



Full wwPDB X-ray Structure Validation Report i

Sep 5, 2023 – 06:13 PM EDT

PDB ID : 8EXD
Title : Crystal structure of Aspergillus fumigatus sterylglucosidase A
Authors : Pereira de Sa, N.; Del Poeta, M.; Airola, M.V.
Deposited on : 2022-10-25
Resolution : 3.80 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 i 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](#) ①) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
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)	:	2.35

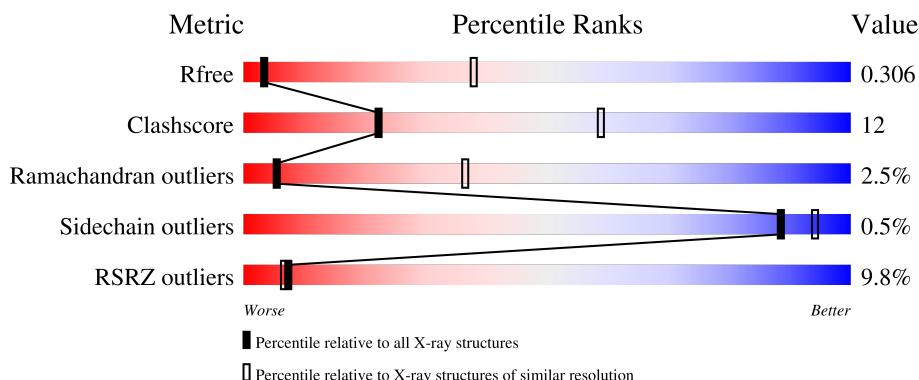
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

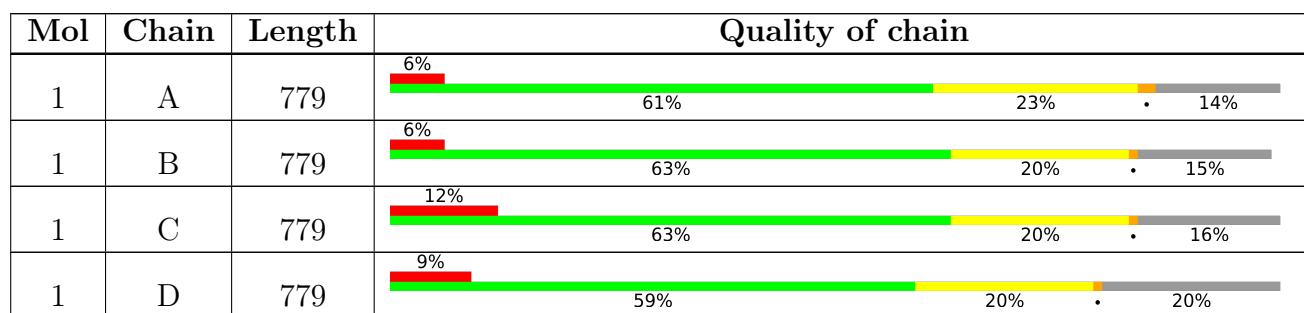
The reported resolution of this entry is 3.80 Å.

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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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.



2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 21118 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 Sterylglucosidase A (SglA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	670	Total	C 5426	N 3486	O 921	S 1002	17	0	0
1	B	659	Total	C 5338	N 3426	O 908	S 987	17	0	0
1	C	655	Total	C 5309	N 3411	O 900	S 981	17	0	0
1	D	623	Total	C 5045	N 3248	O 852	S 929	16	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q4WXA7
A	-18	GLY	-	expression tag	UNP Q4WXA7
A	-17	SER	-	expression tag	UNP Q4WXA7
A	-16	SER	-	expression tag	UNP Q4WXA7
A	-15	HIS	-	expression tag	UNP Q4WXA7
A	-14	HIS	-	expression tag	UNP Q4WXA7
A	-13	HIS	-	expression tag	UNP Q4WXA7
A	-12	HIS	-	expression tag	UNP Q4WXA7
A	-11	HIS	-	expression tag	UNP Q4WXA7
A	-10	HIS	-	expression tag	UNP Q4WXA7
A	-9	SER	-	expression tag	UNP Q4WXA7
A	-8	SER	-	expression tag	UNP Q4WXA7
A	-7	GLY	-	expression tag	UNP Q4WXA7
A	-6	LEU	-	expression tag	UNP Q4WXA7
A	-5	VAL	-	expression tag	UNP Q4WXA7
A	-4	PRO	-	expression tag	UNP Q4WXA7
A	-3	ARG	-	expression tag	UNP Q4WXA7
A	-2	GLY	-	expression tag	UNP Q4WXA7
A	-1	SER	-	expression tag	UNP Q4WXA7
A	0	HIS	-	expression tag	UNP Q4WXA7
B	-19	MET	-	initiating methionine	UNP Q4WXA7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP Q4WXA7
B	-17	SER	-	expression tag	UNP Q4WXA7
B	-16	SER	-	expression tag	UNP Q4WXA7
B	-15	HIS	-	expression tag	UNP Q4WXA7
B	-14	HIS	-	expression tag	UNP Q4WXA7
B	-13	HIS	-	expression tag	UNP Q4WXA7
B	-12	HIS	-	expression tag	UNP Q4WXA7
B	-11	HIS	-	expression tag	UNP Q4WXA7
B	-10	HIS	-	expression tag	UNP Q4WXA7
B	-9	SER	-	expression tag	UNP Q4WXA7
B	-8	SER	-	expression tag	UNP Q4WXA7
B	-7	GLY	-	expression tag	UNP Q4WXA7
B	-6	LEU	-	expression tag	UNP Q4WXA7
B	-5	VAL	-	expression tag	UNP Q4WXA7
B	-4	PRO	-	expression tag	UNP Q4WXA7
B	-3	ARG	-	expression tag	UNP Q4WXA7
B	-2	GLY	-	expression tag	UNP Q4WXA7
B	-1	SER	-	expression tag	UNP Q4WXA7
B	0	HIS	-	expression tag	UNP Q4WXA7
C	-19	MET	-	initiating methionine	UNP Q4WXA7
C	-18	GLY	-	expression tag	UNP Q4WXA7
C	-17	SER	-	expression tag	UNP Q4WXA7
C	-16	SER	-	expression tag	UNP Q4WXA7
C	-15	HIS	-	expression tag	UNP Q4WXA7
C	-14	HIS	-	expression tag	UNP Q4WXA7
C	-13	HIS	-	expression tag	UNP Q4WXA7
C	-12	HIS	-	expression tag	UNP Q4WXA7
C	-11	HIS	-	expression tag	UNP Q4WXA7
C	-10	HIS	-	expression tag	UNP Q4WXA7
C	-9	SER	-	expression tag	UNP Q4WXA7
C	-8	SER	-	expression tag	UNP Q4WXA7
C	-7	GLY	-	expression tag	UNP Q4WXA7
C	-6	LEU	-	expression tag	UNP Q4WXA7
C	-5	VAL	-	expression tag	UNP Q4WXA7
C	-4	PRO	-	expression tag	UNP Q4WXA7
C	-3	ARG	-	expression tag	UNP Q4WXA7
C	-2	GLY	-	expression tag	UNP Q4WXA7
C	-1	SER	-	expression tag	UNP Q4WXA7
C	0	HIS	-	expression tag	UNP Q4WXA7
D	-19	MET	-	initiating methionine	UNP Q4WXA7
D	-18	GLY	-	expression tag	UNP Q4WXA7
D	-17	SER	-	expression tag	UNP Q4WXA7

Continued on next page...

