA	1:A:464:VAL:HG12	2.03	0.41
1:B:435:PRO:HG2	1:B:438:ILE:HD12	2.01	0.41
1:C:256:ALA:HB2	1:C:434:LEU:HD13	2.03	0.41
1:D:112:ASN:HD21	1:D:114:GLU:HG2	1.86	0.41
1:D:115:LEU:HD21	1:D:188:LEU:HB2	2.03	0.41
1:A:107:PHE:HA	1:A:116:THR:O	2.21	0.40
1:A:219:LEU:HD21	1:A:423:ILE:HG12	2.03	0.40
1:A:431:LEU:O	1:A:433:LEU:HD13	2.20	0.40
1:C:228:ASN:O	1:C:232:GLU:HG3	2.20	0.40
1:D:358:GLY:N	1:D:418:ASN:HA	2.35	0.40
1:A:241:VAL:HG13	1:A:265:LEU:HD13	2.03	0.40
1:D:227:LEU:HA	1:D:227:LEU:HD23	1.96	0.40
1:D:56:ILE:HD12	1:D:56:ILE:N	2.36	0.40
1:A:37:ILE:HD11	1:A:41:GLY:C	2.41	0.40
1:C:460:LEU:HD12	1:C:470:LYS:HG2	2.03	0.40
1:A:201:ARG:NH1	2:A:512:HOH:O	2.41	0.40
1:A:234:LEU:HD21	1:A:394:ARG:CZ	2.52	0.40
1:D:474:THR:O	1:D:477:VAL:HG22	2.21	0.40
1:B:219:LEU:HD13	1:B:423:ILE:HG12	2.03	0.40
1:C:270:ILE:N	1:C:270:ILE:HD13	2.28	0.40
1:C:440:TRP:O	1:C:441:ARG:HB3	2.22	0.40
1:D:112:ASN:OD1	1:D:114:GLU:HG2	2.21	0.40
1:D:353:GLY:CA	1:D:421:LYS:HD2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:LEU:HD13	1:D:55:LEU:C	2.42	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	487/503 (97%)	476 (98%)	11 (2%)	0	100	100
1	B	487/503 (97%)	474 (97%)	12 (2%)	1 (0%)	51	63
1	C	487/503 (97%)	472 (97%)	15 (3%)	0	100	100
1	D	467/503 (93%)	449 (96%)	17 (4%)	1 (0%)	51	63
All	All	1928/2012 (96%)	1871 (97%)	55 (3%)	2 (0%)	55	67

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	417	ASP
1	B	417	ASP

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	414/424 (98%)	399 (96%)	15 (4%)	40	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	414/424 (98%)	396 (96%)	18 (4%)	33	45
1	C	414/424 (98%)	391 (94%)	23 (6%)	25	33
1	D	399/424 (94%)	382 (96%)	17 (4%)	33	45
All	All	1641/1696 (97%)	1568 (96%)	73 (4%)	33	45

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	GLU
1	A	130	VAL
1	A	156	GLU
1	A	165	LEU
1	A	212	LEU
1	A	270	ILE
1	A	277	GLU
1	A	394	ARG
1	A	405	LEU
1	A	424	LEU
1	A	476	ARG
1	A	486	LEU
1	A	488	ILE
1	A	496	LEU
1	A	497	LYS
1	C	2	SER
1	C	32	ASN
1	C	73	GLU
1	C	117	VAL
1	C	142	LYS
1	C	156	GLU
1	C	190	HIS
1	C	212	LEU
1	C	219	LEU
1	C	239	ASP
1	C	245	LEU
1	C	260	ARG
1	C	270	ILE
1	C	279	GLU
1	C	296	ILE
1	C	362	ASP
1	C	394	ARG
1	C	405	LEU

