



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:17 PM UTC

PDB ID : 1XSJ / pdb_00001xsj
Title : Structure of a Family 31 alpha glycosidase
Authors : Lovering, A.L.; Lee, S.S.; Kim, Y.W.; Withers, S.G.; Strynadka, N.C.
Deposited on : 2004-10-19
Resolution : 2.10 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
Mogul : 2022.3.0, CSD as543be (2022)
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

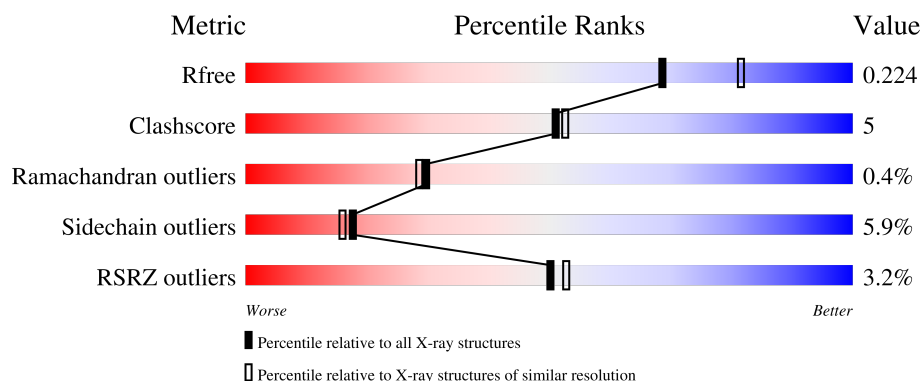
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	778	% 86% 11% ..
1	B	778	3% 83% 14% ..
1	C	778	3% 84% 13% ..
1	D	778	% 86% 12% ..
1	E	778	4% 84% 12% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	778	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TRS	A	2002	-	X	-	-
2	TRS	A	2008	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 38890 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 Putative family 31 glucosidase yicI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			
1	B	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			
1	C	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			
1	D	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			
1	E	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			
1	F	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			

There are 36 discrepancies between the modelled and reference sequences:

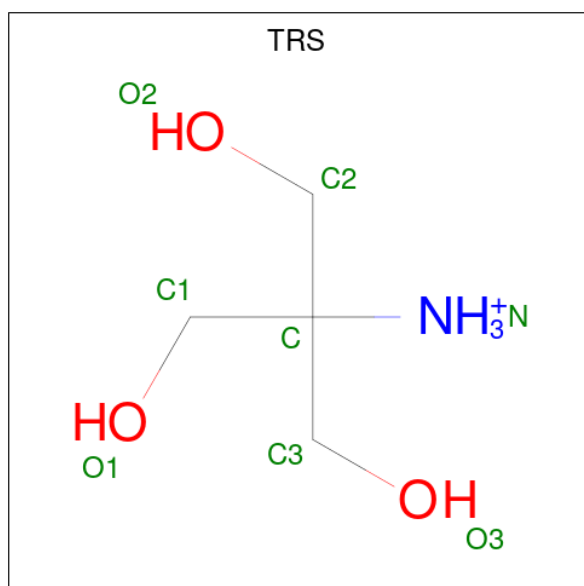
Chain	Residue	Modelled	Actual	Comment	Reference
A	773	HIS	-	expression tag	UNP P31434
A	774	HIS	-	expression tag	UNP P31434
A	775	HIS	-	expression tag	UNP P31434
A	776	HIS	-	expression tag	UNP P31434
A	777	HIS	-	expression tag	UNP P31434
A	778	HIS	-	expression tag	UNP P31434
B	773	HIS	-	expression tag	UNP P31434
B	774	HIS	-	expression tag	UNP P31434
B	775	HIS	-	expression tag	UNP P31434
B	776	HIS	-	expression tag	UNP P31434
B	777	HIS	-	expression tag	UNP P31434
B	778	HIS	-	expression tag	UNP P31434
C	773	HIS	-	expression tag	UNP P31434
C	774	HIS	-	expression tag	UNP P31434
C	775	HIS	-	expression tag	UNP P31434
C	776	HIS	-	expression tag	UNP P31434
C	777	HIS	-	expression tag	UNP P31434

