



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:32 am BST

PDB ID : 6U7I
Title : Faecalibacterium prausnitzii Beta-glucuronidase
Authors : Ervin, S.M.; Redinbo, M.R.
Deposited on : 2019-09-03
Resolution : 2.70 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	:	2.11
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

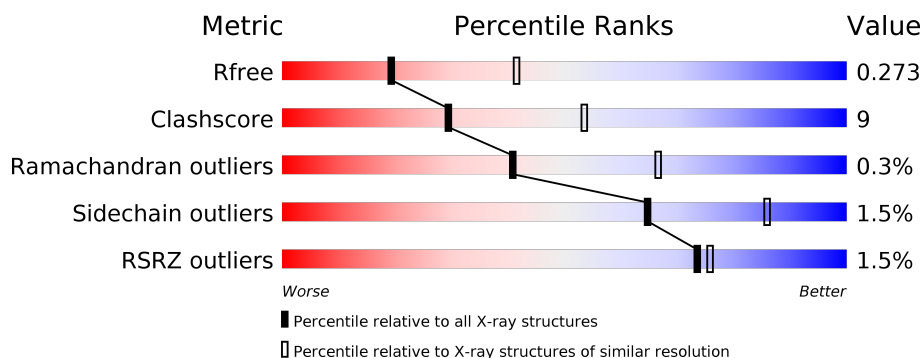
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	597	<div> <div>2%</div> <div>76%</div> <div>24%</div> </div>
1	B	597	<div> <div>2%</div> <div>76%</div> <div>23%</div> <div>.</div> </div>
1	C	597	<div> <div>%</div> <div>78%</div> <div>21%</div> </div>
1	D	597	<div> <div>2%</div> <div>75%</div> <div>24%</div> <div>.</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18998 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 Beta-glucuronidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	S	0	0	0
			4715	3006	811	878	20			
1	B	596	Total	C	N	O	S	0	0	0
			4724	3012	813	879	20			
1	C	597	Total	C	N	O	S	0	0	0
			4732	3017	814	880	21			
1	D	596	Total	C	N	O	S	0	0	0
			4724	3012	813	879	20			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	32	Total	O	0	0
			32	32		
2	B	25	Total	O	0	0
			25	25		
2	C	26	Total	O	0	0
			26	26		
2	D	20	Total	O	0	0
			20	20		

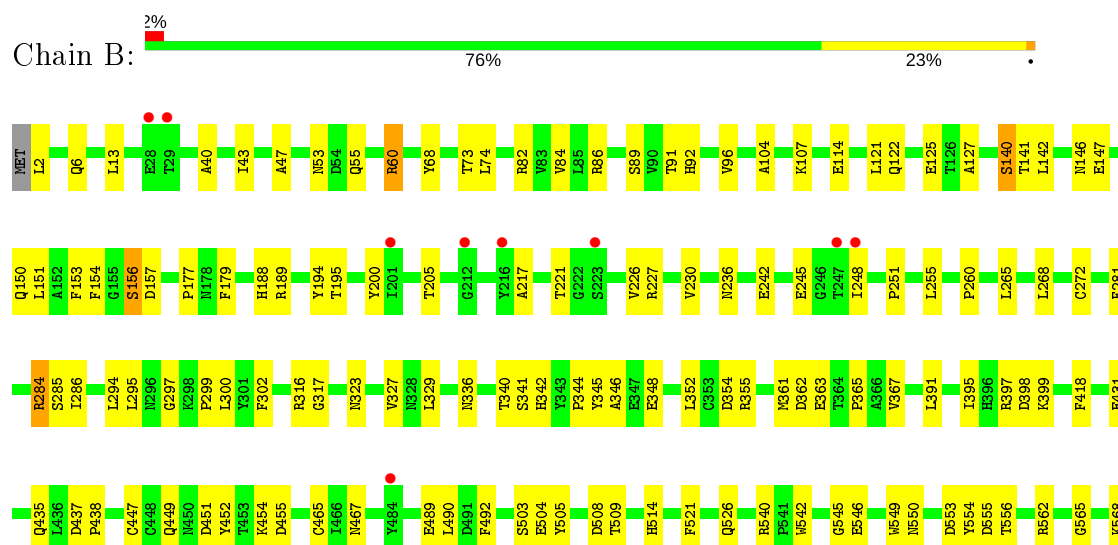
3 Residue-property plots

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: Beta-glucuronidase

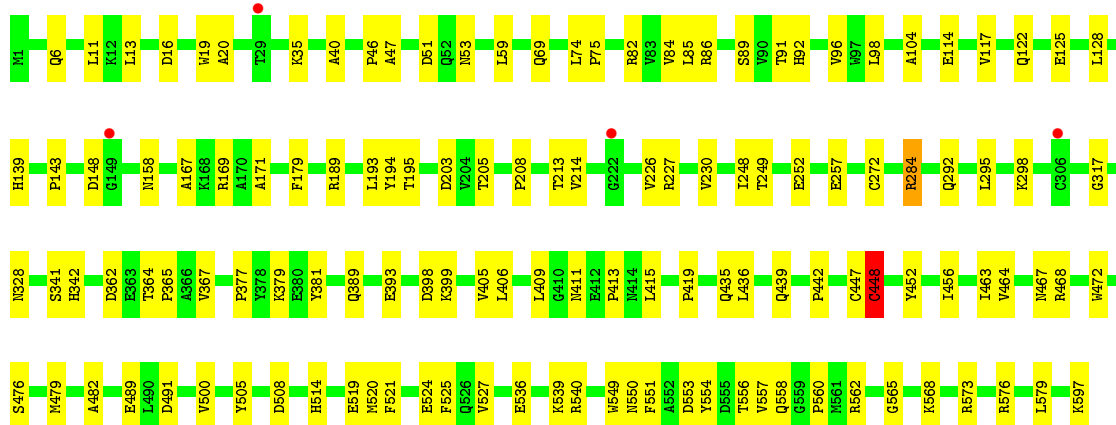
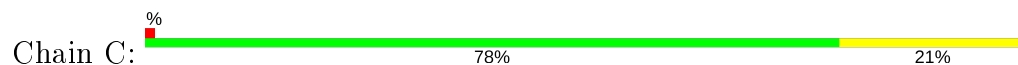


