



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:51 PM UTC

PDB ID : 3PZV / pdb_00003pzv
Title : C2 crystal form of the endo-1,4-beta-glucanase from Bacillus subtilis 168
Authors : Santos, C.R.; Paiva, J.H.; Akao, P.K.; Meza, A.N.; Silva, J.C.; Squina, F.M.;
Ward, R.J.; Ruller, R.; Murakami, M.T.
Deposited on : 2010-12-14
Resolution : 2.87 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

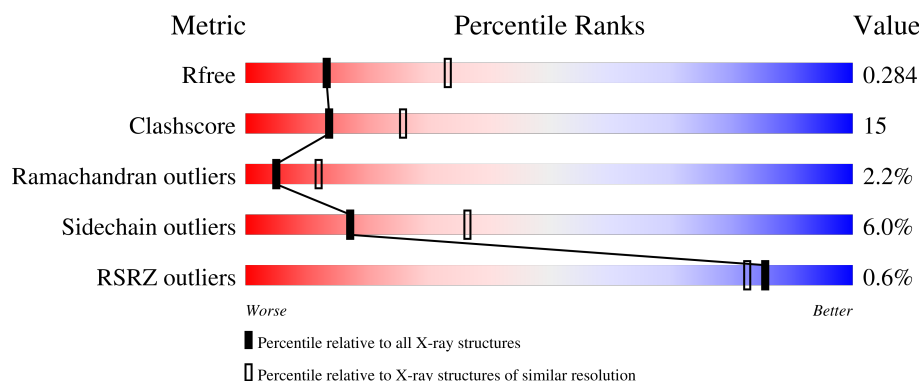
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	327	
1	B	327	
1	C	327	
1	D	327	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9398 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 Endoglucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	0
			2342	1482	402	455	3			
1	B	298	Total	C	N	O	S	0	0	0
			2342	1482	402	455	3			
1	C	298	Total	C	N	O	S	0	0	0
			2342	1482	402	455	3			
1	D	298	Total	C	N	O	S	0	0	0
			2342	1482	402	455	3			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	MET	-	expression tag	UNP P10475
A	7	GLY	-	expression tag	UNP P10475
A	8	SER	-	expression tag	UNP P10475
A	9	SER	-	expression tag	UNP P10475
A	10	HIS	-	expression tag	UNP P10475
A	11	HIS	-	expression tag	UNP P10475
A	12	HIS	-	expression tag	UNP P10475
A	13	HIS	-	expression tag	UNP P10475
A	14	HIS	-	expression tag	UNP P10475
A	15	HIS	-	expression tag	UNP P10475
A	16	SER	-	expression tag	UNP P10475
A	17	SER	-	expression tag	UNP P10475
A	18	GLY	-	expression tag	UNP P10475
A	19	LEU	-	expression tag	UNP P10475
A	20	VAL	-	expression tag	UNP P10475
A	21	PRO	-	expression tag	UNP P10475
A	22	ARG	-	expression tag	UNP P10475
A	23	GLY	-	expression tag	UNP P10475
A	24	SER	-	expression tag	UNP P10475
A	25	HIS	-	expression tag	UNP P10475
A	26	MET	-	expression tag	UNP P10475

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Chain	Residue	Modelled	Actual	Comment	Reference
B	6	MET	-	expression tag	UNP P10475
B	7	GLY	-	expression tag	UNP P10475
B	8	SER	-	expression tag	UNP P10475
B	9	SER	-	expression tag	UNP P10475
B	10	HIS	-	expression tag	UNP P10475
B	11	HIS	-	expression tag	UNP P10475
B	12	HIS	-	expression tag	UNP P10475
B	13	HIS	-	expression tag	UNP P10475
B	14	HIS	-	expression tag	UNP P10475
B	15	HIS	-	expression tag	UNP P10475
B	16	SER	-	expression tag	UNP P10475
B	17	SER	-	expression tag	UNP P10475
B	18	GLY	-	expression tag	UNP P10475
B	19	LEU	-	expression tag	UNP P10475
B	20	VAL	-	expression tag	UNP P10475
B	21	PRO	-	expression tag	UNP P10475
B	22	ARG	-	expression tag	UNP P10475
B	23	GLY	-	expression tag	UNP P10475
B	24	SER	-	expression tag	UNP P10475
B	25	HIS	-	expression tag	UNP P10475
B	26	MET	-	expression tag	UNP P10475
C	6	MET	-	expression tag	UNP P10475
C	7	GLY	-	expression tag	UNP P10475
C	8	SER	-	expression tag	UNP P10475
C	9	SER	-	expression tag	UNP P10475
C	10	HIS	-	expression tag	UNP P10475
C	11	HIS	-	expression tag	UNP P10475
C	12	HIS	-	expression tag	UNP P10475
C	13	HIS	-	expression tag	UNP P10475
C	14	HIS	-	expression tag	UNP P10475
C	15	HIS	-	expression tag	UNP P10475
C	16	SER	-	expression tag	UNP P10475
C	17	SER	-	expression tag	UNP P10475
C	18	GLY	-	expression tag	UNP P10475
C	19	LEU	-	expression tag	UNP P10475
C	20	VAL	-	expression tag	UNP P10475
C	21	PRO	-	expression tag	UNP P10475
C	22	ARG	-	expression tag	UNP P10475
C	23	GLY	-	expression tag	UNP P10475
C	24	SER	-	expression tag	UNP P10475
C	25	HIS	-	expression tag	UNP P10475
C	26	MET	-	expression tag	UNP P10475