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	778	HIS	-	expression tag	UNP P31434
D	773	HIS	-	expression tag	UNP P31434
D	774	HIS	-	expression tag	UNP P31434
D	775	HIS	-	expression tag	UNP P31434
D	776	HIS	-	expression tag	UNP P31434
D	777	HIS	-	expression tag	UNP P31434
D	778	HIS	-	expression tag	UNP P31434
E	773	HIS	-	expression tag	UNP P31434
E	774	HIS	-	expression tag	UNP P31434
E	775	HIS	-	expression tag	UNP P31434
E	776	HIS	-	expression tag	UNP P31434
E	777	HIS	-	expression tag	UNP P31434
E	778	HIS	-	expression tag	UNP P31434
F	773	HIS	-	expression tag	UNP P31434
F	774	HIS	-	expression tag	UNP P31434
F	775	HIS	-	expression tag	UNP P31434
F	776	HIS	-	expression tag	UNP P31434
F	777	HIS	-	expression tag	UNP P31434
F	778	HIS	-	expression tag	UNP P31434

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	4	1	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	4	1	3		
2	A	1	Total	C	N	O	0	0
			8	4	1	3		
2	B	1	Total	C	N	O	0	0
			8	4	1	3		
2	B	1	Total	C	N	O	0	0
			8	4	1	3		
2	C	1	Total	C	N	O	0	0
			8	4	1	3		
2	C	1	Total	C	N	O	0	0
			8	4	1	3		
2	D	1	Total	C	N	O	0	0
			8	4	1	3		
2	E	1	Total	C	N	O	0	0
			8	4	1	3		
2	E	1	Total	C	N	O	0	0
			8	4	1	3		
2	E	1	Total	C	N	O	0	0
			8	4	1	3		
2	F	1	Total	C	N	O	0	0
			8	4	1	3		

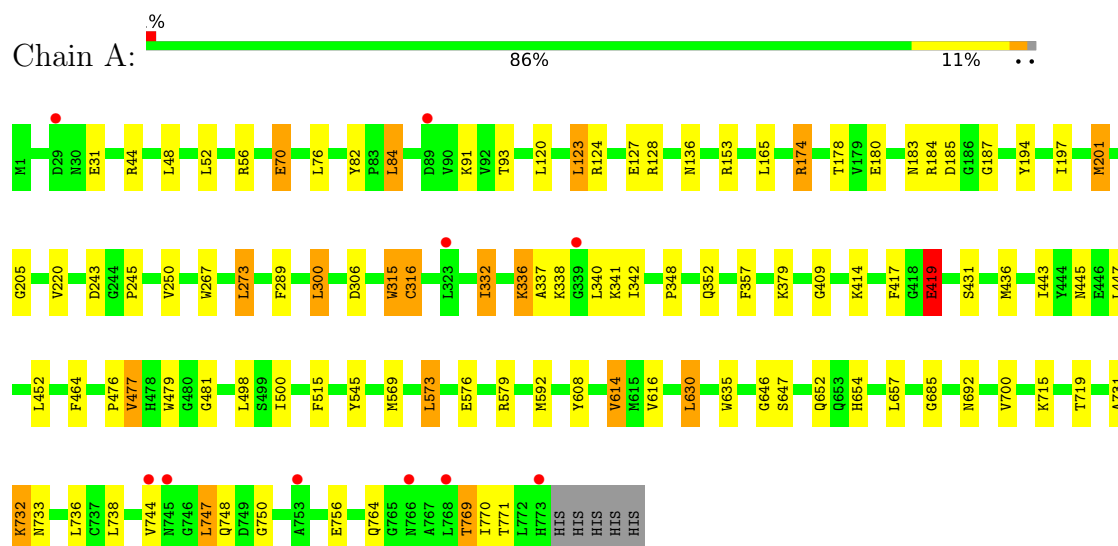
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	295	Total	O	0	0
			295	295		
3	B	208	Total	O	0	0
			208	208		
3	C	234	Total	O	0	0
			234	234		
3	D	267	Total	O	0	0
			267	267		
3	E	243	Total	O	0	0
			243	243		
3	F	191	Total	O	0	0
			191	191		