• Molecule 1: Beta-glucuronidase

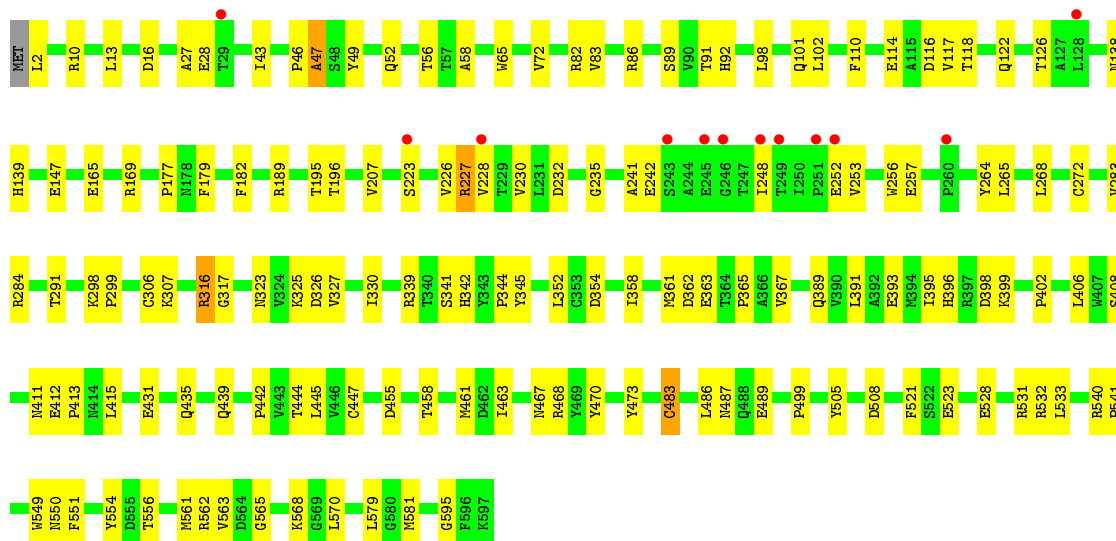
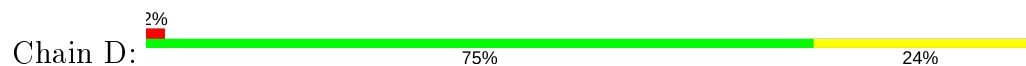




• Molecule 1: Beta-glucuronidase



• Molecule 1: Beta-glucuronidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	122.60Å 129.06Å 161.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.33 – 2.70 41.33 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.8 (41.33-2.70) 91.4 (41.33-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.180 , 0.273 0.180 , 0.273	Depositor DCC
R_{free} test set	1982 reflections (2.91%)	wwPDB-VP
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.908	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18998	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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	0.48	0/4857	0.65	0/6634
1	B	0.48	1/4866 (0.0%)	0.66	1/6645 (0.0%)
1	C	0.49	1/4874 (0.0%)	0.65	0/6655
1	D	0.49	1/4866 (0.0%)	0.65	0/6645
All	All	0.48	3/19463 (0.0%)	0.65	1/26579 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	483	CYS	CB-SG	-5.46	1.73	1.81
1	B	447	CYS	CB-SG	-5.14	1.73	1.81
1	C	447	CYS	CB-SG	-5.12	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	297	GLY	C-N-CA	-5.35	108.33	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	448	CYS	Peptide

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	4715	0	4464	87	1
1	B	4724	0	4477	97	0
1	C	4732	0	4489	76	2
1	D	4724	0	4477	103	0
2	A	32	0	0	3	0
2	B	25	0	0	1	0
2	C	26	0	0	0	0
2	D	20	0	0	3	0
All	All	18998	0	17907	348	2

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 9.