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Chain	Residue	Modelled	Actual	Comment	Reference
D	6	MET	-	expression tag	UNP P10475
D	7	GLY	-	expression tag	UNP P10475
D	8	SER	-	expression tag	UNP P10475
D	9	SER	-	expression tag	UNP P10475
D	10	HIS	-	expression tag	UNP P10475
D	11	HIS	-	expression tag	UNP P10475
D	12	HIS	-	expression tag	UNP P10475
D	13	HIS	-	expression tag	UNP P10475
D	14	HIS	-	expression tag	UNP P10475
D	15	HIS	-	expression tag	UNP P10475
D	16	SER	-	expression tag	UNP P10475
D	17	SER	-	expression tag	UNP P10475
D	18	GLY	-	expression tag	UNP P10475
D	19	LEU	-	expression tag	UNP P10475
D	20	VAL	-	expression tag	UNP P10475
D	21	PRO	-	expression tag	UNP P10475
D	22	ARG	-	expression tag	UNP P10475
D	23	GLY	-	expression tag	UNP P10475
D	24	SER	-	expression tag	UNP P10475
D	25	HIS	-	expression tag	UNP P10475
D	26	MET	-	expression tag	UNP P10475

- Molecule 2 is water.

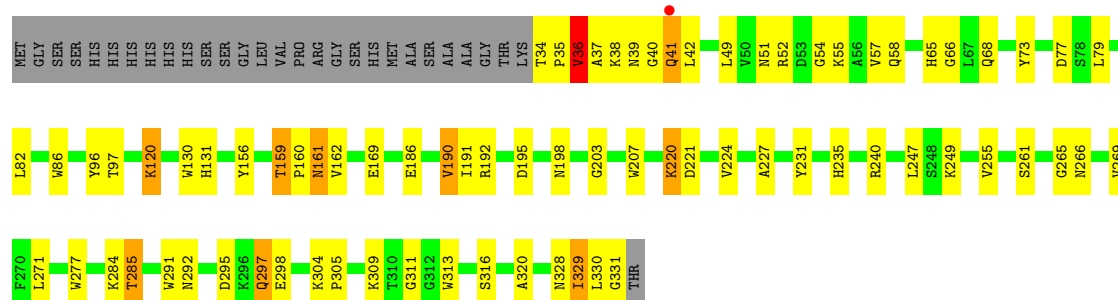
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	9	Total O 9 9	0	0
2	B	11	Total O 11 11	0	0
2	C	7	Total O 7 7	0	0
2	D	3	Total O 3 3	0	0

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.

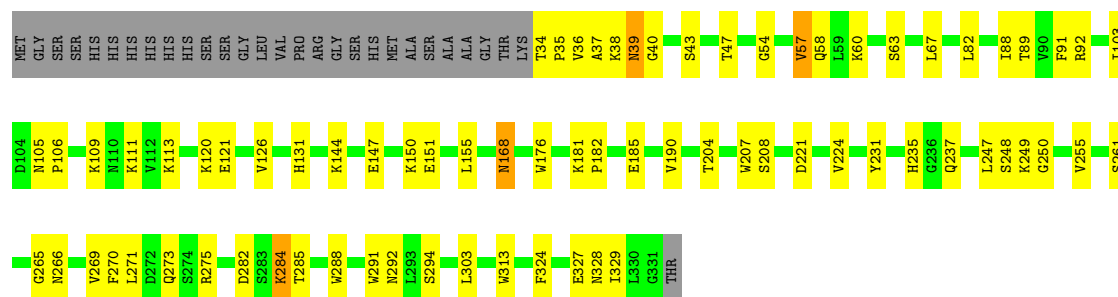
• Molecule 1: Endoglucanase

Chain A: 



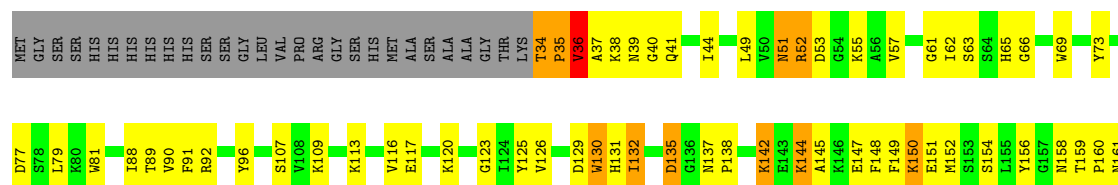
• Molecule 1: Endoglucanase

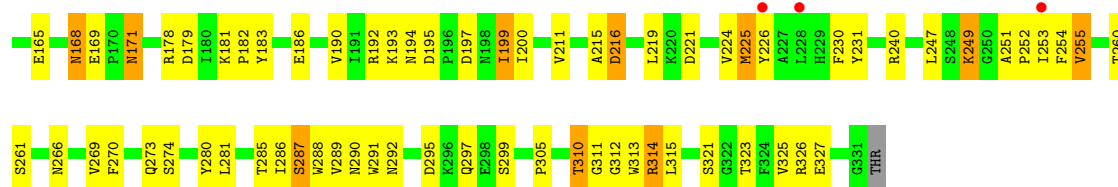
Chain B: 