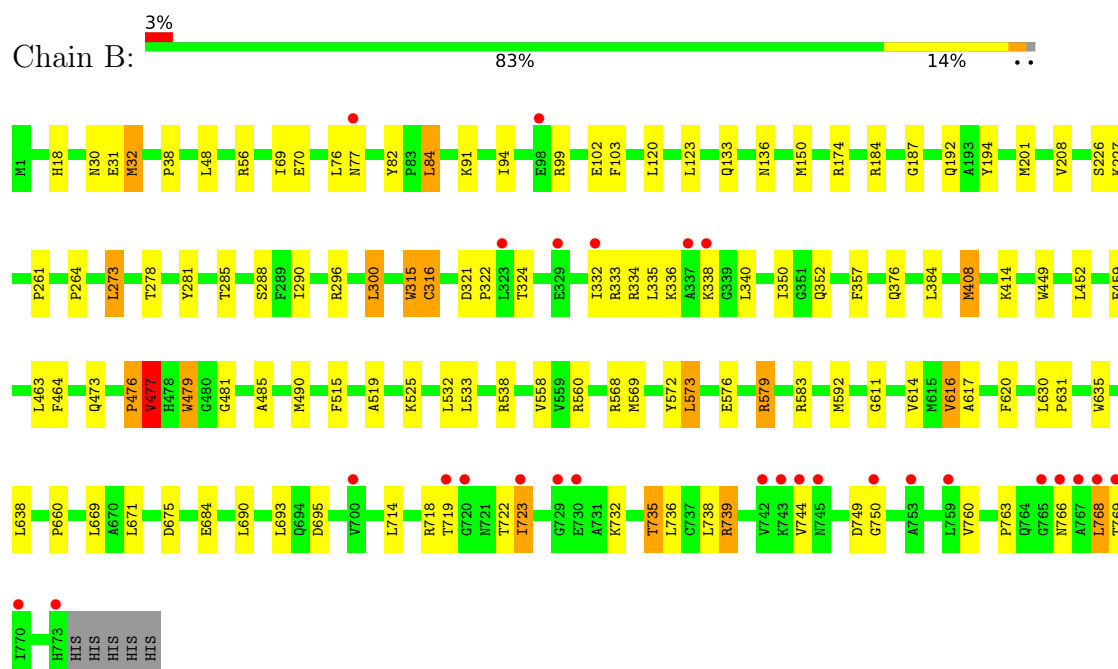
3 Residue-property plots

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.

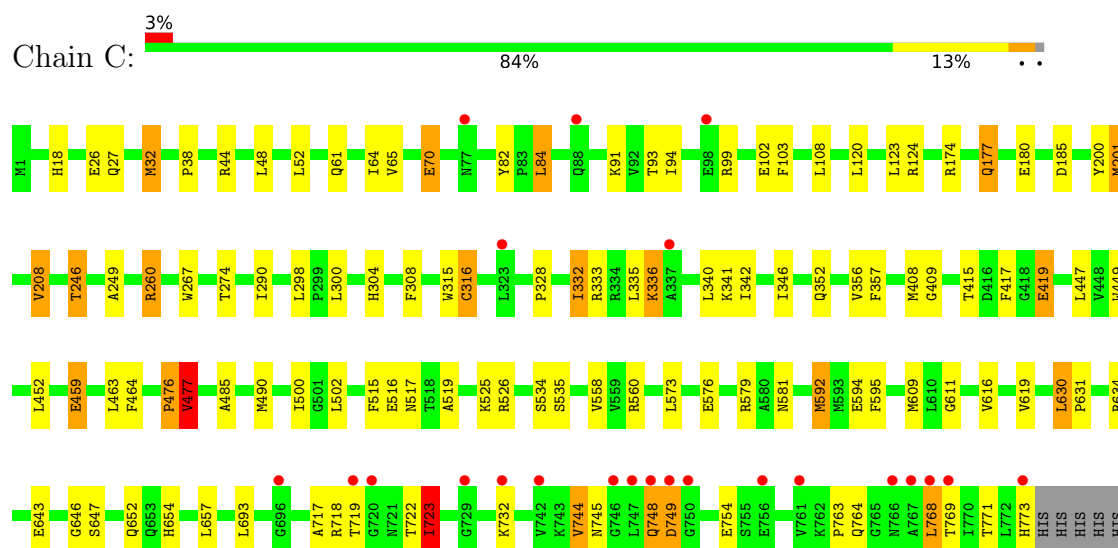
• Molecule 1: Putative family 31 glucosidase yicI