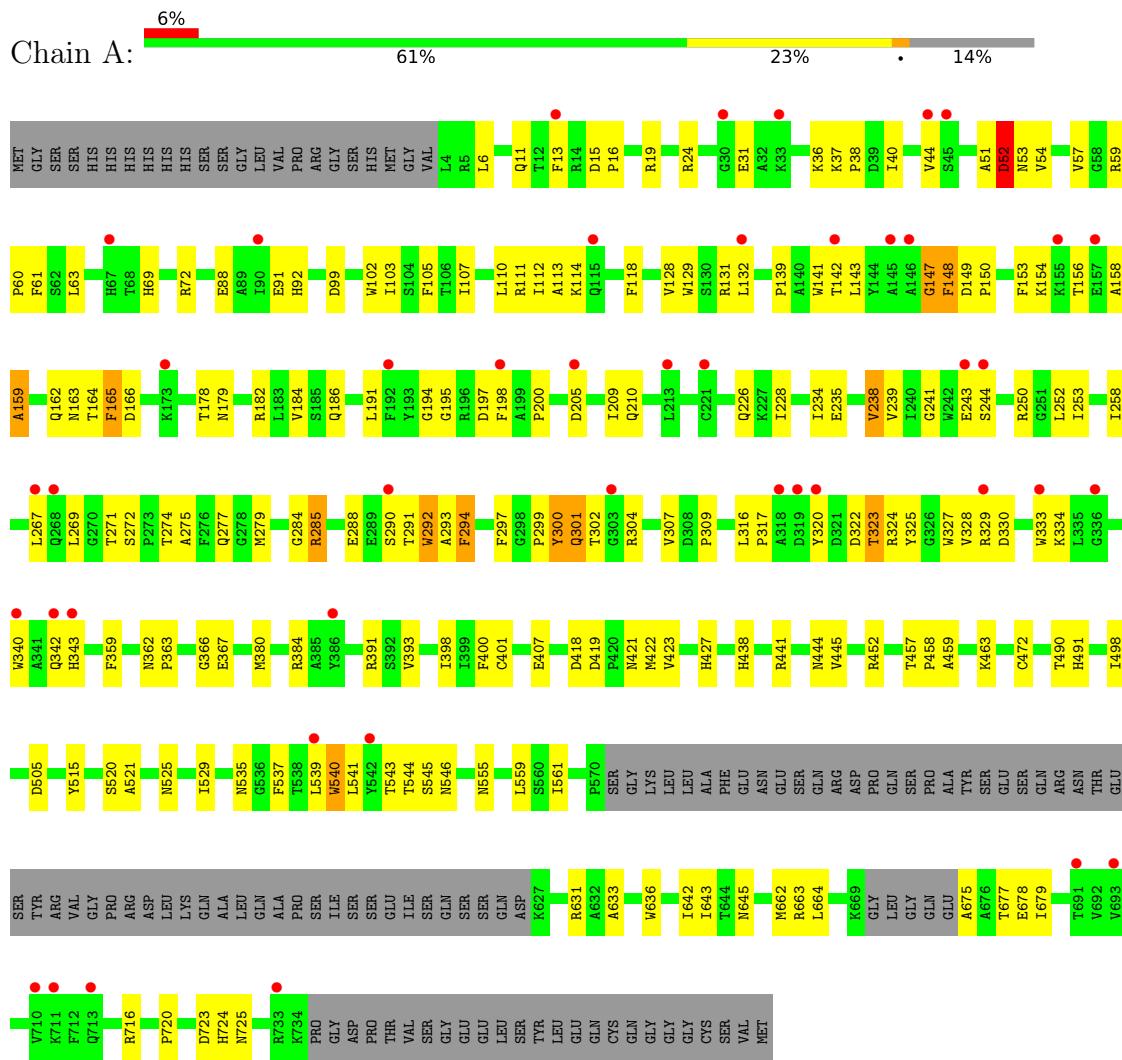
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP Q4WXA7
D	-15	HIS	-	expression tag	UNP Q4WXA7
D	-14	HIS	-	expression tag	UNP Q4WXA7
D	-13	HIS	-	expression tag	UNP Q4WXA7
D	-12	HIS	-	expression tag	UNP Q4WXA7
D	-11	HIS	-	expression tag	UNP Q4WXA7
D	-10	HIS	-	expression tag	UNP Q4WXA7
D	-9	SER	-	expression tag	UNP Q4WXA7
D	-8	SER	-	expression tag	UNP Q4WXA7
D	-7	GLY	-	expression tag	UNP Q4WXA7
D	-6	LEU	-	expression tag	UNP Q4WXA7
D	-5	VAL	-	expression tag	UNP Q4WXA7
D	-4	PRO	-	expression tag	UNP Q4WXA7
D	-3	ARG	-	expression tag	UNP Q4WXA7
D	-2	GLY	-	expression tag	UNP Q4WXA7
D	-1	SER	-	expression tag	UNP Q4WXA7
D	0	HIS	-	expression tag	UNP Q4WXA7

3 Residue-property plots

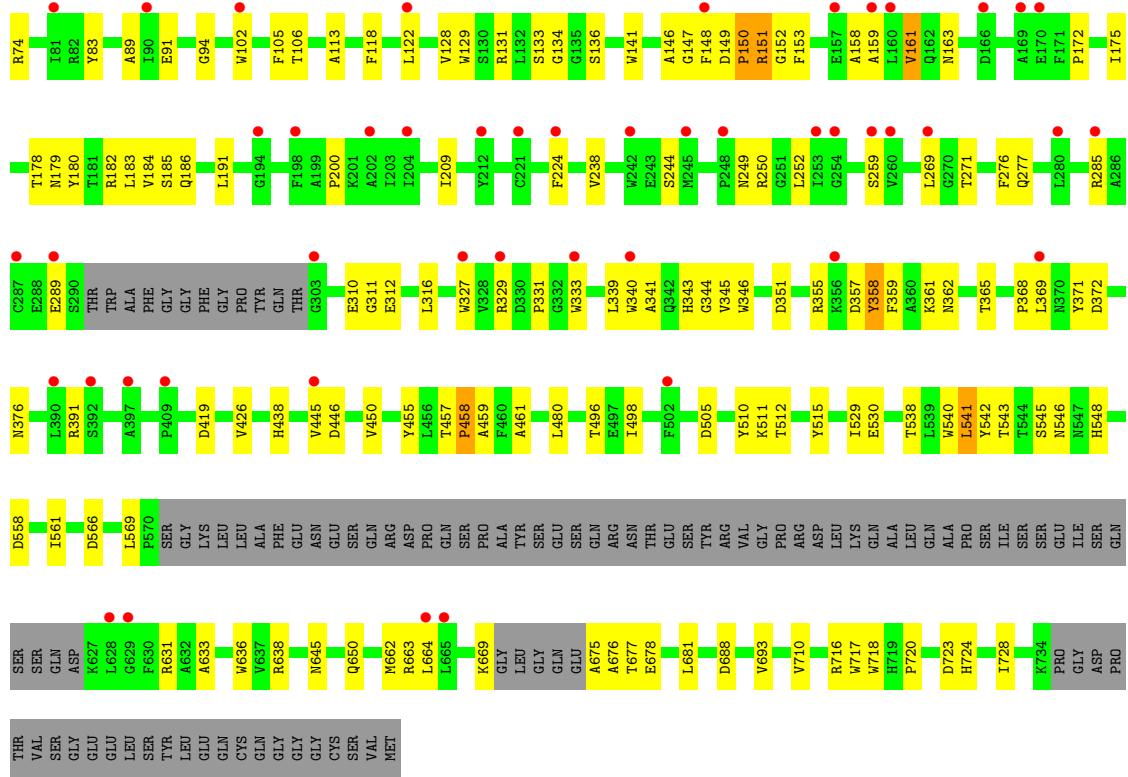
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

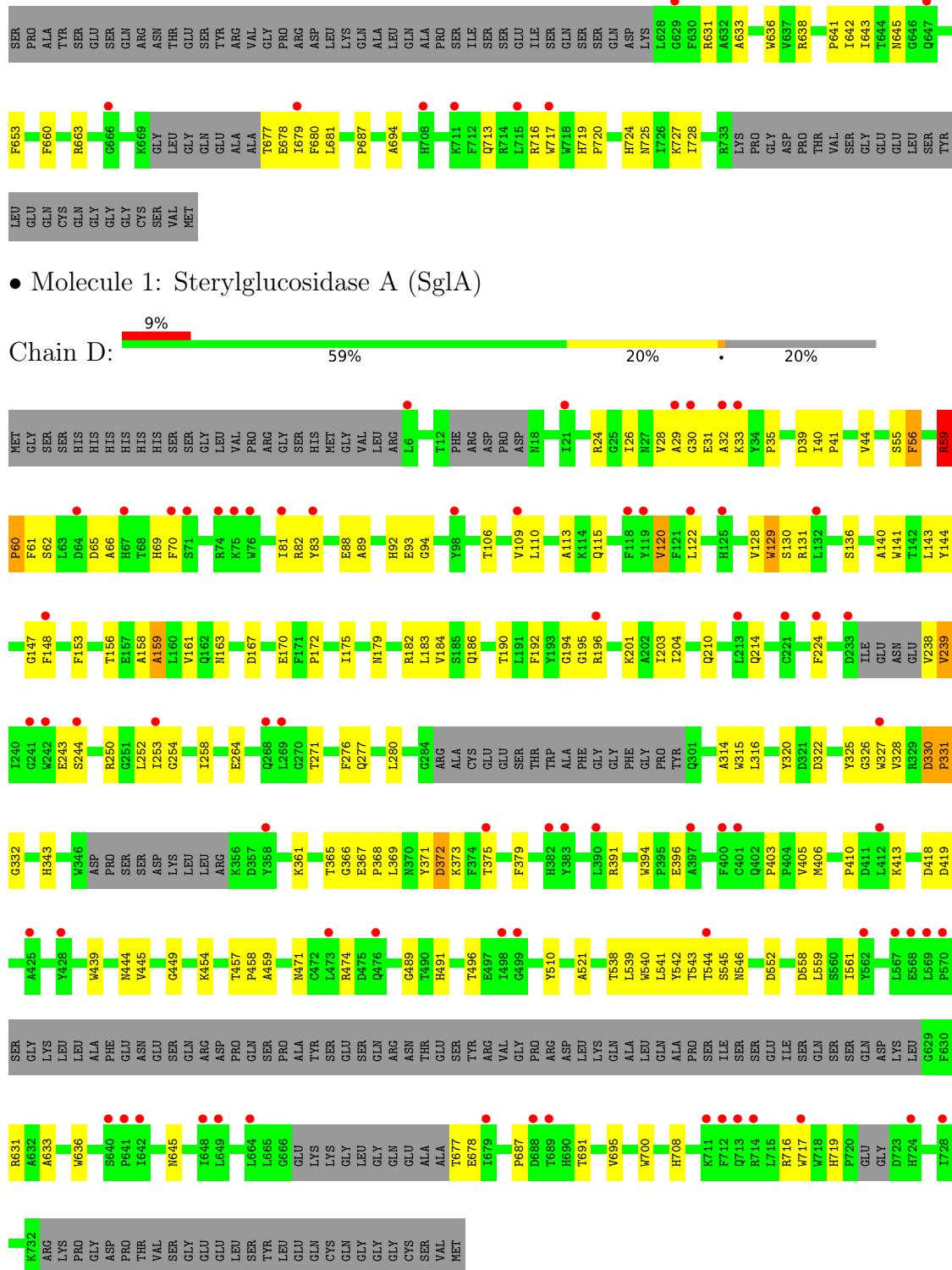
- Molecule 1: Sterylglucosidase A (SgLA)