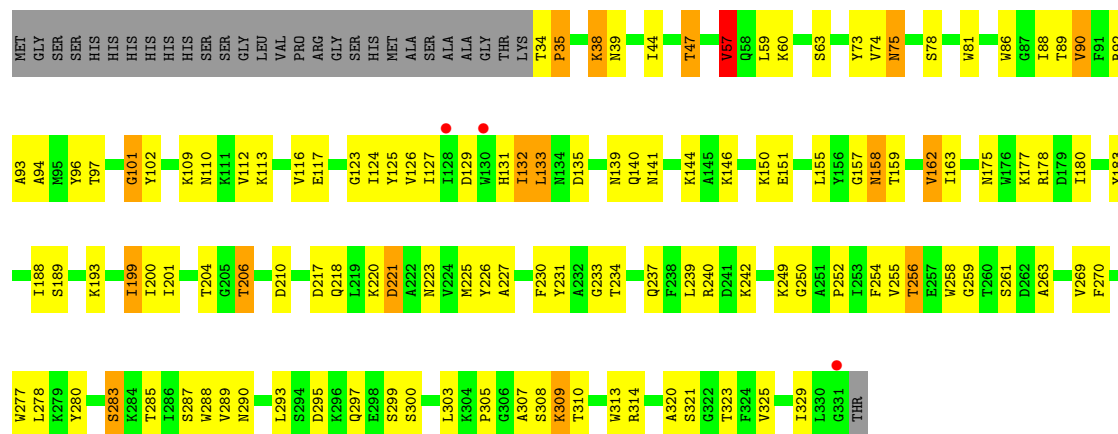
• Molecule 1: Endoglucanase

Chain C: 





• Molecule 1: Endoglucanase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	155.36Å 81.08Å 114.27Å 90.00° 104.29° 90.00°	Depositor
Resolution (Å)	41.46 – 2.87 41.46 – 2.87	Depositor EDS
% Data completeness (in resolution range)	89.8 (41.46-2.87) 89.3 (41.46-2.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.230 , 0.296 0.223 , 0.284	Depositor DCC
R_{free} test set	1531 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	71.4	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 24.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9398	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 4.24% 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

5.1 Standard geometry

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	0.52	1/2396 (0.0%)	1.05	10/3249 (0.3%)
1	B	0.49	0/2396	1.04	12/3249 (0.4%)
1	C	0.35	0/2396	0.90	6/3249 (0.2%)
1	D	0.32	0/2396	0.84	4/3249 (0.1%)
All	All	0.43	1/9584 (0.0%)	0.96	32/12996 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	328	ASN	CG-OD1	-5.31	1.13	1.23

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	ILE	N-CA-C	-11.08	102.28	111.81
1	B	105	ASN	CA-C-N	8.25	127.91	119.82
1	B	105	ASN	C-N-CA	8.25	127.91	119.82
1	A	329	ILE	N-CA-C	-7.84	104.81	111.56
1	C	216	ASP	N-CA-C	-7.71	105.04	114.75
1	B	54	GLY	N-CA-C	7.62	125.89	115.30
1	B	237	GLN	N-CA-C	6.92	119.70	111.33
1	B	37	ALA	N-CA-C	-6.73	103.87	111.14
1	C	195	ASP	CA-C-N	6.66	126.11	118.85
1	C	195	ASP	C-N-CA	6.66	126.11	118.85
1	C	53	ASP	N-CA-C	-6.57	103.68	112.94
1	A	162	VAL	N-CA-C	6.44	117.85	108.58
1	B	39	ASN	N-CA-C	6.28	121.18	112.45
1	C	288	TRP	N-CA-C	6.21	119.61	109.06
1	B	275	ARG	N-CA-C	-6.02	104.72	111.28
1	B	303	LEU	N-CA-C	5.79	118.98	109.72
1	B	43	SER	N-CA-C	5.64	116.52	108.74
1	B	265	GLY	N-CA-C	-5.55	107.44	115.27
1	B	329	ILE	N-CA-C	5.53	115.73	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	THR	CA-C-N	-5.49	114.16	119.87
1	A	159	THR	C-N-CA	-5.49	114.16	119.87
1	D	47	THR	N-CA-C	-5.46	106.97	113.97
1	D	38	LYS	N-CA-C	-5.37	107.38	114.04
1	A	77	ASP	N-CA-C	5.35	116.79	111.07
1	D	199	ILE	N-CA-C	5.30	116.42	109.21
1	A	271	LEU	N-CA-C	5.28	117.94	111.82
1	B	155	LEU	N-CA-C	5.18	116.62	111.07
1	A	54	GLY	N-CA-C	-5.17	108.14	115.43
1	C	193	LYS	N-CA-C	-5.17	107.27	113.21
1	D	57	VAL	N-CA-C	5.16	115.34	108.27
1	A	41	GLN	N-CA-C	5.15	118.01	109.46
1	A	161	ASN	N-CA-C	5.04	117.66	111.82

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	2342	0	2271	52	0
1	B	2342	0	2271	45	0
1	C	2342	0	2271	96	0
1	D	2342	0	2271	77	0
2	A	9	0	0	0	0
2	B	11	0	0	0	0
2	C	7	0	0	0	0
2	D	3	0	0	0	0
All	All	9398	0	9084	268	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 15.