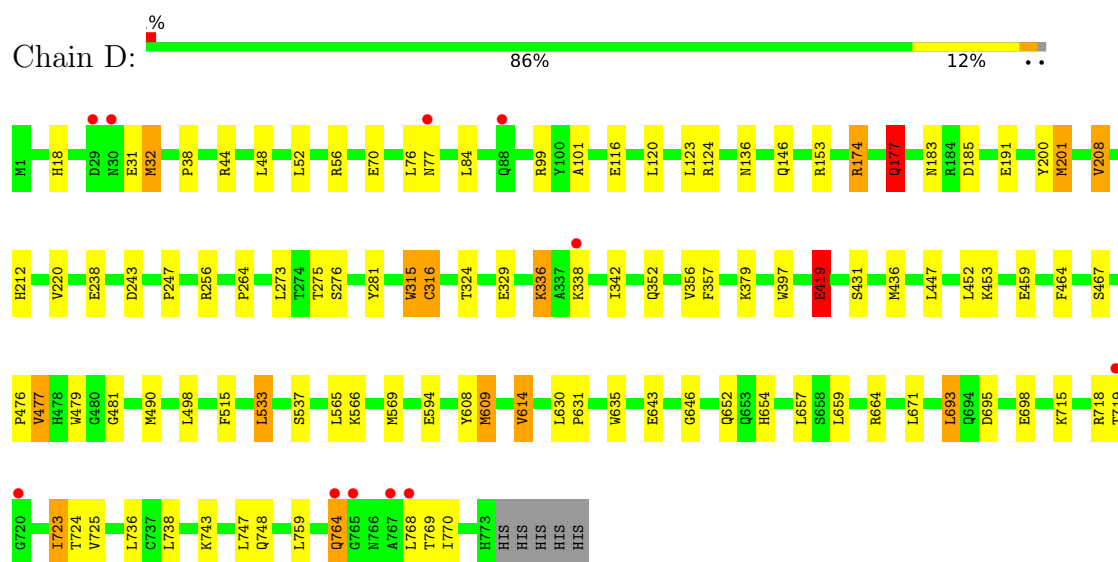
• Molecule 1: Putative family 31 glucosidase yicI



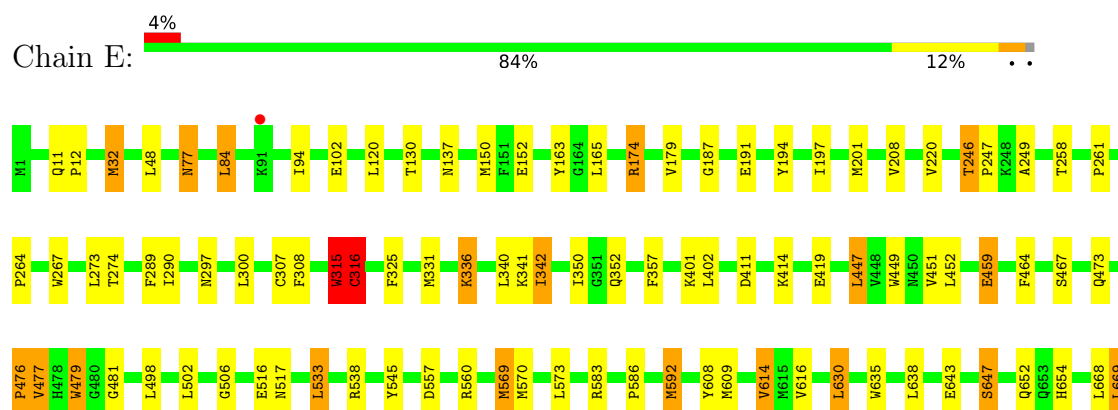
• Molecule 1: Putative family 31 glucosidase yicI