- Molecule 1: Sterylglucosidase A (SgLA)







4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.73Å 112.79Å 139.10Å 90.00° 102.30° 90.00°	Depositor
Resolution (Å)	58.21 – 3.80 76.95 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (58.21-3.80) 99.2 (76.95-3.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	1.42 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R , R_{free}	0.279 , 0.324 0.285 , 0.306	Depositor DCC
R_{free} test set	2000 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	134.4	Xtriage
Anisotropy	0.554	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 136.1	EDS
L-test for twinning ²	$< L > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	21118	wwPDB-VP
Average B, all atoms (Å ²)	177.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $< |L| >$, $< L^2 >$ 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	0.25	0/5596	0.45	0/7613
1	B	0.24	0/5501	0.44	1/7481 (0.0%)
1	C	0.26	0/5472	0.45	1/7443 (0.0%)
1	D	0.28	0/5201	0.45	0/7076
All	All	0.26	0/21770	0.45	2/29613 (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	A	0	3
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	6

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	541	LEU	CA-CB-CG	5.20	127.25	115.30
1	C	541	LEU	CA-CB-CG	5.07	126.96	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	293	ALA	Peptide
1	A	301	GLN	Peptide
1	A	540	TRP	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	59	ARG	Peptide
1	C	59	ARG	Peptide
1	D	59	ARG	Peptide