All (268) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:GLN:OE1	1:A:160:PRO:HA	1.60	1.00
1:C:225:MET:HE2	1:C:254:PHE:HB2	1.48	0.95
1:C:34:THR:N	1:C:35:PRO:HD3	1.90	0.86
1:B:231:TYR:H	1:B:235:HIS:HD2	1.26	0.83
1:B:34:THR:HB	1:B:35:PRO:CD	2.09	0.83
1:C:156:TYR:O	1:C:159:THR:HB	1.79	0.82
1:C:261:SER:HB2	1:C:266:ASN:O	1.81	0.80
1:C:159:THR:HG22	1:C:161:ASN:H	1.47	0.80
1:C:144:LYS:HA	1:C:147:GLU:HB3	1.65	0.79
1:A:231:TYR:H	1:A:235:HIS:HD2	1.28	0.79
1:C:225:MET:HB3	1:C:252:PRO:HB2	1.65	0.77
1:D:280:TYR:O	1:D:283:SER:HB3	1.85	0.77
1:D:290:ASN:OD1	1:D:325:VAL:HG21	1.87	0.75
1:C:65:HIS:CD2	1:C:66:GLY:H	2.06	0.74
1:C:216:ASP:OD1	1:C:249:LYS:HE3	1.88	0.73
1:C:120:LYS:HB3	1:C:120:LYS:NZ	2.06	0.70
1:D:175:ASN:O	1:D:180:ILE:HG13	1.92	0.70
1:A:41:GLN:OE1	1:A:160:PRO:CA	2.39	0.68
1:A:231:TYR:H	1:A:235:HIS:CD2	2.09	0.68
1:C:44:ILE:HD13	1:C:49:LEU:HA	1.74	0.68
1:C:35:PRO:C	1:C:37:ALA:H	2.03	0.65
1:D:225:MET:HG2	1:D:252:PRO:HB2	1.79	0.65
1:D:231:TYR:CD2	1:D:263:ALA:HA	2.31	0.65
1:C:39:ASN:HB3	1:C:51:ASN:HB3	1.79	0.64
1:C:125:TYR:HE1	1:C:160:PRO:O	1.81	0.64
1:C:113:LYS:O	1:C:117:GLU:HG3	1.96	0.64
1:D:295:ASP:HB2	1:D:305:PRO:HA	1.79	0.64
1:B:34:THR:HB	1:B:35:PRO:HD3	1.80	0.63
1:D:35:PRO:HG2	1:D:124:ILE:HG22	1.81	0.63
1:A:221:ASP:HB3	1:A:224:VAL:HG23	1.81	0.62
1:C:221:ASP:HB3	1:C:224:VAL:HG23	1.81	0.62
1:D:39:ASN:HD21	1:D:57:VAL:HG21	1.64	0.62
1:A:329:ILE:C	1:A:331:GLY:H	2.06	0.62
1:A:120:LYS:HA	1:A:161:ASN:ND2	2.14	0.62
1:D:269:VAL:HG21	1:D:320:ALA:HB3	1.83	0.61
1:D:230:PHE:O	1:D:258:TRP:HA	2.00	0.61
1:C:200:ILE:O	1:C:224:VAL:HG13	2.00	0.61
1:C:36:VAL:HG11	1:C:161:ASN:ND2	2.16	0.61
1:B:67:LEU:HD22	1:B:111:LYS:HG3	1.81	0.60
1:D:96:TYR:HA	1:D:131:HIS:HB3	1.83	0.60
1:D:175:ASN:ND2	1:D:178:ARG:H	2.00	0.60
1:D:321:SER:O	1:D:325:VAL:HG23	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:ASN:HD21	1:D:178:ARG:H	1.47	0.60
1:D:44:ILE:HB	1:D:223:ASN:HA	1.85	0.59
1:C:65:HIS:HD2	1:C:66:GLY:H	1.51	0.59
1:D:256:THR:O	1:D:289:VAL:HB	2.03	0.59
1:C:34:THR:N	1:C:35:PRO:CD	2.66	0.58
1:C:291:TRP:CD2	1:C:292:ASN:HB3	2.38	0.58
1:D:113:LYS:O	1:D:117:GLU:HG2	2.04	0.58
1:C:35:PRO:C	1:C:37:ALA:N	2.61	0.58
1:A:159:THR:HG22	1:A:161:ASN:H	1.68	0.58
1:D:151:GLU:O	1:D:155:LEU:HG	2.04	0.58
1:A:195:ASP:OD2	1:A:198:ASN:HB2	2.03	0.57
1:B:261:SER:OG	1:B:266:ASN:O	2.23	0.57
1:B:247:LEU:C	1:B:249:LYS:H	2.13	0.57
1:C:158:ASN:HB2	1:D:314:ARG:HD3	1.87	0.57
1:B:58:GLN:HE22	1:B:282:ASP:HA	1.68	0.57
1:B:34:THR:HB	1:B:35:PRO:HD2	1.84	0.56
1:A:34:THR:OG1	1:A:35:PRO:HD2	2.06	0.56
1:C:179:ASP:C	1:C:182:PRO:HD2	2.30	0.56
1:D:73:TYR:CE1	1:D:309:LYS:HA	2.41	0.56
1:B:285:THR:O	1:B:285:THR:HG22	2.05	0.56
1:C:171:ASN:N	1:C:171:ASN:HD22	2.04	0.56
1:C:148:PHE:CE1	1:C:152:MET:HE3	2.41	0.55
1:D:34:THR:O	1:D:38:LYS:HB2	2.07	0.55
1:A:35:PRO:O	1:A:36:VAL:HG13	2.06	0.55
1:C:159:THR:CG2	1:C:161:ASN:H	2.18	0.55
1:C:270:PHE:HB3	1:C:273:GLN:OE1	2.06	0.55
1:D:254:PHE:CE2	1:D:287:SER:HB2	2.41	0.55
1:B:82:LEU:O	1:B:88:ILE:HG12	2.07	0.54
1:B:221:ASP:HB3	1:B:224:VAL:HG23	1.88	0.54
1:C:148:PHE:HE1	1:C:152:MET:HE3	1.73	0.54
1:C:295:ASP:HB2	1:C:305:PRO:HA	1.88	0.54
1:A:68:GLN:HE22	1:A:96:TYR:HB2	1.73	0.54
1:C:192:ARG:C	1:C:194:ASN:H	2.14	0.54
1:C:51:ASN:HD21	1:C:55:LYS:HB2	1.72	0.54
1:A:156:TYR:O	1:A:159:THR:HB	2.08	0.53
1:A:190:VAL:HG23	1:A:190:VAL:O	2.07	0.53
1:B:63:SER:HA	1:B:92:ARG:HB3	1.89	0.53
1:B:231:TYR:H	1:B:235:HIS:CD2	2.16	0.53
1:C:255:VAL:HG23	1:C:286:ILE:HG21	1.89	0.53
1:A:35:PRO:O	1:A:37:ALA:N	2.37	0.53
1:D:34:THR:N	1:D:35:PRO:CD	2.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:LEU:HD13	1:A:284:LYS:HD3	1.91	0.53
1:C:96:TYR:HA	1:C:131:HIS:HB3	1.89	0.53
1:D:74:VAL:O	1:D:75:ASN:HB3	2.08	0.53
1:B:231:TYR:N	1:B:235:HIS:HD2	2.03	0.52
1:B:47:THR:CG2	1:B:250:GLY:HA2	2.39	0.52
1:B:292:ASN:ND2	1:B:294:SER:OG	2.41	0.52
1:B:204:THR:OG1	1:B:208:SER:HA	2.10	0.52
1:C:135:ASP:OD1	1:C:135:ASP:N	2.43	0.52