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Mol	Chain	Res	Type
1	C	424	LEU
1	C	434	LEU
1	C	485	ARG
1	C	486	LEU
1	C	496	LEU
1	B	2	SER
1	B	35	LEU
1	B	50	ARG
1	B	156	GLU
1	B	165	LEU
1	B	212	LEU
1	B	219	LEU
1	B	270	ILE
1	B	327	LEU
1	B	394	ARG
1	B	398	TRP
1	B	405	LEU
1	B	424	LEU
1	B	463	THR
1	B	472	ARG
1	B	481	PHE
1	B	488	ILE
1	B	497	LYS
1	D	9	TYR
1	D	26	LYS
1	D	46	CYS
1	D	73	GLU
1	D	110	GLU
1	D	212	LEU
1	D	270	ILE
1	D	273	GLU
1	D	274	LEU
1	D	327	LEU
1	D	356	LYS
1	D	394	ARG
1	D	405	LEU
1	D	424	LEU
1	D	476	ARG
1	D	488	ILE
1	D	497	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	282	GLN
1	A	283	GLN
1	C	190	HIS
1	C	282	GLN
1	D	32	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	491/503 (97%)	-0.04	18 (3%)	42 49	10, 22, 49, 74	0
1	B	491/503 (97%)	-0.01	20 (4%)	38 45	11, 23, 63, 79	0
1	C	491/503 (97%)	0.06	23 (4%)	32 39	15, 28, 54, 76	0
1	D	473/503 (94%)	0.22	25 (5%)	27 34	14, 29, 54, 72	0
All	All	1946/2012 (96%)	0.06	86 (4%)	35 42	10, 26, 53, 79	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	LEU	8.0
1	D	275	SER	6.6
1	A	50	ARG	6.3
1	B	465	ASP	6.0
1	D	441	ARG	5.3
1	B	274	LEU	5.2
1	D	358	GLY	4.8
1	B	273	GLU	4.4
1	C	113	GLY	4.3
1	B	464	VAL	4.3
1	C	465	ASP	4.3
1	B	501	LYS	4.2
1	D	165	LEU	4.1
1	C	111	PRO	4.1
1	D	50	ARG	3.9
1	B	165	LEU	3.9
1	B	463	THR	3.9
1	D	111	PRO	3.9
1	A	296	ILE	3.8
1	A	277	GLU	3.7
1	A	440	TRP	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	32	ASN	3.6
1	D	500	ILE	3.5
1	A	273	GLU	3.4
1	B	467	TYR	3.3
1	B	440	TRP	3.2
1	A	465	ASP	3.2
1	D	360	GLN	3.2
1	C	50	ARG	3.1
1	A	464	VAL	3.1
1	B	50	ARG	3.1
1	A	272	THR	3.1
1	A	417	ASP	3.0
1	C	501	LYS	3.0
1	C	490	ASP	3.0
1	D	362	ASP	3.0
1	C	277	GLU	3.0
1	D	49	GLU	2.9
1	A	2	SER	2.9
1	C	497	LYS	2.9
1	C	464	VAL	2.9
1	C	49	GLU	2.9
1	D	21	ARG	2.9
1	A	49	GLU	2.8
1	B	451	SER	2.8
1	C	32	ASN	2.8
1	A	441	ARG	2.7
1	C	463	THR	2.6
1	D	9	TYR	2.6
1	A	111	PRO	2.6
1	D	296	ILE	2.6
1	C	165	LEU	2.6
1	C	493	PRO	2.6
1	B	456	PHE	2.6
1	B	49	GLU	2.6
1	D	359	ALA	2.5
1	B	272	THR	2.5
1	B	458	ASN	2.5
1	D	263	LYS	2.5
1	B	453	ASN	2.4
1	C	210	GLN	2.4
1	D	490	ASP	2.4
1	D	498	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	39	GLN	2.4
1	A	163	GLN	2.4
1	C	164	SER	2.3
1	D	112	ASN	2.3
1	C	498	ASP	2.3
1	A	501	LYS	2.3
1	A	276	ASN	2.3
1	B	441	ARG	2.2
1	C	217	GLU	2.2
1	C	467	TYR	2.2
1	D	277	GLU	2.2
1	B	275	SER	2.2
1	C	500	ILE	2.1
1	C	274	LEU	2.1
1	D	417	ASP	2.1
1	B	500	ILE	2.1
1	D	10	LYS	2.1
1	D	151	GLY	2.1
1	B	276	ASN	2.1
1	C	441	ARG	2.0
1	A	278	PHE	2.0
1	D	280	PHE	2.0
1	D	213	ALA	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.