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	5426	0	5152	123	0
1	B	5338	0	5080	114	0
1	C	5309	0	5041	126	0
1	D	5045	0	4778	120	0
All	All	21118	0	20051	483	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 (483) 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:192:PHE:CZ	1:D:214:GLN:HG2	1.97	0.99
1:B:30:GLY:H	1:B:541:LEU:HD21	1.38	0.88
1:A:291:THR:H	1:A:302:THR:HG21	1.41	0.86
1:B:329:ARG:HD3	1:B:333:TRP:HD1	1.45	0.80
1:A:645:ASN:H	1:A:677:THR:HG22	1.49	0.78
1:D:330:ASP:HB2	1:D:331:PRO:HD2	1.65	0.78
1:D:93:GLU:O	1:D:325:TYR:OH	2.01	0.77
1:D:700:TRP:HB3	1:D:717:TRP:HD1	1.50	0.77
1:C:645:ASN:H	1:C:677:THR:HG22	1.51	0.76
1:A:258:ILE:HB	1:A:275:ALA:HB3	1.68	0.76
1:C:678:GLU:HG2	1:C:716:ARG:HG2	1.66	0.75
1:A:317:PRO:HG2	1:A:320:TYR:HB2	1.68	0.75
1:B:362:ASN:HD21	1:B:365:THR:HG22	1.51	0.74
1:C:329:ARG:HD3	1:C:333:TRP:HD1	1.52	0.74
1:A:322:ASP:O	1:A:327:TRP:NE1	2.21	0.74
1:D:190:THR:O	1:D:194:GLY:HA3	1.86	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:GLY:H	1:A:210:GLN:HB2	1.54	0.72
1:C:158:ALA:HA	1:C:183:LEU:HB3	1.71	0.71
1:C:91:GLU:O	1:C:141:TRP:NE1	2.19	0.71
1:A:329:ARG:HD3	1:A:333:TRP:HD1	1.54	0.71
1:B:150:PRO:O	1:B:152:GLY:N	2.24	0.71
1:D:32:ALA:HA	1:D:59:ARG:HG3	1.73	0.70
1:C:543:THR:HB	1:C:546:ASN:HB2	1.74	0.69
1:A:323:THR:HG22	1:A:323:THR:O	1.93	0.69
1:A:159:ALA:HB2	1:A:184:VAL:HG21	1.72	0.69
1:C:146:ALA:HB2	1:C:333:TRP:HZ2	1.57	0.69
1:A:642:ILE:HG22	1:A:643:ILE:HG13	1.74	0.69
1:D:192:PHE:CZ	1:D:214:GLN:CG	2.75	0.69
1:C:543:THR:HG22	1:C:545:SER:H	1.58	0.69
1:A:322:ASP:O	1:A:324:ARG:N	2.25	0.68
1:B:543:THR:HG22	1:B:545:SER:H	1.59	0.68
1:B:148:PHE:HA	1:B:316:LEU:H	1.58	0.68
1:C:24:ARG:NH2	1:C:636:TRP:O	2.26	0.68
1:C:38:PRO:HD2	1:C:54:VAL:HG13	1.77	0.67
1:D:110:LEU:HB3	1:D:238:VAL:HG11	1.74	0.67
1:C:36:LYS:HD3	1:C:59:ARG:HG3	1.77	0.67
1:D:543:THR:HB	1:D:546:ASN:HB2	1.77	0.67
1:B:31:GLU:OE1	1:B:59:ARG:NH1	2.28	0.66
1:C:54:VAL:HG12	1:C:55:SER:H	1.59	0.66
1:D:24:ARG:NH2	1:D:636:TRP:O	2.29	0.66
1:D:543:THR:HG22	1:D:545:SER:H	1.60	0.66
1:A:107:ILE:HA	1:A:110:LEU:HD12	1.78	0.65
1:A:52:ASP:OD1	1:A:325:TYR:OH	2.14	0.65
1:A:288:GLU:HG2	1:A:304:ARG:HE	1.62	0.65
1:B:645:ASN:H	1:B:677:THR:HG22	1.62	0.64
1:A:197:ASP:HB3	1:A:363:PRO:HG3	1.79	0.64
1:D:372:ASP:OD1	1:D:373:LYS:N	2.31	0.64
1:B:446:ASP:HB3	1:B:455:TYR:HE2	1.63	0.64
1:C:95:PRO:HG3	1:C:327:TRP:HE3	1.63	0.64
1:C:11:GLN:O	1:C:535:ASN:ND2	2.29	0.63
1:C:175:ILE:HG12	1:C:175:ILE:O	1.98	0.63
1:C:540:TRP:CE2	1:C:541:LEU:HD12	2.33	0.63
1:A:11:GLN:O	1:A:535:ASN:ND2	2.27	0.63
1:C:42:SER:O	1:C:163:ASN:ND2	2.30	0.63
1:B:30:GLY:N	1:B:541:LEU:HD21	2.12	0.63
1:B:357:ASP:OD1	1:B:358:TYR:N	2.31	0.63
1:B:693:VAL:HG13	1:B:728:ILE:HG12	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:511:LYS:HG3	1:B:512:THR:HG23	1.81	0.62
1:D:31:GLU:HB3	1:D:59:ARG:HH11	1.64	0.62
1:A:299:PRO:HB3	1:A:302:THR:HB	1.80	0.62
1:C:162:GLN:O	1:C:171:PHE:CZ	2.52	0.62
1:D:158:ALA:HB1	1:D:183:LEU:HB3	1.80	0.62
1:D:330:ASP:O	1:D:332:GLY:N	2.29	0.62
1:B:158:ALA:HB1	1:B:184:VAL:HG13	1.82	0.62
1:B:128:VAL:HG11	1:B:179:ASN:HB2	1.82	0.61
1:B:329:ARG:HD3	1:B:333:TRP:CD1	2.30	0.61
1:C:54:VAL:O	1:C:92:HIS:NE2	2.31	0.61
1:D:238:VAL:HG12	1:D:239:VAL:HG23	1.81	0.61
1:A:24:ARG:NH2	1:A:636:TRP:O	2.33	0.61
1:C:280:LEU:HD22	1:C:285:ARG:HB2	1.80	0.61
1:B:541:LEU:HD23	1:B:542:TYR:N	2.16	0.61
1:C:159:ALA:HB2	1:C:184:VAL:HG21	1.82	0.61
1:B:662:MET:HE3	1:B:664:LEU:HD23	1.82	0.60
1:D:143:LEU:HB3	1:D:148:PHE:CD2	2.35	0.60
1:B:372:ASP:O	1:B:376:ASN:ND2	2.34	0.60
1:B:19:ARG:NH1	1:B:676:ALA:O	2.33	0.60
1:C:642:ILE:HG22	1:C:643:ILE:HG13	1.83	0.60
1:D:254:GLY:HA2	1:D:369:LEU:HG	1.82	0.60
1:A:182:ARG:NH2	1:A:271:THR:O	2.35	0.60
1:B:678:GLU:HG2	1:B:716:ARG:HG2	1.84	0.59
1:C:541:LEU:HD23	1:C:542:TYR:N	2.17	0.59
1:B:540:TRP:CE2	1:B:541:LEU:HD12	2.37	0.59
1:A:36:LYS:HD3	1:A:59:ARG:HD3	1.83	0.59
1:B:548:HIS:NE2	1:B:566:ASP:OD1	2.32	0.59
1:B:161:VAL:HG12	1:B:163:ASN:H	1.68	0.59
1:A:36:LYS:HB2	1:A:59:ARG:HG2	1.84	0.59
1:A:329:ARG:HD3	1:A:333:TRP:CD1	2.35	0.59
1:A:401:CYS:N	1:A:423:VAL:O	2.35	0.58
1:A:158:ALA:HB1	1:A:184:VAL:HG13	1.85	0.58
1:D:322:ASP:HB3	1:D:327:TRP:CZ3	2.38	0.58
1:D:148:PHE:CZ	1:D:184:VAL:HB	2.39	0.58
1:B:69:HIS:ND1	1:B:542:TYR:OH	2.36	0.58
1:A:457:THR:O	1:A:459:ALA:N	2.37	0.58
1:C:353:LEU:HD23	1:C:356:LYS:HB3	1.86	0.58
1:B:113:ALA:HB1	1:B:118:PHE:HD2	1.68	0.57
1:A:148:PHE:HA	1:A:316:LEU:N	2.19	0.57
1:D:391:ARG:NH2	1:D:419:ASP:OD2	2.29	0.57
1:D:700:TRP:HB3	1:D:717:TRP:CD1	2.36	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:LEU:HD13	1:C:7:ARG:HG3	1.86	0.57
1:C:329:ARG:HD3	1:C:333:TRP:CD1	2.36	0.57
1:D:182:ARG:NH2	1:D:271:THR:O	2.37	0.57
1:D:33:LYS:HB3	1:D:136:SER:HB3	1.87	0.57
1:B:61:PHE:HE2	1:B:66:ALA:HA	1.70	0.56
1:B:249:ASN:OD1	1:B:250:ARG:N	2.33	0.56
1:D:30:GLY:HA3	1:D:541:LEU:HD21	1.86	0.56
1:A:128:VAL:HG11	1:A:179:ASN:HB2	1.86	0.56
1:D:190:THR:HG23	1:D:253:ILE:HG13	1.87	0.56
1:D:201:LYS:HG2	1:D:332:GLY:HA2	1.87	0.56
1:A:92:HIS:HE1	1:A:99:ASP:HB2	1.71	0.56
1:D:94:GLY:HA3	1:D:325:TYR:CZ	2.41	0.56
1:D:277:GLN:HA	1:D:280:LEU:HD12	1.87	0.56
1:A:334:LYS:HE3	1:A:342:GLN:HB2	1.87	0.56
1:A:441:ARG:NH2	1:A:520:SER:OG	2.38	0.56
1:B:496:THR:O	1:B:538:THR:OG1	2.25	0.55
1:B:147:GLY:HA2	1:B:316:LEU:HD12	1.88	0.55
1:B:250:ARG:HD2	1:B:371:TYR:HE2	1.71	0.55
1:A:103:ILE:O	1:A:107:ILE:HG12	2.06	0.55
1:C:200:PRO:HD2	1:C:343:HIS:CD2	2.42	0.55
1:C:49:PHE:HZ	1:C:163:ASN:HB3	1.70	0.55
1:B:61:PHE:CE2	1:B:66:ALA:HA	2.42	0.55
1:C:131:ARG:HB3	1:C:136:SER:HA	1.88	0.55
1:A:463:LYS:HD2	1:A:472:CYS:HB2	1.89	0.55
1:A:537:PHE:HE2	1:A:539:LEU:HG	1.71	0.55
1:A:15:ASP:HB2	1:A:16:PRO:HD2	1.88	0.54
1:C:157:GLU:O	1:C:159:ALA:N	2.39	0.54
1:A:662:MET:HE3	1:A:664:LEU:HD23	1.90	0.54
1:B:362:ASN:HB3	1:B:369:LEU:HD21	1.90	0.54
1:B:645:ASN:N	1:B:677:THR:HG22	2.21	0.54
1:D:365:THR:OG1	1:D:366:GLY:N	2.40	0.54
1:C:346:TRP:CZ3	1:C:348:PRO:HA	2.42	0.54
1:D:55:SER:OG	1:D:92:HIS:NE2	2.40	0.54
1:B:333:TRP:CZ3	1:B:339:LEU:HD13	2.43	0.53
1:C:14:ARG:NH1	1:C:18:ASN:O	2.37	0.53
1:B:681:LEU:HD21	1:B:728:ILE:HG21	1.89	0.53
1:D:140:ALA:HB1	1:D:144:TYR:HE2	1.73	0.53
1:A:111:ARG:HG3	1:A:114:LYS:HE3	1.91	0.53
1:D:322:ASP:HB3	1:D:327:TRP:HZ3	1.73	0.53
1:D:546:ASN:ND2	1:D:552:ASP:OD1	2.41	0.53
1:A:186:GLN:HB3	1:A:252:LEU:HG	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ARG:NH2	1:A:419:ASP:OD2	2.37	0.53
1:B:200:PRO:HD2	1:B:343:HIS:CD2	2.43	0.53
1:C:523:ASP:OD1	1:C:638:ARG:NH1	2.34	0.53
1:A:200:PRO:HD2	1:A:343:HIS:CD2	2.44	0.53
1:A:228:ILE:HG22	1:A:235:GLU:HG3	1.91	0.53
1:A:274:THR:H	1:A:277:GLN:HB2	1.74	0.53
1:B:310:GLU:O	1:B:312:GLU:N	2.41	0.53
1:D:83:TYR:HB3	1:D:122:LEU:HD23	1.91	0.53
1:B:391:ARG:NH2	1:B:419:ASP:OD2	2.28	0.53
1:C:41:PRO:HB3	1:C:553:ASN:HB3	1.91	0.52
1:A:162:GLN:OE1	1:A:555:ASN:HA	2.09	0.52
1:A:148:PHE:HA	1:A:316:LEU:H	1.74	0.52
1:B:28:VAL:HG13	1:B:29:ALA:HB2	1.92	0.52
1:C:162:GLN:O	1:C:171:PHE:HZ	1.92	0.52
1:C:174:MET:HB2	1:C:176:TRP:NE1	2.23	0.52
1:C:510:TYR:OH	1:C:558:ASP:OD2	2.19	0.52
1:A:148:PHE:CD1	1:A:153:PHE:HZ	2.28	0.52
1:B:457:THR:O	1:B:459:ALA:N	2.41	0.52
1:C:339:LEU:HD11	1:C:343:HIS:CE1	2.45	0.52
1:A:294:PHE:CD1	1:A:297:PHE:HB3	2.45	0.52