1:C:90:VAL:HA	1:C:125:TYR:O	2.10	0.51
1:C:215:ALA:HB2	1:C:251:ALA:CB	2.40	0.51
1:C:321:SER:O	1:C:325:VAL:HG23	2.11	0.51
1:D:94:ALA:HB1	1:D:131:HIS:ND1	2.24	0.51
1:A:295:ASP:HB2	1:A:305:PRO:HA	1.91	0.51
1:B:324:PHE:O	1:B:328:ASN:ND2	2.42	0.51
1:B:207:TRP:O	1:B:208:SER:HB2	2.10	0.51
1:C:226:TYR:HE2	1:C:252:PRO:HD2	1.75	0.51
1:D:60:LYS:HB3	1:D:329:ILE:HG12	1.92	0.51
1:C:252:PRO:O	1:C:253:ILE:HD13	2.10	0.51
1:B:106:PRO:O	1:B:109:LYS:HG2	2.10	0.51
1:B:91:PHE:O	1:B:126:VAL:HA	2.11	0.51
1:B:103:ILE:HD12	1:B:144:LYS:HD2	1.92	0.51
1:C:129:ASP:HA	1:C:165:GLU:HB3	1.92	0.51
1:C:291:TRP:CG	1:C:292:ASN:HB3	2.46	0.51
1:D:132:ILE:HG22	1:D:135:ASP:OD2	2.10	0.51
1:C:230:PHE:C	1:C:231:TYR:CD2	2.89	0.51
1:D:112:VAL:O	1:D:116:VAL:HG23	2.11	0.51
1:B:181:LYS:O	1:B:185:GLU:HG2	2.10	0.50
1:B:176:TRP:HE1	1:B:181:LYS:HD2	1.76	0.50
1:D:35:PRO:HD2	1:D:123:GLY:O	2.11	0.50
1:C:254:PHE:CE2	1:C:287:SER:HB2	2.47	0.50
1:A:297:GLN:O	1:A:297:GLN:HG3	2.12	0.50
1:C:266:ASN:HA	1:C:299:SER:HB2	1.93	0.50
1:D:188:ILE:HG12	1:D:200:ILE:HD13	1.94	0.49
1:C:290:ASN:CG	1:C:291:TRP:H	2.20	0.49
1:C:178:ARG:O	1:C:182:PRO:HG2	2.11	0.49
1:A:97:THR:HG21	1:A:130:TRP:CE2	2.47	0.49
1:C:290:ASN:CG	1:C:291:TRP:N	2.71	0.49
1:D:92:ARG:HA	1:D:127:ILE:HB	1.93	0.49
1:D:293:LEU:O	1:D:293:LEU:HG	2.11	0.49
1:A:304:LYS:HD2	1:A:316:SER:O	2.12	0.49
1:C:62:ILE:CG1	1:C:63:SER:H	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:LYS:HB3	1:C:120:LYS:HZ1	1.74	0.49
1:B:82:LEU:HD21	1:B:313:TRP:HZ3	1.77	0.49
1:D:231:TYR:HD1	1:D:259:GLY:HA3	1.76	0.49
1:C:323:THR:O	1:C:327:GLU:HB2	2.13	0.49
1:D:255:VAL:O	1:D:288:TRP:HA	2.13	0.49
1:A:68:GLN:HE22	1:A:96:TYR:CB	2.25	0.48
1:D:269:VAL:HG21	1:D:320:ALA:CB	2.42	0.48
1:D:204:THR:HB	1:D:210:ASP:O	2.13	0.48
1:C:77:ASP:HB2	1:C:310:THR:HG22	1.94	0.48
1:D:93:ALA:O	1:D:129:ASP:HB3	2.13	0.48
1:D:139:ASN:OD1	1:D:183:TYR:HB2	2.14	0.48
1:B:36:VAL:O	1:B:40:GLY:N	2.45	0.48
1:C:221:ASP:HB3	1:C:224:VAL:CG2	2.42	0.48
1:D:158:ASN:O	1:D:159:THR:C	2.56	0.48
1:C:131:HIS:HA	1:C:168:ASN:HB2	1.95	0.48
1:A:82:LEU:O	1:A:86:TRP:HB2	2.13	0.47
1:A:169:GLU:OE1	1:A:207:TRP:HD1	1.97	0.47
1:B:47:THR:HG22	1:B:250:GLY:HA2	1.95	0.47
1:B:113:LYS:NZ	1:B:151:GLU:OE2	2.47	0.47
1:C:129:ASP:OD1	1:C:129:ASP:C	2.57	0.47
1:C:171:ASN:N	1:C:171:ASN:ND2	2.62	0.47
1:D:44:ILE:HD13	1:D:199:ILE:HD12	1.95	0.47
1:C:181:LYS:N	1:C:182:PRO:CD	2.78	0.47
1:D:141:ASN:HB3	1:D:144:LYS:HB2	1.97	0.47
1:A:68:GLN:NE2	1:A:96:TYR:HB2	2.29	0.47
1:B:67:LEU:HD22	1:B:111:LYS:CG	2.45	0.47
1:D:162:VAL:C	1:D:163:ILE:HG13	2.40	0.47
1:A:221:ASP:HB3	1:A:224:VAL:CG2	2.43	0.47
1:C:255:VAL:HG23	1:C:286:ILE:CG2	2.45	0.47
1:C:291:TRP:HA	1:C:292:ASN:HA	1.64	0.47
1:B:284:LYS:HE2	1:B:284:LYS:HB3	1.66	0.46
1:C:142:LYS:HB2	1:C:183:TYR:CD1	2.49	0.46
1:A:291:TRP:CG	1:A:292:ASN:HB3	2.51	0.46
1:C:36:VAL:CG2	1:C:36:VAL:O	2.63	0.46
1:A:39:ASN:O	1:A:51:ASN:HB2	2.15	0.46
1:C:73:TYR:HH	1:C:295:ASP:CG	2.23	0.46
1:C:314:ARG:H	1:C:314:ARG:HG2	1.51	0.46
1:D:110:ASN:O	1:D:113:LYS:HB2	2.14	0.46
1:C:35:PRO:O	1:C:37:ALA:N	2.48	0.46
1:C:61:GLY:HA3	1:C:90:VAL:O	2.16	0.46
1:A:265:GLY:O	1:A:298:GLU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:LEU:CD1	1:A:284:LYS:HD3	2.46	0.45
1:C:226:TYR:CE2	1:C:252:PRO:HD2	2.51	0.45
1:D:226:TYR:N	1:D:226:TYR:CD2	2.84	0.45
1:A:58:GLN:HB2	1:A:285:THR:HG22	1.97	0.45
1:A:120:LYS:HB2	1:A:120:LYS:HE3	1.65	0.45
1:B:60:LYS:HG2	1:B:288:TRP:CE2	2.51	0.45
1:C:148:PHE:O	1:C:150:LYS:N	2.50	0.45
1:D:201:ILE:CG2	1:D:227:ALA:HB2	2.47	0.45
1:D:218:GLN:NE2	1:D:249:LYS:O	2.48	0.45
1:C:116:VAL:HA	1:C:126:VAL:HG11	1.99	0.45
1:D:146:LYS:O	1:D:150:LYS:HB2	2.16	0.45
1:A:311:GLY:HA2	1:A:313:TRP:CE2	2.52	0.45
1:C:65:HIS:HB2	1:C:292:ASN:OD1	2.17	0.45
1:D:90:VAL:HA	1:D:125:TYR:O	2.17	0.45
1:D:63:SER:HB2	1:D:92:ARG:HB3	1.98	0.45
1:A:51:ASN:ND2	1:A:55:LYS:HB2	2.31	0.44
1:A:203:GLY:HA2	1:A:227:ALA:HB3	1.98	0.44
1:C:199:ILE:H	1:C:199:ILE:HG12	1.59	0.44