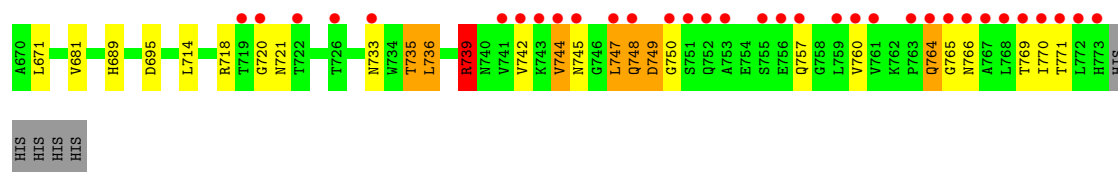


• Molecule 1: Putative family 31 glucosidase yicI

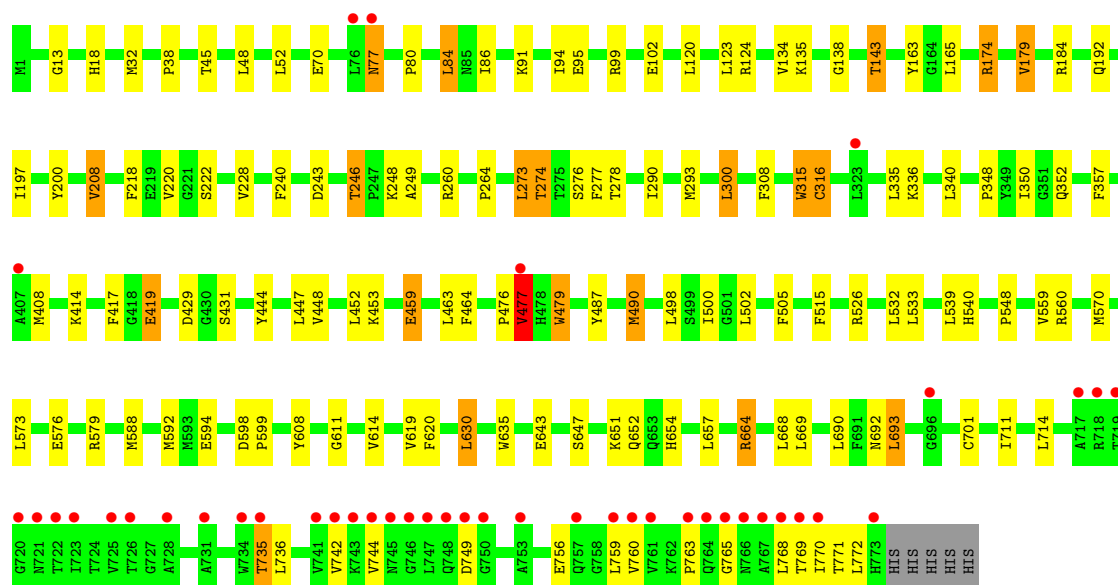
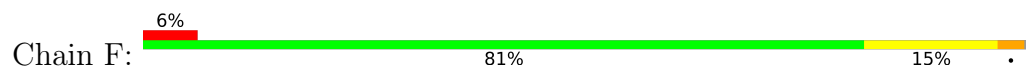


• Molecule 1: Putative family 31 glucosidase yicI





- Molecule 1: Putative family 31 glucosidase yicI



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.53Å 224.44Å 154.12Å 90.00° 101.75° 90.00°	Depositor
Resolution (Å)	29.98 – 2.10 29.98 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.2 (29.98-2.10) 93.0 (29.98-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.90 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.180 , 0.220 0.187 , 0.224	Depositor DCC
R_{free} test set	16704 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.5	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	0.95	EDS
Total number of atoms	38890	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TRS

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	0.92	1/6409 (0.0%)	1.03	15/8711 (0.2%)
1	B	0.87	5/6409 (0.1%)	1.00	13/8711 (0.1%)
1	C	0.88	5/6409 (0.1%)	1.01	9/8711 (0.1%)
1	D	0.94	7/6409 (0.1%)	1.06	18/8711 (0.2%)
1	E	0.93	6/6409 (0.1%)	1.04	15/8711 (0.2%)
1	F	0.86	2/6409 (0.0%)	1.02	17/8711 (0.2%)
All	All	0.90	26/38454 (0.1%)	1.03	87/52266 (0.2%)

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	1
1	B	0	1
1	C	1	0
1	D	0	1
1	E	0	1
1	F	1	0
All	All	2	4