All (348) 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:83:VAL:H	1:D:118:THR:HG22	1.20	1.05
1:C:122:GLN:N	1:C:125:GLU:OE2	1.98	0.95
1:D:447:CYS:HB2	1:D:458:THR:HG21	1.51	0.91
1:D:2:LEU:O	1:D:86:ARG:NH1	2.07	0.88
1:C:114:GLU:OE2	1:C:194:TYR:OH	1.92	0.88
1:B:227:ARG:HH11	1:B:242:GLU:HG2	1.39	0.85
1:B:227:ARG:HH11	1:B:242:GLU:CG	1.91	0.83
1:D:89:SER:HB3	1:D:189:ARG:HD2	1.60	0.82
1:D:182:PHE:O	1:D:316:ARG:NH2	2.19	0.75
1:D:83:VAL:N	1:D:118:THR:HG22	1.99	0.75
1:B:295:LEU:HB2	1:B:300:LEU:HD22	1.68	0.73
1:B:344:PRO:HD3	1:B:365:PRO:HD3	1.71	0.73
1:B:227:ARG:HH11	1:B:242:GLU:CD	1.92	0.72
1:D:86:ARG:HD2	1:D:114:GLU:OE2	1.90	0.71
1:D:470:TYR:OH	1:D:489:GLU:OE1	2.06	0.71
1:D:83:VAL:H	1:D:118:THR:CG2	2.00	0.70
1:A:212:GLY:HA2	1:A:253:VAL:HG11	1.72	0.70
1:A:89:SER:HB3	1:A:189:ARG:HD2	1.73	0.70
1:D:523:GLU:HB3	1:D:579:LEU:HB3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ASP:OD2	1:A:211:ASP:N	2.18	0.69
1:C:74:LEU:HD12	1:C:75:PRO:HD2	1.73	0.69
1:B:227:ARG:NH1	1:B:242:GLU:CD	2.47	0.67
1:D:27:ALA:O	2:D:601:HOH:O	2.14	0.66
1:B:227:ARG:NH1	1:B:242:GLU:HG2	2.09	0.66
1:B:151:LEU:HD11	1:B:157:ASP:HB2	1.78	0.65
1:C:362:ASP:OD2	1:C:398:ASP:OD2	2.15	0.65
1:C:527:VAL:HG21	1:C:579:LEU:HD22	1.78	0.65
1:D:257:GLU:OE1	1:D:298:LYS:NZ	2.29	0.65
1:A:528:GLU:OE1	2:A:601:HOH:O	2.15	0.64
1:B:227:ARG:NH1	1:B:242:GLU:CG	2.59	0.64
1:C:96:VAL:HB	1:C:104:ALA:HB3	1.80	0.63
1:B:336:ASN:HD22	1:B:593:THR:HG23	1.62	0.63
1:B:189:ARG:HH21	1:B:345:TYR:C	2.02	0.63
1:A:13:LEU:HD11	1:B:6:GLN:HE22	1.64	0.63
1:A:226:VAL:HG22	1:A:272:CYS:HB2	1.82	0.61
1:B:245:GLU:OE2	2:B:601:HOH:O	2.15	0.61
1:C:284:ARG:NH2	1:C:439:GLN:OE1	2.33	0.61
1:D:528:GLU:OE2	1:D:531:ARG:NH1	2.33	0.61
1:B:141:THR:O	1:B:142:LEU:HD23	2.01	0.60
1:D:56:THR:HG23	1:D:58:ALA:H	1.66	0.60
1:B:336:ASN:ND2	1:B:593:THR:HG23	2.17	0.60
1:C:11:LEU:HD11	1:D:13:LEU:HD21	1.83	0.60
1:B:226:VAL:HG22	1:B:272:CYS:HB2	1.84	0.60
1:B:556:THR:HG22	1:B:565:GLY:HA2	1.83	0.60
1:C:203:ASP:OD1	1:C:399:LYS:NZ	2.30	0.59
1:A:295:LEU:HB2	1:A:300:LEU:HD22	1.85	0.59
1:B:540:ARG:HD3	1:B:542:TRP:CZ2	2.38	0.59
1:B:284:ARG:CZ	1:B:286:ILE:HD11	2.32	0.59
1:A:474:ASN:ND2	1:C:158:ASN:OD1	2.25	0.59
1:D:82:ARG:HA	1:D:118:THR:HG21	1.84	0.59
1:B:556:THR:CG2	1:B:565:GLY:HA2	2.33	0.59
1:A:151:LEU:HD11	1:A:157:ASP:HB2	1.83	0.59
1:B:391:LEU:O	1:B:395:ILE:HG13	2.03	0.59
1:D:367:VAL:HG23	1:D:411:ASN:HD22	1.68	0.58
1:A:16:ASP:OD2	1:A:190:PRO:HB3	2.03	0.58
1:A:470:TYR:OH	1:A:489:GLU:OE1	2.20	0.58
1:C:452:TYR:CE2	1:C:489:GLU:HG3	2.38	0.58
1:A:579:LEU:HD13	1:D:579:LEU:HD13	1.86	0.57
1:C:47:ALA:HA	1:C:317:GLY:HA3	1.86	0.57
1:D:406:LEU:HD12	1:D:442:PRO:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:ARG:NH1	1:B:114:GLU:OE2	2.37	0.57
1:D:89:SER:CB	1:D:189:ARG:HD2	2.33	0.57
1:A:532:ARG:NH1	2:A:601:HOH:O	2.11	0.57
1:B:114:GLU:OE2	1:B:194:TYR:OH	2.20	0.57
1:A:89:SER:CB	1:A:189:ARG:HD2	2.35	0.57
1:A:6:GLN:OE1	1:B:13:LEU:HD11	2.04	0.56
1:B:189:ARG:NH2	1:B:344:PRO:O	2.38	0.56
1:A:138:ASN:HB2	1:A:147:GLU:OE2	2.05	0.56
1:A:312:THR:O	1:A:314:HIS:N	2.35	0.56