1:C:107:SER:C	1:C:109:LYS:N	2.75	0.44
1:A:186:GLU:O	1:A:190:VAL:HG13	2.17	0.44
1:B:247:LEU:C	1:B:249:LYS:N	2.76	0.44
1:B:269:VAL:HG12	1:B:271:LEU:HG	1.99	0.44
1:C:52:ARG:O	1:C:52:ARG:NH1	2.51	0.44
1:C:260:THR:HG22	1:C:274:SER:OG	2.16	0.44
1:D:86:TRP:CD1	1:D:86:TRP:N	2.84	0.44
1:A:42:LEU:HD13	1:A:49:LEU:HD21	1.99	0.44
1:D:127:ILE:HD13	1:D:256:THR:HG22	1.99	0.44
1:C:62:ILE:CG1	1:C:63:SER:N	2.80	0.44
1:D:102:TYR:HE1	1:D:109:LYS:HB3	1.83	0.44
1:D:234:THR:OG1	1:D:263:ALA:N	2.50	0.43
1:B:131:HIS:HA	1:B:168:ASN:HB2	2.00	0.43
1:D:261:SER:OG	1:D:300:SER:HB3	2.19	0.43
1:C:39:ASN:HB3	1:C:51:ASN:CB	2.47	0.43
1:A:240:ARG:HG2	1:A:277:TRP:CZ3	2.53	0.43
1:D:81:TRP:HD1	1:D:313:TRP:CZ3	2.36	0.43
1:A:51:ASN:CG	1:A:55:LYS:HB2	2.43	0.43
1:B:35:PRO:CG	1:B:89:THR:HG22	2.49	0.43
1:A:291:TRP:CD2	1:A:292:ASN:HB3	2.54	0.43
1:D:88:ILE:HD12	1:D:90:VAL:O	2.19	0.43
1:B:270:PHE:HB3	1:B:273:GLN:OE1	2.19	0.43
1:C:280:TYR:HD2	1:C:281:LEU:HD23	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:VAL:O	1:D:75:ASN:CB	2.67	0.43
1:D:89:THR:O	1:D:90:VAL:HB	2.18	0.43
1:C:132:ILE:O	1:C:132:ILE:HG13	2.18	0.42
1:D:129:ASP:OD2	1:D:131:HIS:ND1	2.41	0.42
1:D:220:LYS:O	1:D:221:ASP:C	2.62	0.42
1:D:237:GLN:O	1:D:240:ARG:N	2.52	0.42
1:A:96:TYR:HA	1:A:131:HIS:HB3	2.00	0.42
1:A:329:ILE:O	1:A:331:GLY:N	2.51	0.42
1:C:91:PHE:N	1:C:125:TYR:O	2.42	0.42
1:D:59:LEU:N	1:D:287:SER:OG	2.45	0.42
1:A:255:VAL:HG12	1:A:255:VAL:O	2.18	0.42
1:C:148:PHE:C	1:C:150:LYS:N	2.77	0.42
1:C:151:GLU:HG3	1:D:81:TRP:CZ3	2.54	0.42
1:D:277:TRP:O	1:D:280:TYR:HB3	2.19	0.42
1:A:73:TYR:CD1	1:A:309:LYS:HA	2.54	0.42
1:B:324:PHE:O	1:B:327:GLU:HB2	2.20	0.42
1:C:150:LYS:O	1:C:154:SER:HB2	2.20	0.42
1:D:96:TYR:O	1:D:101:GLY:HA3	2.20	0.42
1:B:111:LYS:HA	1:B:111:LYS:HD3	1.72	0.42
1:C:63:SER:OG	1:C:92:ARG:HD3	2.20	0.42
1:A:220:LYS:H	1:A:220:LYS:HD3	1.85	0.42
1:D:75:ASN:OD1	1:D:78:SER:N	2.48	0.42
1:B:291:TRP:CD2	1:B:292:ASN:HB3	2.55	0.41
1:C:137:ASN:HA	1:C:138:PRO:HD2	1.86	0.41
1:D:158:ASN:O	1:D:158:ASN:ND2	2.51	0.41
1:B:120:LYS:HE3	1:B:120:LYS:HB3	1.78	0.41
1:D:227:ALA:HA	1:D:254:PHE:O	2.19	0.41
1:C:260:THR:HB	1:C:269:VAL:HG13	2.02	0.41
1:D:239:LEU:HD12	1:D:242:LYS:HD3	2.03	0.41
1:C:169:GLU:O	1:C:171:ASN:ND2	2.53	0.41
1:D:81:TRP:CD1	1:D:313:TRP:CE3	3.08	0.41
1:B:82:LEU:C	1:B:88:ILE:HG12	2.44	0.41
1:C:41:GLN:HB3	1:C:52:ARG:HG3	2.03	0.41
1:A:41:GLN:CD	1:A:198:ASN:OD1	2.64	0.41
1:D:47:THR:HG22	1:D:250:GLY:O	2.20	0.41
1:B:181:LYS:HB3	1:B:182:PRO:HD3	2.02	0.41
1:C:230:PHE:O	1:C:231:TYR:CD2	2.74	0.41
1:A:40:GLY:HA3	1:A:52:ARG:HE	1.86	0.41
1:A:35:PRO:C	1:A:37:ALA:N	2.78	0.41
1:C:315:LEU:HD21	1:C:326:ARG:NH1	2.35	0.41
1:B:39:ASN:ND2	1:B:57:VAL:HG21	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:VAL:O	1:B:288:TRP:HA	2.21	0.41
1:C:159:THR:HA	1:C:160:PRO:HD2	1.91	0.41
1:A:41:GLN:NE2	1:A:198:ASN:OD1	2.54	0.40
1:A:269:VAL:HG21	1:A:320:ALA:HB3	2.02	0.40
1:B:34:THR:CB	1:B:35:PRO:CD	2.84	0.40
1:C:254:PHE:CD1	1:C:254:PHE:C	2.99	0.40
1:D:189:SER:O	1:D:193:LYS:HG3	2.20	0.40
1:A:192:ARG:HA	1:A:192:ARG:HD3	1.82	0.40
1:A:261:SER:HB2	1:A:266:ASN:O	2.20	0.40
1:C:35:PRO:HD2	1:C:123:GLY:O	2.20	0.40
1:C:81:TRP:CZ2	1:C:312:GLY:HA2	2.56	0.40
1:C:130:TRP:CZ2	1:C:145:ALA:HA	2.56	0.40
1:C:254:PHE:HE1	1:C:289:VAL:HG23	1.86	0.40
1:D:206:THR:O	1:D:206:THR:HG22	2.20	0.40
1:A:65:HIS:O	1:A:66:GLY:C	2.65	0.40
1:C:66:GLY:HA3	1:C:69:TRP:CE3	2.56	0.40
1:C:311:GLY:HA2	1:C:313:TRP:CE2	2.56	0.40
1:D:233:GLY:HA2	1:D:270:PHE:CD2	2.56	0.40
1:D:307:ALA:O	1:D:308:SER:C	2.63	0.40
1:D:329:ILE:O	1:D:329:ILE:HG22	2.21	0.40
1:D:39:ASN:ND2	1:D:57:VAL:HG11	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	296/327 (90%)	284 (96%)	9 (3%)	3 (1%)	12	25
1	B	296/327 (90%)	277 (94%)	17 (6%)	2 (1%)	18	35
1	C	296/327 (90%)	242 (82%)	45 (15%)	9 (3%)	3	8
1	D	296/327 (90%)	244 (82%)	40 (14%)	12 (4%)	2	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1184/1308 (90%)	1047 (88%)	111 (9%)	26 (2%)	5	12