1:A:645:ASN:ND2	1:A:675:ALA:O	2.42	0.52
1:B:60:PRO:HD2	1:B:105:PHE:HE2	1.75	0.52
1:C:83:TYR:HB3	1:C:122:LEU:HD23	1.91	0.52
1:B:83:TYR:HB3	1:B:122:LEU:HD23	1.92	0.52
1:C:128:VAL:HG11	1:C:179:ASN:HB2	1.91	0.52
1:C:202:ALA:HA	1:C:333:TRP:CE3	2.44	0.52
1:B:344:GLY:O	1:B:355:ARG:HG3	2.10	0.52
1:A:198:PHE:HE2	1:A:253:ILE:HA	1.75	0.51
1:B:106:THR:HG21	1:B:224:PHE:HZ	1.75	0.51
1:D:192:PHE:CD2	1:D:192:PHE:C	2.84	0.51
1:A:132:LEU:HD13	1:A:150:PRO:HG3	1.91	0.51
1:B:498:ILE:HD13	1:B:529:ILE:HD11	1.93	0.51
1:C:157:GLU:HG3	1:C:281:THR:HG21	1.92	0.51
1:A:11:GLN:HG3	1:A:490:THR:HG23	1.92	0.51
1:D:61:PHE:CD1	1:D:66:ALA:HA	2.46	0.51
1:A:178:THR:HG22	1:A:267:LEU:HD21	1.93	0.51
1:B:28:VAL:HG22	1:B:542:TYR:HB3	1.93	0.51
1:B:60:PRO:HD2	1:B:105:PHE:CE2	2.46	0.51
1:D:128:VAL:HG11	1:D:179:ASN:HB2	1.92	0.51
1:C:43:TYR:HE1	1:C:164:THR:HA	1.76	0.51
1:C:88:GLU:HG3	1:C:139:PRO:HA	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:642:ILE:HD11	1:C:680:PHE:HB2	1.93	0.51
1:A:226:GLN:HA	1:A:393:VAL:HG11	1.93	0.51
1:C:28:VAL:HG13	1:C:29:ALA:HB2	1.92	0.51
1:C:540:TRP:CZ2	1:C:541:LEU:HD12	2.46	0.51
1:C:694:ALA:HB3	1:C:727:LYS:HB3	1.93	0.51
1:A:205:ASP:H	1:A:328:VAL:HG23	1.76	0.50
1:B:146:ALA:HB3	1:B:148:PHE:HE2	1.75	0.50
1:C:449:GLY:HA2	1:C:454:LYS:HD3	1.92	0.50
1:D:540:TRP:CE2	1:D:541:LEU:HD12	2.46	0.50
1:D:633:ALA:HA	1:D:636:TRP:CE2	2.46	0.50
1:A:678:GLU:HG2	1:A:716:ARG:HG2	1.93	0.50
1:B:14:ARG:NH1	1:B:18:ASN:O	2.41	0.50
1:C:384:ARG:NE	1:C:417:ASP:OD2	2.41	0.50
1:B:134:GLY:N	1:B:161:VAL:HG22	2.26	0.50
1:D:62:SER:OG	1:D:65:ASP:OD2	2.29	0.50
1:A:61:PHE:HD2	1:A:544:THR:HG21	1.75	0.50
1:A:662:MET:HE2	1:A:679:ILE:HD11	1.93	0.50
1:A:113:ALA:HB1	1:A:118:PHE:HD2	1.77	0.50
1:C:268:GLN:O	1:C:292:TRP:NE1	2.40	0.50
1:B:141:TRP:HB2	1:B:327:TRP:HZ2	1.77	0.50
1:B:510:TYR:OH	1:B:558:ASP:OD2	2.28	0.50
1:A:543:THR:HB	1:A:546:ASN:HB2	1.93	0.50
1:B:677:THR:OG1	1:B:717:TRP:HB3	2.12	0.50
1:B:543:THR:HB	1:B:546:ASN:HB2	1.94	0.50
1:D:147:GLY:HA2	1:D:316:LEU:HD12	1.94	0.50
1:C:156:THR:HG22	1:C:309:PRO:HB3	1.94	0.49
1:D:88:GLU:OE2	1:D:131:ARG:NE	2.44	0.49
1:B:645:ASN:ND2	1:B:675:ALA:O	2.45	0.49
1:C:174:MET:HB2	1:C:176:TRP:CD1	2.48	0.49
1:A:165:PHE:HD1	1:A:166:ASP:H	1.60	0.49
1:C:173:LYS:HE2	1:C:437:LYS:HD2	1.93	0.49
1:C:256:GLN:NE2	1:C:369:LEU:O	2.46	0.49
1:D:61:PHE:CZ	1:D:109:VAL:HG13	2.48	0.49
1:B:24:ARG:NH2	1:B:636:TRP:O	2.46	0.49
1:B:141:TRP:HB2	1:B:327:TRP:CZ2	2.47	0.49
1:D:510:TYR:OH	1:D:558:ASP:OD2	2.22	0.49
1:D:541:LEU:HD23	1:D:542:TYR:N	2.26	0.49
1:B:131:ARG:HB3	1:B:136:SER:HA	1.94	0.49
1:C:202:ALA:O	1:C:209:ILE:N	2.46	0.49
1:C:633:ALA:HA	1:C:636:TRP:CE2	2.47	0.49
1:D:129:TRP:CD1	1:D:143:LEU:HD21	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:SER:HB3	1:D:143:LEU:HD11	1.95	0.49
1:D:143:LEU:HD22	1:D:148:PHE:CE2	2.47	0.49
1:D:558:ASP:OD1	1:D:631:ARG:NH2	2.46	0.49
1:B:179:ASN:HA	1:B:182:ARG:HB2	1.94	0.49
1:B:271:THR:HB	1:B:289:GLU:OE1	2.12	0.49
1:D:65:ASP:HB3	1:D:69:HIS:CE1	2.47	0.49
1:D:115:GLN:HB3	1:D:708:HIS:NE2	2.28	0.49
1:A:633:ALA:HA	1:A:636:TRP:CE2	2.48	0.49
1:C:160:LEU:CD2	1:C:175:ILE:HD13	2.43	0.49
1:B:277:GLN:HE22	1:B:289:GLU:HA	1.77	0.49
1:C:36:LYS:HG3	1:C:37:LYS:HG3	1.94	0.49
1:C:141:TRP:HA	1:C:144:TYR:CE1	2.48	0.48
1:C:276:PHE:CG	1:C:353:LEU:HD11	2.48	0.48
1:A:51:ALA:O	1:A:53:ASN:N	2.46	0.48
1:A:238:VAL:HG13	1:A:239:VAL:HG23	1.95	0.48
1:C:49:PHE:CZ	1:C:163:ASN:HB3	2.49	0.48
1:C:172:PRO:O	1:C:172:PRO:HG2	2.12	0.48
1:A:88:GLU:OE2	1:A:131:ARG:NE	2.42	0.48
1:B:333:TRP:HZ3	1:B:339:LEU:HD13	1.78	0.48
1:C:546:ASN:ND2	1:C:552:ASP:OD1	2.47	0.48
1:D:444:ASN:OD1	1:D:445:VAL:N	2.42	0.48
1:C:103:ILE:O	1:C:107:ILE:HG12	2.12	0.48
1:D:394:TRP:HE1	1:D:396:GLU:HB2	1.79	0.48
1:A:31:GLU:OE2	1:A:545:SER:N	2.46	0.48
1:B:285:ARG:NH2	1:B:351:ASP:OD2	2.45	0.48
1:C:95:PRO:HG3	1:C:327:TRP:CE3	2.45	0.48
1:C:339:LEU:HD11	1:C:343:HIS:HE1	1.78	0.48
1:A:258:ILE:HG21	1:A:359:PHE:HD2	1.79	0.48
1:C:243:GLU:HA	1:C:400:PHE:HB2	1.94	0.48
1:A:723:ASP:O	1:A:724:HIS:ND1	2.47	0.48
1:B:633:ALA:HA	1:B:636:TRP:CE2	2.49	0.48
1:C:541:LEU:HD23	1:C:542:TYR:C	2.34	0.48
1:A:292:TRP:C	1:A:299:PRO:HB2	2.34	0.48
1:C:238:VAL:HG13	1:C:239:VAL:HG23	1.96	0.48
1:C:307:VAL:HG12	1:C:309:PRO:HD2	1.96	0.48
1:D:695:VAL:HG21	1:D:717:TRP:HE1	1.78	0.48
1:C:663:ARG:HG3	1:C:725:ASN:HB3	1.96	0.47
1:A:148:PHE:HD1	1:A:153:PHE:HZ	1.61	0.47
1:B:37:LYS:HB2	1:B:55:SER:HB2	1.96	0.47
1:C:285:ARG:NH2	1:C:348:PRO:O	2.46	0.47
1:D:367:GLU:N	1:D:368:PRO:HD2	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:543:THR:HG22	1:D:545:SER:N	2.29	0.47
1:B:561:ILE:HD12	1:B:636:TRP:CZ3	2.49	0.47
1:C:308:ASP:N	1:C:309:PRO:HD2	2.28	0.47
1:D:192:PHE:HE2	1:D:214:GLN:HE21	1.56	0.47
1:A:92:HIS:CE1	1:A:99:ASP:HB2	2.49	0.47
1:B:498:ILE:HG21	1:B:529:ILE:HD11	1.96	0.47
1:B:180:TYR:HA	1:B:185:SER:HB2	1.97	0.47
1:B:530:GLU:OE2	1:B:638:ARG:NE	2.38	0.47
1:C:280:LEU:HD11	1:C:351:ASP:HB3	1.97	0.47
1:C:720:PRO:HG2	1:C:724:HIS:NE2	2.30	0.47
1:D:26:ILE:HA	1:D:539:LEU:H	1.79	0.47
1:D:65:ASP:HB3	1:D:69:HIS:HE1	1.80	0.47
1:D:167:ASP:OD1	1:D:170:GLU:N	2.48	0.47
1:D:678:GLU:HG2	1:D:716:ARG:HG2	1.97	0.47
1:A:143:LEU:O	1:A:147:GLY:N	2.45	0.47
1:D:190:THR:O	1:D:194:GLY:CA	2.60	0.47
1:A:322:ASP:HB3	1:A:327:TRP:CZ2	2.50	0.47
1:B:676:ALA:HB2	1:B:718:TRP:NE1	2.30	0.47
1:A:156:THR:HA	1:A:309:PRO:HG3	1.96	0.47
1:C:391:ARG:NH2	1:C:419:ASP:OD2	2.48	0.47
1:D:375:THR:HA	1:D:379:PHE:HB3	1.97	0.47
1:A:521:ALA:O	1:A:525:ASN:ND2	2.35	0.46
1:A:362:ASN:HB3	1:A:366:GLY:H	1.79	0.46
1:C:277:GLN:HE21	1:C:287:CYS:HB3	1.80	0.46
1:B:693:VAL:HG22	1:B:728:ILE:HG23	1.98	0.46
1:B:723:ASP:O	1:B:724:HIS:ND1	2.48	0.46
1:D:439:TRP:HB2	1:D:521:ALA:HB2	1.98	0.46
1:A:63:LEU:HG	1:A:105:PHE:CE2	2.51	0.46
1:A:391:ARG:NH2	1:A:421:ASN:HB3	2.31	0.46
1:D:94:GLY:HA2	1:D:141:TRP:CD1	2.51	0.46
1:C:291:THR:O	1:C:302:THR:N	2.49	0.46
1:A:6:LEU:HD21	1:A:13:PHE:CD1	2.51	0.46
1:B:650:GLN:HG2	1:B:663:ARG:HB3	1.98	0.46
1:D:31:GLU:HB3	1:D:59:ARG:NH1	2.30	0.46
1:B:445:VAL:HG13	1:B:461:ALA:HB1	1.97	0.46
1:D:59:ARG:HA	1:D:59:ARG:HD3	1.66	0.46
1:D:540:TRP:CZ2	1:D:541:LEU:HD12	2.51	0.46
1:A:362:ASN:HB3	1:A:367:GLU:H	1.81	0.46
1:A:720:PRO:HG2	1:A:724:HIS:NE2	2.31	0.46
1:C:677:THR:OG1	1:C:717:TRP:HB3	2.16	0.46
1:A:91:GLU:O	1:A:141:TRP:NE1	2.45	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:PRO:HG2	1:A:142:THR:HG23	1.98	0.45
1:C:25:GLY:HA3	1:C:80:THR:HB	1.99	0.45
1:D:40:ILE:HA	1:D:44:VAL:HG11	1.98	0.45
1:D:159:ALA:HB2	1:D:184:VAL:HG22	1.98	0.45
1:D:645:ASN:HB3	1:D:719:HIS:NE2	2.31	0.45
1:C:452:ARG:HG3	1:C:479:PHE:CE2	2.50	0.45
1:D:28:VAL:HA	1:D:29:ALA:HA	1.72	0.45
1:A:54:VAL:HG22	1:A:92:HIS:CG	2.52	0.45
1:A:294:PHE:HB3	1:A:297:PHE:O	2.16	0.45
1:C:333:TRP:CZ3	1:C:339:LEU:HD13	2.52	0.45
1:D:645:ASN:H	1:D:677:THR:HG22	1.81	0.45
1:D:687:PRO:O	1:D:691:THR:OG1	2.20	0.45
1:B:340:TRP:HB3	1:B:345:VAL:HG21	1.99	0.45
1:B:541:LEU:HD23	1:B:542:TYR:C	2.37	0.45
1:C:22:THR:HB	1:C:641:PRO:O	2.16	0.45
1:A:540:TRP:CD1	1:A:559:LEU:HD13	2.51	0.45
1:C:85:PHE:HE1	1:C:122:LEU:HB3	1.81	0.45
1:C:160:LEU:HD12	1:C:160:LEU:HA	1.81	0.45
1:A:57:VAL:HG22	1:A:102:TRP:HA	1.99	0.45
1:C:341:ALA:HB1	1:C:348:PRO:HD3	1.99	0.45
1:D:471:ASN:OD1	1:D:474:ARG:NH1	2.50	0.45