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	32	MET	SD-CE	-11.62	1.50	1.79
1	B	201	MET	SD-CE	-9.55	1.55	1.79
1	C	32	MET	SD-CE	-9.38	1.56	1.79
1	A	201	MET	SD-CE	-9.25	1.56	1.79
1	C	490	MET	SD-CE	-8.19	1.59	1.79
1	E	150	MET	SD-CE	-7.75	1.60	1.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	201	MET	SD-CE	-6.89	1.62	1.79
1	D	32	MET	SD-CE	-6.67	1.62	1.79
1	D	477	VAL	N-CA	-6.31	1.38	1.46
1	C	316	CYS	CA-C	-6.28	1.45	1.53
1	D	609	MET	SD-CE	6.07	1.94	1.79
1	F	490	MET	SD-CE	-6.04	1.64	1.79
1	B	32	MET	SD-CE	-6.03	1.64	1.79
1	E	609	MET	SD-CE	5.97	1.94	1.79
1	B	264	PRO	CA-C	5.38	1.55	1.52
1	B	150	MET	SD-CE	-5.26	1.66	1.79
1	C	201	MET	SD-CE	-5.20	1.66	1.79
1	D	77	ASN	CA-C	5.18	1.59	1.52
1	E	130	THR	CA-CB	5.17	1.60	1.53
1	C	723	ILE	CA-CB	5.15	1.60	1.54
1	F	77	ASN	CA-C	5.09	1.59	1.52
1	D	490	MET	SD-CE	-5.09	1.66	1.79
1	E	569	MET	SD-CE	-5.07	1.66	1.79
1	D	614	VAL	CA-CB	5.06	1.60	1.54
1	B	77	ASN	CA-C	5.04	1.59	1.53
1	E	477	VAL	N-CA	-5.04	1.40	1.46