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	LEU
1	C	35	PRO
1	C	40	GLY
1	D	217	ASP
1	C	51	ASN
1	C	149	PHE
1	C	297	GLN
1	D	133	LEU
1	D	157	GLY
1	D	221	ASP
1	D	283	SER
1	A	297	GLN
1	B	248	SER
1	C	130	TRP
1	C	135	ASP
1	D	75	ASN
1	A	36	VAL
1	C	255	VAL
1	D	206	THR
1	B	168	ASN
1	D	35	PRO
1	D	90	VAL
1	D	97	THR
1	D	297	GLN
1	C	36	VAL
1	D	101	GLY

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	248/270 (92%)	239 (96%)	9 (4%)	31	56
1	B	248/270 (92%)	241 (97%)	7 (3%)	38	62
1	C	248/270 (92%)	220 (89%)	28 (11%)	5	11
1	D	248/270 (92%)	232 (94%)	16 (6%)	15	32
All	All	992/1080 (92%)	932 (94%)	60 (6%)	17	36

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	VAL
1	A	38	LYS
1	A	57	VAL
1	A	79	LEU
1	A	120	LYS
1	A	190	VAL
1	A	220	LYS
1	A	249	LYS
1	A	285	THR
1	B	38	LYS
1	B	57	VAL
1	B	121	GLU
1	B	147	GLU
1	B	150	LYS
1	B	190	VAL
1	B	284	LYS
1	C	34	THR
1	C	36	VAL
1	C	38	LYS
1	C	52	ARG
1	C	57	VAL
1	C	79	LEU
1	C	88	ILE
1	C	89	THR
1	C	132	ILE
1	C	142	LYS
1	C	144	LYS
1	C	150	LYS
1	C	168	ASN
1	C	171	ASN
1	C	186	GLU
1	C	190	VAL
1	C	197	ASP