1:A:189:ARG:HH21	1:A:345:TYR:C	2.08	0.56
1:B:556:THR:HG21	1:B:562:ARG:HB3	1.86	0.56
1:B:146:ASN:HB3	1:B:150:GLN:HB3	1.87	0.56
1:B:553:ASP:OD2	1:B:572:THR:HA	2.06	0.56
1:D:556:THR:HG22	1:D:565:GLY:HA2	1.87	0.56
1:A:326:ASP:O	1:A:330:ILE:HG13	2.05	0.56
1:C:464:VAL:HB	1:C:500:VAL:HG22	1.87	0.56
1:D:326:ASP:O	1:D:330:ILE:HG13	2.06	0.56
1:D:323:ASN:O	1:D:327:VAL:HG23	2.06	0.56
1:A:228:VAL:HG23	1:A:248:ILE:HD11	1.87	0.56
1:B:508:ASP:O	1:B:521:PHE:HA	2.06	0.55
1:D:467:ASN:O	1:D:468:ARG:HD3	2.06	0.55
1:B:82:ARG:O	1:B:195:THR:HA	2.07	0.55
1:B:122:GLN:O	1:B:125:GLU:HG3	2.07	0.55
1:A:180:ASP:OD2	1:A:562:ARG:NH2	2.38	0.55
1:D:228:VAL:HB	1:D:268:LEU:HD11	1.89	0.55
1:A:431:GLU:HA	1:A:431:GLU:OE2	2.06	0.54
1:D:556:THR:HG21	1:D:562:ARG:HB3	1.90	0.54
1:B:556:THR:HG21	1:B:562:ARG:CB	2.37	0.54
1:C:389:GLN:O	1:C:393:GLU:HG3	2.07	0.54
1:D:455:ASP:OD1	2:D:602:HOH:O	2.18	0.54
1:B:189:ARG:HE	1:B:346:ALA:HA	1.72	0.54
1:A:330:ILE:HG23	1:A:335:ALA:HB3	1.90	0.54
1:B:265:LEU:HD11	1:B:354:ASP:HB3	1.90	0.54
1:D:101:GLN:NE2	1:D:102:LEU:O	2.41	0.53
1:B:327:VAL:HG21	1:B:352:LEU:HD22	1.90	0.53
1:C:51:ASP:O	1:D:325:LYS:HE2	2.08	0.53
1:C:556:THR:HG21	1:C:562:ARG:HB3	1.90	0.53
1:C:556:THR:HG23	1:C:557:VAL:O	2.07	0.53
1:D:508:ASP:O	1:D:521:PHE:HA	2.09	0.53
1:A:407:TRP:HE1	1:A:441:ARG:HB2	1.73	0.53
1:A:86:ARG:HD2	1:A:114:GLU:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:TYR:OH	1:A:534:ASP:OD1	2.23	0.53
1:B:177:PRO:HB3	1:B:179:PHE:CZ	2.44	0.53
1:B:546:GLU:OE1	1:B:587:ARG:NH2	2.38	0.53
1:A:227:ARG:HB3	1:A:242:GLU:OE2	2.09	0.53
1:D:299:PRO:HG2	1:D:595:GLY:HA2	1.91	0.53
1:A:370:GLY:HA2	1:A:377:PRO:HG3	1.90	0.52
1:B:340:THR:O	1:B:340:THR:OG1	2.27	0.52
1:A:96:VAL:HG13	1:A:131:VAL:HG22	1.91	0.52
1:B:156:SER:OG	1:D:473:TYR:O	2.24	0.52
1:D:264:TYR:O	1:D:265:LEU:HD12	2.09	0.52
1:D:327:VAL:HG13	1:D:358:ILE:HD12	1.90	0.52
1:A:53:ASN:OD1	1:A:55:GLN:HG3	2.10	0.52
1:B:348:GLU:N	1:B:348:GLU:OE1	2.35	0.52
1:A:153:PHE:HB2	1:A:178:ASN:HA	1.91	0.52
1:D:138:ASN:HB2	1:D:147:GLU:OE1	2.09	0.52
1:D:86:ARG:CD	1:D:114:GLU:OE2	2.58	0.52
1:C:208:PRO:HB3	1:C:214:VAL:HG22	1.91	0.51
1:C:16:ASP:CG	1:C:46:PRO:HD3	2.30	0.51
1:D:444:THR:HA	1:D:461:MET:HB3	1.92	0.51
1:A:6:GLN:NE2	1:B:73:THR:O	2.44	0.51
1:B:236:ASN:HD22	1:B:236:ASN:N	2.08	0.51
1:A:142:LEU:HD22	1:A:366:ALA:HA	1.91	0.51
1:D:256:TRP:CD1	1:D:265:LEU:CD1	2.94	0.51
1:D:550:ASN:OD1	1:D:551:PHE:N	2.42	0.51
1:A:177:PRO:HB3	1:A:179:PHE:CZ	2.46	0.51
1:A:339:ARG:NH1	1:A:363:GLU:OE1	2.43	0.51
1:B:147:GLU:O	1:B:150:GLN:HB2	2.11	0.51
1:C:20:ALA:HB1	1:C:40:ALA:HB1	1.93	0.51
1:C:19:TRP:CD1	1:C:19:TRP:N	2.79	0.51
1:C:508:ASP:OD1	1:C:568:LYS:NZ	2.32	0.50
1:D:28:GLU:HG3	1:D:65:TRP:CZ2	2.46	0.50
1:A:339:ARG:NH1	1:A:446:VAL:HG21	2.26	0.50
1:B:205:THR:HG23	1:B:399:LYS:HD2	1.93	0.50
1:B:53:ASN:OD1	1:B:55:GLN:HG3	2.12	0.50
1:C:556:THR:HG22	1:C:565:GLY:HA2	1.93	0.50
1:B:230:VAL:HG21	1:B:248:ILE:HD11	1.93	0.50
1:D:291:THR:HA	1:D:499:PRO:HG3	1.93	0.50
1:A:85:LEU:HD23	1:A:103:ILE:HD11	1.94	0.50
1:A:143:PRO:HB2	1:A:179:PHE:CD2	2.47	0.49