1:D:153:PHE:CZ	1:D:184:VAL:HG11	2.52	0.45
1:D:330:ASP:CB	1:D:331:PRO:HD2	2.39	0.45
1:A:63:LEU:HD23	1:A:63:LEU:HA	1.80	0.44
1:B:250:ARG:HD2	1:B:371:TYR:CE2	2.51	0.44
1:B:446:ASP:HB3	1:B:455:TYR:CE2	2.47	0.44
1:A:418:ASP:OD1	1:A:491:HIS:NE2	2.48	0.44
1:B:175:ILE:O	1:B:178:THR:HG22	2.16	0.44
1:C:258:ILE:HG12	1:C:356:LYS:O	2.18	0.44
1:C:333:TRP:CH2	1:C:339:LEU:HD22	2.52	0.44
1:D:250:ARG:HD2	1:D:253:ILE:O	2.17	0.44
1:C:540:TRP:HA	1:C:541:LEU:HA	1.72	0.44
1:A:269:LEU:HA	1:A:292:TRP:O	2.17	0.44
1:A:285:ARG:O	1:A:309:PRO:HD2	2.17	0.44
1:B:15:ASP:HB3	1:B:21:ILE:HD11	1.98	0.44
1:C:15:ASP:HB3	1:C:21:ILE:HD11	2.00	0.44
1:A:561:ILE:HD12	1:A:636:TRP:CZ3	2.52	0.44
1:B:341:ALA:HB2	1:B:346:TRP:NE1	2.32	0.44
1:A:162:GLN:C	1:A:164:THR:H	2.20	0.44
1:A:300:TYR:CG	1:A:300:TYR:O	2.70	0.44
1:D:540:TRP:HA	1:D:541:LEU:HA	1.77	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ILE:HG23	1:A:234:ILE:HG13	2.00	0.44
1:A:327:TRP:HH2	1:A:329:ARG:NH2	2.15	0.44
1:C:191:LEU:HD22	1:C:209:ILE:HG21	2.00	0.44
1:C:443:TYR:HA	1:C:463:LYS:O	2.18	0.44
1:D:148:PHE:CD2	1:D:153:PHE:HZ	2.36	0.44
1:B:153:PHE:HB3	1:B:159:ALA:O	2.17	0.44
1:B:540:TRP:CZ2	1:B:541:LEU:HD12	2.53	0.44
1:C:148:PHE:CE2	1:C:317:PRO:HD3	2.53	0.44
1:D:192:PHE:O	1:D:210:GLN:HG3	2.17	0.44
1:A:143:LEU:HB3	1:A:148:PHE:CE1	2.52	0.43
1:B:150:PRO:HB2	1:B:151:ARG:H	1.58	0.43
1:C:28:VAL:HA	1:C:29:ALA:HA	1.77	0.43
1:D:94:GLY:HA3	1:D:325:TYR:OH	2.18	0.43
1:A:407:GLU:HA	1:A:452:ARG:HH12	1.83	0.43
1:D:147:GLY:O	1:D:315:TRP:HA	2.18	0.43
1:A:284:GLY:HA2	1:A:309:PRO:HB2	2.01	0.43
1:A:243:GLU:HA	1:A:400:PHE:HB2	2.00	0.43
1:A:250:ARG:HD2	1:A:253:ILE:O	2.19	0.43
1:B:128:VAL:O	1:B:133:SER:OG	2.31	0.43
1:B:688:ASP:N	1:B:688:ASP:OD1	2.49	0.43
1:C:146:ALA:HB2	1:C:333:TRP:CZ2	2.45	0.43
1:A:63:LEU:HD22	1:A:112:ILE:HD12	1.99	0.43
1:A:279:MET:SD	1:A:340:TRP:HD1	2.42	0.43
1:B:69:HIS:CG	1:B:542:TYR:HH	2.37	0.43
1:B:186:GLN:HB3	1:B:252:LEU:HG	2.00	0.43
1:D:31:GLU:OE2	1:D:544:THR:OG1	2.21	0.43
1:C:561:ILE:HD12	1:C:636:TRP:CZ3	2.54	0.43
1:A:419:ASP:HB3	1:A:422:MET:HB3	2.01	0.43
1:B:172:PRO:HB2	1:B:175:ILE:HB	2.01	0.43
1:C:403:PRO:HG3	1:C:424:HIS:HE2	1.84	0.43
1:B:89:ALA:HB1	1:B:102:TRP:CE2	2.54	0.43
1:B:541:LEU:HD22	1:B:543:THR:OG1	2.18	0.43
1:C:162:GLN:O	1:C:171:PHE:CE1	2.71	0.43
1:D:264:GLU:HG3	1:D:371:TYR:HE2	1.83	0.43
1:A:69:HIS:CE1	1:A:544:THR:HB	2.53	0.42
1:C:681:LEU:O	1:C:713:GLN:HB3	2.19	0.42
1:D:496:THR:O	1:D:538:THR:OG1	2.31	0.42
1:A:38:PRO:HG2	1:A:40:ILE:HD11	2.00	0.42
1:B:259:SER:HA	1:B:276:PHE:HB2	2.00	0.42
1:D:106:THR:HG21	1:D:224:PHE:HZ	1.83	0.42
1:B:48:PHE:CZ	1:B:161:VAL:HG11	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ARG:HA	1:B:59:ARG:HD3	1.76	0.42
1:D:82:ARG:NE	1:D:243:GLU:OE1	2.46	0.42
1:D:326:GLY:O	1:D:328:VAL:HG23	2.19	0.42
1:A:114:LYS:HG3	1:A:238:VAL:HB	2.01	0.42
1:A:543:THR:HG22	1:A:545:SER:H	1.84	0.42
1:A:274:THR:N	1:A:277:GLN:HB2	2.34	0.42
1:C:49:PHE:HZ	1:C:163:ASN:CB	2.33	0.42
1:D:35:PRO:C	1:D:59:ARG:HH21	2.22	0.42
1:D:186:GLN:HB3	1:D:252:LEU:HG	2.02	0.42
1:D:201:LYS:HB3	1:D:343:HIS:CE1	2.55	0.42
1:C:307:VAL:CG1	1:C:309:PRO:HD2	2.50	0.42
1:C:310:GLU:N	1:C:310:GLU:OE1	2.53	0.42
1:D:28:VAL:HG13	1:D:29:ALA:HB2	2.02	0.42
1:B:515:TYR:CE2	1:B:631:ARG:HA	2.55	0.42
1:A:69:HIS:CE1	1:A:72:ARG:HH12	2.38	0.42
1:B:56:PHE:HD2	1:B:89:ALA:HB2	1.85	0.42
1:C:158:ALA:HB1	1:C:184:VAL:HG13	2.01	0.42
1:A:241:GLY:HA3	1:A:398:ILE:O	2.19	0.42
1:A:380:MET:O	1:A:384:ARG:HG3	2.20	0.42
1:D:41:PRO:O	1:D:163:ASN:ND2	2.48	0.42
1:D:405:VAL:HG12	1:D:406:MET:HG3	2.02	0.42
1:D:449:GLY:O	1:D:454:LYS:N	2.52	0.42
1:A:40:ILE:HG23	1:A:44:VAL:HG13	2.00	0.42
1:B:191:LEU:HD22	1:B:209:ILE:HG21	2.02	0.42
1:C:127:ASP:OD2	1:C:136:SER:OG	2.38	0.42
1:D:56:PHE:CD1	1:D:89:ALA:HA	2.55	0.42
1:D:330:ASP:HB2	1:D:331:PRO:CD	2.43	0.42
1:D:394:TRP:NE1	1:D:396:GLU:HB2	2.34	0.42
1:A:272:SER:HB3	1:A:290:SER:O	2.20	0.41
1:B:146:ALA:HB3	1:B:148:PHE:CE2	2.55	0.41
1:B:540:TRP:HA	1:B:541:LEU:HA	1.78	0.41
1:C:717:TRP:CE2	1:C:719:HIS:HB3	2.55	0.41
1:D:60:PRO:HG2	1:D:109:VAL:HG11	2.01	0.41
1:A:37:LYS:HA	1:A:38:PRO:HA	1.93	0.41
1:B:361:LYS:HA	1:B:368:PRO:HA	2.02	0.41
1:C:275:ALA:O	1:C:276:PHE:HB3	2.19	0.41
1:A:498:ILE:HG21	1:A:529:ILE:HD11	2.02	0.41
1:C:638:ARG:HH21	1:C:653:PHE:HB3	1.84	0.41
1:D:258:ILE:HG13	1:D:276:PHE:HD2	1.84	0.41
1:A:362:ASN:HB3	1:A:366:GLY:N	2.35	0.41
1:A:515:TYR:CE1	1:A:631:ARG:HA	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:ASP:O	1:B:359:PHE:N	2.54	0.41
1:B:438:HIS:ND1	1:B:505:ASP:OD1	2.54	0.41
1:B:543:THR:HG22	1:B:545:SER:N	2.32	0.41
1:D:361:LYS:HG2	1:D:367:GLU:HA	2.03	0.41
1:A:15:ASP:OD1	1:A:19:ARG:N	2.49	0.41
1:C:160:LEU:HD22	1:C:175:ILE:HD13	2.03	0.41
1:C:560:SER:O	1:C:631:ARG:NH2	2.54	0.41
1:D:60:PRO:HB2	1:D:61:PHE:H	1.70	0.41
1:D:161:VAL:HG12	1:D:163:ASN:H	1.85	0.41
1:D:316:LEU:HD13	1:D:320:TYR:CE2	2.55	0.41
1:A:275:ALA:O	1:A:279:MET:HB2	2.21	0.41
1:C:126:GLN:HA	1:C:137:GLY:HA3	2.03	0.41
1:C:172:PRO:O	1:C:174:MET:N	2.53	0.41
1:C:333:TRP:HH2	1:C:339:LEU:HD22	1.84	0.41
1:C:391:ARG:HH22	1:C:419:ASP:CG	2.24	0.41
1:D:561:ILE:HD12	1:D:636:TRP:CZ3	2.56	0.41
1:A:663:ARG:HG3	1:A:725:ASN:HB3	2.02	0.41
1:A:307:VAL:HG12	1:A:309:PRO:HD3	2.03	0.41
1:B:310:GLU:O	1:B:312:GLU:HG2	2.20	0.41
1:C:660:PHE:HE2	1:C:679:ILE:HD13	1.86	0.41
1:D:403:PRO:HB3	1:D:410:PRO:HD3	2.03	0.41
1:A:113:ALA:HB1	1:A:118:PHE:CD2	2.56	0.41
1:B:71:SER:HB2	1:B:710:VAL:HG22	2.03	0.41
1:B:720:PRO:HG2	1:B:724:HIS:NE2	2.35	0.41
1:C:141:TRP:HA	1:C:144:TYR:CD1	2.56	0.41
1:C:148:PHE:HB2	1:C:315:TRP:C	2.42	0.41
1:C:173:LYS:HE2	1:C:437:LYS:CD	2.50	0.41
1:C:681:LEU:HD21	1:C:728:ILE:HG21	2.03	0.41
1:D:81:ILE:HB	1:D:120:VAL:HG22	2.02	0.41
1:A:438:HIS:ND1	1:A:505:ASP:OD1	2.53	0.41
1:B:450:VAL:HG11	1:B:458:PRO:HG3	2.03	0.41
1:B:569:LEU:HD23	1:B:569:LEU:HA	1.94	0.41
1:D:156:THR:HG21	1:D:314:ALA:N	2.36	0.41
1:B:91:GLU:HG2	1:B:94:GLY:O	2.21	0.40
1:B:426:VAL:HG11	1:B:480:LEU:HD13	2.04	0.40
1:B:541:LEU:HD23	1:B:542:TYR:H	1.86	0.40
1:C:224:PHE:HD2	1:C:242:TRP:HH2	1.69	0.40
1:D:194:GLY:CA	1:D:253:ILE:HD11	2.51	0.40
1:D:695:VAL:HG11	1:D:717:TRP:NE1	2.36	0.40
1:A:191:LEU:HD22	1:A:209:ILE:HG21	2.03	0.40
1:C:124:PRO:HG2	1:C:244:SER:O	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:GLN:O	1:D:190:THR:OG1	2.30	0.40
1:D:418:ASP:OD1	1:D:491:HIS:NE2	2.53	0.40
1:D:457:THR:C	1:D:459:ALA:H	2.25	0.40
1:B:74:ARG:HD2	1:B:74:ARG:HA	1.96	0.40
1:D:540:TRP:CD1	1:D:559:LEU:HD13	2.56	0.40
1:A:444:ASN:OD1	1:A:445:VAL:N	2.53	0.40
1:B:669:LYS:HA	1:B:669:LYS:HD2	1.88	0.40
1:C:172:PRO:HG2	1:C:175:ILE:HG22	2.04	0.40
1:C:175:ILE:O	1:C:175:ILE:CG1	2.68	0.40
1:C:276:PHE:HA	1:C:279:MET:HB2	2.03	0.40
1:C:353:LEU:HD23	1:C:356:LYS:CB	2.49	0.40
1:D:413:LYS:HD2	1:D:489:GLY:HA2	2.02	0.40
1:C:160:LEU:HD23	1:C:175:ILE:HD13	2.04	0.40
1:D:26:ILE:HA	1:D:539:LEU:N	2.36	0.40
1:D:70:PHE:HE2	1:D:113:ALA:HB2	1.87	0.40
1:D:172:PRO:HB2	1:D:175:ILE:HB	2.03	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	664/779 (85%)	597 (90%)	47 (7%)	20 (3%)	4 33
1	B	651/779 (84%)	593 (91%)	41 (6%)	17 (3%)	5 36
1	C	643/779 (82%)	588 (91%)	44 (7%)	11 (2%)	9 43
1	D	607/779 (78%)	550 (91%)	41 (7%)	16 (3%)	5 36
All	All	2565/3116 (82%)	2328 (91%)	173 (7%)	64 (2%)	5 36