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Mol	Chain	Res	Type
1	C	199	ILE
1	C	211	VAL
1	C	219	LEU
1	C	225	MET
1	C	240	ARG
1	C	247	LEU
1	C	249	LYS
1	C	285	THR
1	C	287	SER
1	C	310	THR
1	C	314	ARG
1	D	57	VAL
1	D	126	VAL
1	D	132	ILE
1	D	133	LEU
1	D	140	GLN
1	D	158	ASN
1	D	162	VAL
1	D	177	LYS
1	D	256	THR
1	D	278	LEU
1	D	285	THR
1	D	299	SER
1	D	303	LEU
1	D	309	LYS
1	D	310	THR
1	D	323	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	ASN
1	A	139	ASN
1	A	140	GLN
1	A	141	ASN
1	A	209	GLN
1	A	235	HIS
1	A	297	GLN
1	B	39	ASN
1	B	134	ASN
1	B	140	GLN
1	B	158	ASN

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Mol	Chain	Res	Type
1	B	223	ASN
1	B	235	HIS
1	B	244	ASN
1	B	292	ASN
1	B	297	GLN
1	C	41	GLN
1	C	137	ASN
1	C	140	GLN
1	C	141	ASN
1	C	171	ASN
1	C	198	ASN
1	C	209	GLN
1	C	235	HIS
1	D	39	ASN
1	D	65	HIS
1	D	105	ASN
1	D	140	GLN
1	D	141	ASN
1	D	175	ASN
1	D	194	ASN
1	D	223	ASN
1	D	235	HIS

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 oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	298/327 (91%)	-0.35	1 (0%) 90 89	48, 63, 79, 90	0
1	B	298/327 (91%)	-0.22	0 100 100	47, 68, 87, 107	0
1	C	298/327 (91%)	0.11	3 (1%) 79 74	52, 84, 100, 115	1 (0%)
1	D	298/327 (91%)	0.21	3 (1%) 79 74	62, 103, 121, 129	1 (0%)
All	All	1192/1308 (91%)	-0.06	7 (0%) 85 82	47, 77, 114, 129	2 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	253	ILE	2.9
1	D	130	TRP	2.6
1	C	228	LEU	2.6
1	D	331	GLY	2.5
1	A	41	GLN	2.1
1	D	128	ILE	2.1
1	C	226	TYR	2.1

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 oligosaccharides 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.