1:A:250:ILE:HB	1:A:253:VAL:HG12	1.95	0.49
1:D:232:ASP:OD1	1:D:235:GLY:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:415:LEU:HD13	1:D:458:THR:HG23	1.94	0.49
1:C:226:VAL:HG22	1:C:272:CYS:HB2	1.94	0.49
1:D:327:VAL:HG21	1:D:352:LEU:HG	1.95	0.49
1:B:514:HIS:O	1:C:576:ARG:HD3	2.13	0.49
1:A:32:ASP:O	1:A:34:ALA:N	2.45	0.48
1:D:363:GLU:OE2	1:D:411:ASN:HB2	2.14	0.48
1:B:340:THR:O	1:B:363:GLU:HB3	2.13	0.48
1:C:328:ASN:ND2	1:D:52:GLN:O	2.46	0.48
1:D:2:LEU:O	1:D:86:ARG:CZ	2.61	0.48
1:D:344:PRO:HD3	1:D:365:PRO:HD3	1.95	0.48
1:C:19:TRP:HB3	1:C:69:GLN:O	2.14	0.48
1:A:200:TYR:CE2	1:A:202:GLU:HG3	2.49	0.48
1:C:364:THR:OG1	1:C:409:LEU:O	2.18	0.48
1:D:406:LEU:HD13	1:D:463:ILE:HD12	1.94	0.48
1:C:367:VAL:HG23	1:C:411:ASN:HD22	1.77	0.48
1:C:448:CYS:O	1:C:468:ARG:NH1	2.46	0.48
1:A:561:MET:CE	1:C:560:PRO:HB2	2.44	0.48
1:D:10:ARG:NH1	1:D:196:THR:HG22	2.28	0.48
1:D:165:GLU:O	1:D:169:ARG:HG3	2.12	0.48
1:B:341:SER:HB2	1:B:342:HIS:ND1	2.29	0.48
1:C:413:PRO:HG2	1:C:415:LEU:HD21	1.96	0.48
1:B:121:LEU:HD12	1:B:127:ALA:CB	2.44	0.48
1:D:43:ILE:HD11	1:D:49:TYR:HB2	1.95	0.48
1:A:461:MET:O	1:A:498:LYS:NZ	2.29	0.47
1:B:121:LEU:HD12	1:B:127:ALA:HB3	1.95	0.47
1:B:397:ARG:HH21	1:B:398:ASP:CG	2.17	0.47
1:B:302:PHE:HB2	1:B:545:GLY:HA3	1.95	0.47
1:B:579:LEU:HD13	1:C:579:LEU:HG	1.96	0.47
1:A:82:ARG:O	1:A:195:THR:HA	2.14	0.47
1:D:265:LEU:HD21	1:D:354:ASP:HB3	1.95	0.47
1:A:467:ASN:O	1:A:468:ARG:NH1	2.38	0.47
1:B:89:SER:HB3	1:B:189:ARG:HD2	1.96	0.47
1:C:419:PRO:HB3	1:C:456:ILE:HG12	1.97	0.47
1:D:116:ASP:OD2	1:D:118:THR:HG23	2.15	0.47
1:D:226:VAL:HG22	1:D:272:CYS:HB2	1.95	0.47
1:D:307:LYS:HE3	1:D:307:LYS:HB3	1.69	0.47
1:D:83:VAL:O	1:D:117:VAL:HG12	2.15	0.47
1:D:354:ASP:CG	1:D:402:PRO:HD2	2.35	0.47
1:D:549:TRP:HA	1:D:550:ASN:HA	1.67	0.47
1:C:143:PRO:HB2	1:C:179:PHE:CD2	2.50	0.47
1:B:43:ILE:HG21	1:B:68:TYR:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:PHE:CD1	1:D:563:VAL:HG13	2.50	0.46
1:A:36:PRO:HA	1:A:69:GLN:HE22	1.80	0.46
1:D:2:LEU:O	1:D:86:ARG:NH2	2.48	0.46
1:A:490:LEU:HD13	1:A:540:ARG:HG3	1.97	0.46
1:D:361:MET:HG3	1:D:406:LEU:HD23	1.98	0.46
1:D:431:GLU:O	1:D:435:GLN:HG3	2.15	0.46
1:A:203:ASP:HB3	1:A:219:LYS:HG3	1.96	0.46
1:C:379:LYS:HD2	1:C:379:LYS:HA	1.74	0.46
1:D:540:ARG:HA	1:D:541:PRO:HD3	1.86	0.46
1:A:304:GLY:HA3	1:A:547:PHE:CD2	2.50	0.46
1:D:207:VAL:HG22	1:D:439:GLN:HG2	1.98	0.46
1:D:47:ALA:HA	1:D:317:GLY:HA3	1.97	0.46
1:A:407:TRP:NE1	1:A:441:ARG:HB2	2.31	0.46
1:C:230:VAL:HG23	1:C:248:ILE:HD13	1.96	0.46
1:A:536:GLU:HA	1:A:539:LYS:HE3	1.96	0.46
1:C:82:ARG:O	1:C:195:THR:HA	2.16	0.46
1:C:84:VAL:O	1:C:193:LEU:HD22	2.16	0.46
1:D:177:PRO:HB3	1:D:179:PHE:CZ	2.50	0.46
1:B:153:PHE:O	1:B:154:PHE:HB2	2.16	0.46
1:D:28:GLU:H	1:D:28:GLU:CD	2.17	0.46
1:D:256:TRP:HD1	1:D:265:LEU:CD1	2.28	0.46
1:D:306:CYS:SG	1:D:339:ARG:HD3	2.56	0.46
1:C:98:LEU:HD22	1:C:117:VAL:HG21	1.97	0.45
1:D:549:TRP:HZ2	1:D:554:TYR:HH	1.62	0.45
1:A:508:ASP:N	1:A:568:LYS:HG2	2.31	0.45
1:C:213:THR:HG23	1:C:249:THR:HG22	1.98	0.45
1:D:341:SER:HA	1:D:342:HIS:HA	1.74	0.45