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	ASP
1	A	149	ASP
1	A	294	PHE
1	A	300	TYR
1	A	323	THR
1	B	51	ALA
1	B	149	ASP
1	B	150	PRO
1	B	151	ARG
1	B	358	TYR
1	C	44	VAL
1	C	173	LYS
1	D	60	PRO
1	D	330	ASP
1	A	244	SER
1	A	541	LEU
1	B	161	VAL
1	D	120	VAL
1	D	195	GLY
1	D	372	ASP
1	A	238	VAL
1	A	285	ARG
1	B	52	ASP
1	B	60	PRO
1	B	244	SER
1	C	50	ASP
1	C	238	VAL
1	D	159	ALA
1	D	196	ARG
1	D	331	PRO
1	A	292	TRP
1	A	301	GLN
1	B	183	LEU
1	C	129	TRP
1	C	158	ALA
1	D	39	ASP
1	D	203	ILE
1	D	244	SER
1	A	129	TRP
1	A	147	GLY
1	A	148	PHE
1	A	159	ALA
1	A	163	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	458	PRO
1	B	129	TRP
1	B	238	VAL
1	B	269	LEU
1	B	311	GLY
1	B	458	PRO
1	C	49	PHE
1	C	244	SER
1	C	687	PRO
1	D	239	VAL
1	A	154	LYS
1	C	60	PRO
1	D	59	ARG
1	D	129	TRP
1	B	59	ARG
1	D	204	ILE
1	A	194	GLY
1	B	331	PRO
1	D	458	PRO
1	C	253	ILE
1	A	60	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	569/661 (86%)	565 (99%)	4 (1%)	84 91
1	B	562/661 (85%)	562 (100%)	0	100 100
1	C	559/661 (85%)	553 (99%)	6 (1%)	73 85
1	D	530/661 (80%)	529 (100%)	1 (0%)	93 97
All	All	2220/2644 (84%)	2209 (100%)	11 (0%)	88 94