1:A:212:GLY:HA2	1:A:253:VAL:CG1	2.45	0.45
1:A:569:GLY:O	1:A:578:LYS:NZ	2.40	0.45
1:C:85:LEU:HD12	1:C:86:ARG:N	2.32	0.45
1:D:227:ARG:HG2	1:D:227:ARG:HH11	1.81	0.45
1:B:455:ASP:OD2	1:B:455:ASP:C	2.56	0.45
1:C:342:HIS:O	1:C:365:PRO:HA	2.17	0.45
1:C:467:ASN:O	1:C:468:ARG:HD3	2.16	0.45
1:A:467:ASN:CG	1:A:504:GLU:HB2	2.37	0.45
1:B:489:GLU:O	1:B:492:PHE:HB3	2.17	0.45
1:C:167:ALA:O	1:C:171:ALA:N	2.49	0.45
1:A:549:TRP:HA	1:A:550:ASN:HA	1.71	0.45
1:A:50:ASN:HB3	1:A:60:ARG:HA	1.99	0.45
1:C:536:GLU:HA	1:C:539:LYS:HD2	1.99	0.44
1:D:483:CYS:O	1:D:487:ASN:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:THR:HA	1:D:92:HIS:HA	1.72	0.44
1:C:292:GLN:NE2	1:C:597:LYS:HE2	2.32	0.44
1:A:344:PRO:HD3	1:A:365:PRO:HD3	1.99	0.44
1:B:362:ASP:OD2	1:B:398:ASP:OD2	2.35	0.44
1:B:451:ASP:OD2	1:B:454:LYS:HD2	2.17	0.44
1:D:406:LEU:CD1	1:D:442:PRO:HB2	2.47	0.44
1:C:479:MET:HA	1:C:482:ALA:HB3	1.98	0.44
1:A:476:SER:HB3	1:A:520:MET:SD	2.57	0.44
1:B:340:THR:HG23	1:B:361:MET:O	2.17	0.44
1:D:268:LEU:HD12	1:D:268:LEU:HA	1.81	0.44
1:D:354:ASP:OD2	1:D:402:PRO:HD2	2.17	0.44
1:A:399:LYS:NZ	2:A:606:HOH:O	2.47	0.44
1:B:549:TRP:HE1	1:B:554:TYR:HH	1.66	0.44
1:D:486:LEU:HD22	1:D:533:LEU:HD22	1.99	0.44
1:A:387:HIS:HE1	1:A:426:TRP:CZ3	2.36	0.44
1:A:66:VAL:HG22	1:A:133:CYS:HB3	2.00	0.44
1:B:549:TRP:HA	1:B:550:ASN:HA	1.72	0.44
1:B:74:LEU:HB2	1:B:121:LEU:CD2	2.47	0.44
1:A:177:PRO:HB3	1:A:179:PHE:CE1	2.53	0.44
1:A:177:PRO:HG2	1:A:557:VAL:HG11	2.00	0.44
1:A:259:ARG:HA	1:A:260:PRO:C	2.38	0.44
1:A:423:TYR:HB2	1:A:457:THR:HG22	2.00	0.44
1:B:60:ARG:NH2	1:B:555:ASP:OD2	2.50	0.44
1:B:107:LYS:NZ	1:B:140:SER:OG	2.51	0.44
1:C:549:TRP:HA	1:C:550:ASN:HA	1.69	0.44
1:A:355:ARG:NH2	1:B:40:ALA:O	2.52	0.43
1:C:74:LEU:HD12	1:C:75:PRO:CD	2.44	0.43
1:D:389:GLN:NE2	1:D:393:GLU:OE1	2.48	0.43
1:A:142:LEU:HA	1:A:142:LEU:HD23	1.78	0.43
1:A:341:SER:HA	1:A:342:HIS:HA	1.83	0.43
1:A:508:ASP:O	1:A:521:PHE:HA	2.17	0.43
1:C:53:ASN:HB3	1:C:59:LEU:HD22	1.99	0.43
1:D:253:VAL:HG21	1:D:283:VAL:HG11	2.00	0.43
1:D:570:LEU:HD12	1:D:581:MET:HA	2.01	0.43
1:A:356:GLU:HA	1:A:356:GLU:OE1	2.18	0.43
1:C:377:PRO:O	1:C:381:TYR:HB2	2.18	0.43
1:C:89:SER:HB3	1:C:189:ARG:HD2	2.01	0.43
1:D:72:VAL:O	1:D:126:THR:HA	2.18	0.43
1:A:74:LEU:HD12	1:A:75:PRO:HD2	2.00	0.43
1:A:19:TRP:HE3	1:A:68:TYR:HB3	1.83	0.43
1:A:336:ASN:HD22	1:A:593:THR:HB	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:THR:HA	1:A:92:HIS:HA	1.69	0.43
1:B:323:ASN:HB3	1:B:352:LEU:CD1	2.49	0.43
1:A:141:THR:O	1:A:142:LEU:HD23	2.19	0.43
1:C:550:ASN:OD1	1:C:551:PHE:N	2.52	0.43
1:A:250:ILE:HB	1:A:253:VAL:CG1	2.48	0.43
1:B:591:ILE:HG23	1:B:596:PHE:CD1	2.54	0.43
1:C:508:ASP:O	1:C:521:PHE:HA	2.18	0.43
1:D:230:VAL:HG23	1:D:248:ILE:HD12	2.01	0.43
1:A:206:ILE:HD12	1:A:281:PHE:HB3	2.00	0.43
1:B:268:LEU:HA	1:B:268:LEU:HD12	1.88	0.43
1:C:257:GLU:OE1	1:C:298:LYS:NZ	2.30	0.43
1:B:341:SER:HA	1:B:342:HIS:HA	1.59	0.42
1:B:91:THR:HA	1:B:92:HIS:HA	1.69	0.42
1:D:362:ASP:OD2	1:D:398:ASP:OD2	2.37	0.42
1:A:97:TRP:HA	1:A:101:GLN:O	2.19	0.42
1:B:255:LEU:HD23	1:B:255:LEU:HA	1.80	0.42