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ASP
1	A	165	PHE
1	A	330	ASP
1	A	427	HIS
1	C	61	PHE
1	C	148	PHE
1	C	171	PHE
1	C	172	PRO
1	C	292	TRP
1	C	371	TYR
1	D	56	PHE

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

Mol	Chain	Res	Type
1	A	92	HIS
1	B	362	ASN
1	C	427	HIS
1	C	555	ASN
1	D	402	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 [\(i\)](#)

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	670/779 (86%)	0.41	44 (6%) 18 14	89, 179, 220, 239	0
1	B	659/779 (84%)	0.44	49 (7%) 14 11	86, 179, 223, 238	0
1	C	655/779 (84%)	0.63	90 (13%) 3 3	30, 180, 218, 249	0
1	D	623/779 (79%)	0.51	72 (11%) 4 5	93, 190, 224, 243	0
All	All	2607/3116 (83%)	0.50	255 (9%) 7 7	30, 182, 223, 249	0

All (255) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	629	GLY	7.8
1	B	159	ALA	7.7
1	D	570	PRO	6.9
1	C	350	SER	6.4
1	C	260	VAL	6.3
1	C	279	MET	5.8
1	D	242	TRP	5.8
1	A	45	SER	5.7
1	C	344	GLY	5.6
1	D	33	LYS	5.4
1	A	244	SER	5.0
1	C	198	PHE	4.8
1	B	333	TRP	4.7
1	C	290	SER	4.7
1	A	333	TRP	4.6
1	D	32	ALA	4.5
1	C	264	GLU	4.5
1	D	21	ILE	4.4
1	D	688	ASP	4.4
1	D	71	SER	4.4
1	C	318	ALA	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	253	ILE	4.3
1	C	276	PHE	4.3
1	C	319	ASP	4.3
1	C	380	MET	4.3
1	B	327	TRP	4.2
1	D	233	ASP	4.2
1	D	109	VAL	4.1
1	B	160	LEU	4.1
1	A	33	LYS	4.1
1	C	121	PHE	4.1
1	B	198	PHE	4.1
1	A	268	GLN	4.1
1	A	157	GLU	4.0
1	C	234	ILE	3.9
1	C	242	TRP	3.9
1	C	183	LEU	3.9
1	A	44	VAL	3.8
1	C	340	TRP	3.8
1	D	476	GLN	3.7
1	C	177	SER	3.7
1	C	165	PHE	3.7
1	D	569	LEU	3.7
1	C	187	THR	3.7
1	C	146	ALA	3.7
1	B	204	ILE	3.7
1	A	145	ALA	3.6
1	D	125	HIS	3.6
1	A	132	LEU	3.6
1	C	343	HIS	3.6
1	C	200	PRO	3.6
1	D	568	GLU	3.6
1	A	342	GLN	3.5
1	C	334	LYS	3.5
1	C	666	GLY	3.5
1	A	319	ASP	3.5
1	B	340	TRP	3.5
1	B	289	GLU	3.5
1	C	253	ILE	3.5
1	D	397	ALA	3.4
1	D	641	PRO	3.4
1	D	679	ILE	3.4
1	B	194	GLY	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	146	ALA	3.3
1	A	155	LYS	3.3
1	D	499	GLY	3.3
1	D	401	CYS	3.3
1	D	253	ILE	3.3
1	A	30	GLY	3.2
1	B	170	GLU	3.2
1	C	252	LEU	3.2
1	A	711	LYS	3.2
1	A	733	ARG	3.2
1	C	289	GLU	3.2
1	C	11	GLN	3.1
1	C	283	SER	3.1
1	D	648	ILE	3.1
1	D	70	PHE	3.1
1	C	452	ARG	3.1
1	A	386	TYR	3.1
1	C	495	PHE	3.1
1	D	221	CYS	3.1
1	D	642	ILE	3.1
1	C	116	TYR	3.0
1	B	287	CYS	3.0
1	D	425	ALA	3.0
1	D	717	TRP	3.0
1	A	329	ARG	3.0
1	B	303	GLY	3.0
1	B	221	CYS	3.0
1	D	30	GLY	3.0
1	C	715	LEU	3.0
1	D	75	LYS	3.0
1	D	244	SER	3.0
1	C	286	ALA	2.9
1	C	534	ALA	2.9
1	B	254	GLY	2.9
1	C	498	ILE	2.9
1	C	284	GLY	2.9
1	C	406	MET	2.9
1	A	320	TYR	2.9
1	B	280	LEU	2.9
1	B	664	LEU	2.9
1	C	207	ILE	2.9
1	B	260	VAL	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	83	TYR	2.9
1	D	412	LEU	2.9
1	C	280	LEU	2.9
1	D	122	LEU	2.9
1	C	647	GLN	2.8
1	D	81	ILE	2.8
1	A	13	PHE	2.8
1	A	198	PHE	2.8
1	B	445	VAL	2.8
1	C	351	ASP	2.8
1	D	714	ARG	2.8
1	D	390	LEU	2.8
1	C	47	GLY	2.8
1	C	206	GLY	2.8
1	B	148	PHE	2.8
1	B	392	SER	2.7
1	C	28	VAL	2.7
1	B	369	LEU	2.7
1	C	550	TRP	2.7
1	D	6	LEU	2.7
1	A	221	CYS	2.7
1	D	67	HIS	2.7
1	C	337	GLU	2.7
1	D	713	GLN	2.7
1	D	728	ILE	2.7
1	B	169	ALA	2.6
1	B	329	ARG	2.6
1	B	245	MET	2.6
1	C	404	PRO	2.6
1	C	256	GLN	2.6
1	D	196	ARG	2.6
1	B	390	LEU	2.6
1	A	318	ALA	2.6
1	B	166	ASP	2.6
1	B	67	HIS	2.6
1	A	213	LEU	2.6
1	A	243	GLU	2.5
1	C	330	ASP	2.5
1	C	243	GLU	2.5
1	C	212	TYR	2.5
1	C	193	TYR	2.5
1	C	423	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	74	ARG	2.5
1	C	190	THR	2.5
1	C	96	GLY	2.5
1	C	336	GLY	2.5
1	C	717	TRP	2.5
1	A	90	ILE	2.5
1	B	259	SER	2.5
1	A	336	GLY	2.5
1	A	67	HIS	2.5
1	C	262	PRO	2.4
1	B	157	GLU	2.4
1	A	142	THR	2.4
1	C	454	LYS	2.4
1	D	383	TYR	2.4
1	D	711	LYS	2.4
1	D	148	PHE	2.4
1	D	327	TRP	2.4
1	D	268	GLN	2.4
1	C	259	SER	2.4
1	C	90	ILE	2.4
1	B	628	LEU	2.4
1	A	115	GLN	2.4
1	B	102	TRP	2.4
1	C	711	LYS	2.4
1	D	132	LEU	2.4
1	B	224	PHE	2.4
1	D	118	PHE	2.4
1	C	679	ILE	2.3
1	D	119	TYR	2.4
1	D	724	HIS	2.3
1	A	340	TRP	2.3
1	C	567	LEU	2.3
1	D	382	HIS	2.3
1	D	562	TYR	2.3
1	D	358	TYR	2.3
1	C	201	LYS	2.3
1	C	629	GLY	2.3
1	D	375	THR	2.3
1	D	428	TYR	2.3
1	C	8	VAL	2.3
1	D	64	ASP	2.3
1	D	76	TRP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	205	ASP	2.3
1	C	316	LEU	2.3
1	D	224	PHE	2.2
1	A	343	HIS	2.2
1	C	240	ILE	2.2
1	D	689	THR	2.2
1	C	170	GLU	2.2
1	A	710	VAL	2.2
1	A	691	THR	2.2
1	B	59	ARG	2.2
1	C	708	HIS	2.2
1	D	712	PHE	2.2
1	C	83	TYR	2.2
1	C	132	LEU	2.2
1	C	335	LEU	2.2
1	D	98	TYR	2.2
1	D	241	GLY	2.2
1	C	224	PHE	2.2
1	A	267	LEU	2.2
1	C	196	ARG	2.2
1	D	567	LEU	2.2
1	D	664	LEU	2.2
1	B	502	PHE	2.2
1	B	202	ALA	2.2
1	B	397	ALA	2.2
1	A	290	SER	2.2
1	B	665	LEU	2.1
1	C	320	TYR	2.1
1	D	473	LEU	2.1
1	C	21	ILE	2.1
1	A	303	GLY	2.1
1	C	167	ASP	2.1
1	B	248	PRO	2.1
1	D	29	ALA	2.1
1	C	143	LEU	2.1
1	B	242	TRP	2.1
1	C	244	SER	2.1
1	C	288	GLU	2.1
1	B	212	TYR	2.1
1	D	269	LEU	2.1
1	C	342	GLN	2.1
1	A	173	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	713	GLN	2.1
1	D	640	SER	2.1
1	A	542	TYR	2.1
1	C	70	PHE	2.1
1	D	498	ILE	2.1
1	B	285	ARG	2.1
1	A	192	PHE	2.1
1	C	490	THR	2.1
1	D	649	LEU	2.1
1	C	304	ARG	2.1
1	D	213	LEU	2.1
1	C	261	ILE	2.1
1	B	90	ILE	2.0
1	D	544	THR	2.0
1	B	356	LYS	2.0
1	B	81	ILE	2.0
1	C	13	PHE	2.0
1	B	269	LEU	2.0
1	B	122	LEU	2.0
1	D	400	PHE	2.0
1	C	268	GLN	2.0
1	A	539	LEU	2.0
1	B	409	PRO	2.0
1	A	693	VAL	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 [\(i\)](#)

There are no ligands in this entry.

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.