1:B:549:TRP:HZ2	1:B:554:TYR:HH	1.64	0.42
1:B:584:LEU:HD23	1:B:584:LEU:HA	1.90	0.42
1:B:96:VAL:CG1	1:B:104:ALA:HB3	2.49	0.42
1:D:412:GLU:N	1:D:413:PRO:HD3	2.34	0.42
1:D:396:HIS:O	1:D:399:LYS:HG2	2.20	0.42
1:A:412:GLU:HB3	1:A:448:CYS:HB3	2.01	0.42
1:C:139:HIS:CD2	1:C:381:TYR:CZ	3.08	0.42
1:C:86:ARG:HD2	1:C:114:GLU:HG3	2.00	0.42
1:D:122:GLN:NE2	2:D:609:HOH:O	2.45	0.42
1:D:16:ASP:CG	1:D:46:PRO:HD3	2.39	0.42
1:B:265:LEU:HD22	1:B:281:PHE:O	2.19	0.42
1:B:342:HIS:HB3	1:B:367:VAL:HG21	2.01	0.42
1:C:69:GLN:HG2	1:C:128:LEU:HD11	2.01	0.42
1:B:188:HIS:CE1	1:B:316:ARG:HB3	2.55	0.42
1:B:509:THR:OG1	1:B:526:GLN:HB2	2.19	0.42
1:A:258:PRO:O	1:A:261:GLY:N	2.53	0.42
1:A:299:PRO:HG2	1:A:595:GLY:HA2	2.02	0.42
1:B:490:LEU:HD13	1:B:540:ARG:HD2	2.01	0.42
1:D:82:ARG:O	1:D:195:THR:HA	2.19	0.42
1:D:56:THR:HG23	1:D:58:ALA:N	2.33	0.42
1:C:553:ASP:O	1:C:573:ARG:HG3	2.19	0.42
1:B:431:GLU:O	1:B:435:GLN:HG3	2.19	0.42
1:B:452:TYR:CD2	1:B:489:GLU:HG3	2.55	0.42
1:B:508:ASP:OD1	1:B:568:LYS:HE3	2.19	0.42
1:D:110:PHE:O	1:D:189:ARG:NH1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:444:THR:OG1	1:D:445:LEU:N	2.53	0.42
1:C:405:VAL:O	1:C:442:PRO:HD2	2.19	0.42
1:C:472:TRP:CZ2	1:C:508:ASP:HB2	2.55	0.42
1:D:532:ARG:HD2	1:D:532:ARG:HA	1.81	0.42
1:C:205:THR:OG1	1:C:399:LYS:NZ	2.53	0.41
1:C:476:SER:HB3	1:C:520:MET:SD	2.60	0.41
1:C:436:LEU:HD23	1:C:436:LEU:HA	1.81	0.41
1:D:189:ARG:NH2	1:D:345:TYR:C	2.74	0.41
1:B:47:ALA:HA	1:B:317:GLY:HA3	2.02	0.41
1:C:549:TRP:HZ2	1:C:554:TYR:HH	1.66	0.41
1:C:85:LEU:HD12	1:C:86:ARG:H	1.86	0.41
1:D:139:HIS:CE1	1:D:147:GLU:HB2	2.56	0.41
1:D:98:LEU:HA	1:D:98:LEU:HD12	1.60	0.41
1:A:339:ARG:HD3	1:A:361:MET:SD	2.60	0.41
1:B:200:TYR:O	1:B:221:THR:HG23	2.20	0.41
1:B:294:LEU:HD23	1:B:299:PRO:HA	2.03	0.41
1:D:363:GLU:HG3	1:D:408:SER:HB3	2.03	0.41
1:C:13:LEU:HB2	1:C:193:LEU:O	2.21	0.41
1:C:91:THR:HA	1:C:92:HIS:HA	1.68	0.41
1:B:465:CYS:HB3	1:B:503:SER:OG	2.20	0.41
1:A:105:GLN:HE21	1:A:105:GLN:HB2	1.75	0.41
1:B:329:LEU:HD23	1:B:329:LEU:HA	1.86	0.41
1:B:467:ASN:ND2	1:B:504:GLU:OE2	2.54	0.41
1:A:21:PHE:HB2	1:A:43:ILE:CG2	2.51	0.41
1:D:241:ALA:HB2	1:D:248:ILE:CG2	2.51	0.41
1:D:28:GLU:OE2	1:D:28:GLU:N	2.35	0.41
1:A:266:TYR:HB2	1:A:281:PHE:CE1	2.56	0.40
1:C:406:LEU:HD13	1:C:463:ILE:HD12	2.02	0.40
1:C:514:HIS:HB3	1:C:524:GLU:OE2	2.21	0.40
1:B:217:ALA:HA	1:B:245:GLU:HB3	2.03	0.40
1:C:519:GLU:O	1:C:525:PHE:HB2	2.21	0.40
1:D:227:ARG:HG3	1:D:242:GLU:OE2	2.21	0.40
1:B:437:ASP:HA	1:B:438:PRO:HD2	1.93	0.40
1:C:341:SER:HB2	1:C:342:HIS:CE1	2.57	0.40
1:C:491:ASP:OD2	1:C:540:ARG:NH2	2.48	0.40
1:B:151:LEU:HA	1:B:151:LEU:HD23	1.88	0.40
1:B:82:ARG:NH1	1:B:84:VAL:HG21	2.36	0.40
1:B:2:LEU:O	1:B:86:ARG:NH2	2.54	0.40
1:A:519:GLU:HA	1:C:558:GLN:OE1	2.20	0.40
1:D:391:LEU:O	1:D:395:ILE:HG13	2.21	0.40
1:D:508:ASP:N	1:D:568:LYS:HG2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:ALA:HB1	1:C:40:ALA:CB	2.52	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:ASP:OD2	1:C:249:THR:OG1[3_556]	2.00	0.20
1:C:169:ARG:NH2	1:C:252:GLU:OE2[3_556]	2.07	0.13

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	593/597 (99%)	549 (93%)	42 (7%)	2 (0%)	41	66
1	B	594/597 (100%)	547 (92%)	45 (8%)	2 (0%)	41	66
1	C	595/597 (100%)	565 (95%)	29 (5%)	1 (0%)	47	73
1	D	594/597 (100%)	562 (95%)	30 (5%)	2 (0%)	41	66
All	All	2376/2388 (100%)	2223 (94%)	146 (6%)	7 (0%)	41	66

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	448	CYS
1	A	243	SER
1	B	251	PRO
1	D	47	ALA
1	D	252	GLU
1	A	33	PRO
1	B	260	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	491/496 (99%)	484 (99%)	7 (1%)	67	86
1	B	492/496 (99%)	483 (98%)	9 (2%)	59	83
1	C	493/496 (99%)	485 (98%)	8 (2%)	62	85
1	D	492/496 (99%)	486 (99%)	6 (1%)	71	88
All	All	1968/1984 (99%)	1938 (98%)	30 (2%)	65	86

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

Mol	Chain	Res	Type
1	A	10	ARG
1	A	14	SER
1	A	39	ASP
1	A	284	ARG
1	A	355	ARG
1	A	408	SER
1	A	505	TYR
1	B	60	ARG
1	B	140	SER
1	B	156	SER
1	B	284	ARG
1	B	285	SER
1	B	355	ARG
1	B	418	PHE
1	B	449	GLN
1	B	505	TYR
1	C	6	GLN
1	C	35	LYS
1	C	148	ASP
1	C	227	ARG
1	C	284	ARG
1	C	295	LEU
1	C	435	GLN
1	C	505	TYR

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Mol	Chain	Res	Type
1	D	223	SER
1	D	227	ARG
1	D	284	ARG
1	D	316	ARG
1	D	505	TYR
1	D	561	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	411	ASN
1	B	30	GLN
1	B	236	ASN
1	D	101	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 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	595/597 (99%)	-0.06	10 (1%) 70 72	32, 47, 61, 72	0
1	B	596/597 (99%)	0.03	9 (1%) 73 76	31, 49, 69, 90	0
1	C	597/597 (100%)	-0.02	4 (0%) 87 89	32, 46, 61, 78	0
1	D	596/597 (99%)	0.01	12 (2%) 65 67	32, 48, 63, 84	0
All	All	2384/2388 (99%)	-0.01	35 (1%) 73 76	31, 47, 63, 90	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	ILE	3.4
1	D	249	THR	3.2
1	D	248	ILE	3.1
1	B	216	TYR	3.0
1	D	223	SER	2.9
1	B	248	ILE	2.8
1	D	228	VAL	2.8
1	D	243	SER	2.8
1	C	29	THR	2.7
1	A	26	CYS	2.7
1	A	219	LYS	2.6
1	D	252	GLU	2.6
1	B	201	ILE	2.5
1	B	247	THR	2.5
1	A	23	LEU	2.4
1	C	149	GLY	2.4
1	B	28	GLU	2.3
1	A	30	GLN	2.3
1	B	484	TYR	2.3
1	A	245	GLU	2.3
1	C	222	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	212	GLY	2.2
1	D	29	THR	2.2
1	A	27	ALA	2.2
1	D	246	GLY	2.2
1	A	31	PHE	2.2
1	D	245	GLU	2.1
1	B	223	SER	2.1
1	A	484	TYR	2.1
1	D	251	PRO	2.1
1	C	306	CYS	2.0
1	D	128	LEU	2.0
1	D	260	PRO	2.0
1	A	28	GLU	2.0
1	B	29	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.