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	316	CYS	N-CA-C	11.41	126.82	111.30
1	E	476	PRO	CA-C-N	10.65	141.14	121.97
1	E	476	PRO	C-N-CA	10.65	141.14	121.97
1	D	315	TRP	CA-C-N	10.47	137.22	122.46
1	D	315	TRP	C-N-CA	10.47	137.22	122.46
1	A	316	CYS	N-CA-C	10.36	125.39	111.30
1	F	315	TRP	CA-C-N	10.06	136.38	122.19
1	F	315	TRP	C-N-CA	10.06	136.38	122.19
1	C	315	TRP	CA-C-N	10.02	137.09	122.36
1	C	315	TRP	C-N-CA	10.02	137.09	122.36
1	F	316	CYS	N-CA-C	9.88	125.07	111.74
1	D	476	PRO	CA-C-N	9.69	139.41	121.97
1	D	476	PRO	C-N-CA	9.69	139.41	121.97
1	E	477	VAL	CB-CA-C	9.03	126.10	111.29
1	A	315	TRP	CA-C-N	8.96	135.09	122.46
1	A	315	TRP	C-N-CA	8.96	135.09	122.46
1	B	316	CYS	N-CA-C	8.75	129.44	110.80
1	A	476	PRO	CA-C-N	8.64	137.52	121.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	476	PRO	C-N-CA	8.64	137.52	121.97
1	B	315	TRP	CA-C-N	8.39	137.56	121.54
1	B	315	TRP	C-N-CA	8.39	137.56	121.54
1	B	476	PRO	CA-C-N	8.31	136.93	121.97
1	B	476	PRO	C-N-CA	8.31	136.93	121.97
1	C	476	PRO	CA-C-N	8.22	136.77	121.97
1	C	476	PRO	C-N-CA	8.22	136.77	121.97
1	F	476	PRO	N-CA-C	8.19	123.04	111.33
1	E	316	CYS	N-CA-C	8.00	127.84	110.80
1	C	316	CYS	N-CA-C	7.84	122.78	111.56
1	A	76	LEU	N-CA-C	7.39	119.03	110.97
1	A	477	VAL	CB-CA-C	7.17	123.06	111.29
1	D	419	GLU	CA-CB-CG	7.14	128.39	114.10
1	E	614	VAL	N-CA-C	7.14	118.10	108.11
1	B	477	VAL	CB-CA-C	7.13	122.99	111.29
1	D	477	VAL	CB-CA-C	7.00	122.77	111.29
1	F	264	PRO	O-C-N	6.71	124.30	121.15
1	C	316	CYS	CB-CA-C	6.55	120.20	111.82
1	E	476	PRO	O-C-N	6.52	130.95	122.86
1	F	476	PRO	CA-C-N	6.51	133.68	121.97
1	F	476	PRO	C-N-CA	6.51	133.68	121.97
1	A	419	GLU	N-CA-C	6.48	121.46	112.45
1	F	315	TRP	O-C-N	6.38	130.86	122.95
1	D	476	PRO	O-C-N	6.34	130.74	123.00
1	C	315	TRP	O-C-N	6.33	130.80	122.95
1	D	659	LEU	N-CA-C	-6.10	102.73	108.22
1	F	315	TRP	N-CA-C	6.04	119.10	110.10
1	E	315	TRP	CA-C-N	5.96	132.92	121.54
1	E	315	TRP	C-N-CA	5.96	132.92	121.54
1	D	664	ARG	N-CA-CB	-5.92	101.34	110.04
1	C	476	PRO	O-C-N	5.90	130.17	122.86
1	A	419	GLU	CA-CB-CG	5.89	125.88	114.10
1	A	476	PRO	O-C-N	5.88	130.57	122.64
1	A	614	VAL	N-CA-C	5.86	116.32	108.11
1	D	614	VAL	N-CA-C	5.79	116.21	108.11
1	B	476	PRO	O-C-N	5.72	129.95	122.86
1	F	477	VAL	CB-CA-C	5.58	120.45	111.29
1	D	70	GLU	N-CA-C	5.57	118.31	109.50
1	D	315	TRP	O-C-N	5.57	129.72	122.87
1	A	315	TRP	O-C-N	5.55	129.64	122.81
1	B	315	TRP	O-C-N	5.55	129.41	122.86
1	D	419	GLU	CB-CG-CD	5.48	121.92	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	76	LEU	N-CA-C	5.46	117.67	111.11
1	F	570	MET	N-CA-C	5.42	120.86	113.16
1	E	307	CYS	N-CA-C	5.38	117.84	111.33
1	E	264	PRO	O-C-N	5.36	123.67	121.15
1	F	70	GLU	N-CA-C	5.30	117.44	109.23
1	C	477	VAL	CB-CA-C	5.29	119.97	111.29
1	E	739	ARG	CG-CD-NE	-5.29	100.35	112.00
1	E	342	ILE	N-CA-C	5.29	115.52	108.11
1	F	264	PRO	CA-C-O	-5.29	116.55	120.73
1	A	337	ALA	N-CA-C	-5.28	105.60	111.36
1	D	256	ARG	N-CA-C	-5.24	105.57	111.28
1	E	476	PRO	CA-C-O	5.23	129.68	122.31
1	E	721	ASN	N-CA-C	-5.19	105.29	113.02
1	B	476	PRO	N-CA-C	5.18	118.48	111.22
1	F	138	GLY	N-CA-C	5.18	117.01	110.38
1	E	570	MET	N-CA-C	5.15	120.61	113.45
1	D	264	PRO	O-C-N	5.13	123.56	121.15
1	F	476	PRO	CA-C-O	5.12	129.69	122.31
1	B	750	GLY	N-CA-C	5.10	118.03	110.42
1	B	350	ILE	CA-C-N	5.08	125.17	120.34
1	B	350	ILE	C-N-CA	5.08	125.17	120.34
1	A	70	GLU	N-CA-C	5.06	117.67	109.06
1	A	445	ASN	N-CA-C	5.05	117.44	111.33
1	F	316	CYS	CB-CA-C	5.04	118.89	111.73
1	D	177	GLN	N-CA-C	5.02	117.93	109.95
1	B	616	VAL	N-CA-C	5.01	115.80	108.53
1	F	316	CYS	CA-CB-SG	-5.01	102.88	114.40

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	316	CYS	CA
1	F	316	CYS	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	315	TRP	Peptide
1	B	315	TRP	Peptide
1	D	315	TRP	Peptide
1	E	315	TRP	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	6226	0	5934	56	0
1	B	6226	0	5934	67	0
1	C	6226	0	5934	66	0
1	D	6226	0	5934	57	0
1	E	6226	0	5934	64	0
1	F	6226	0	5934	73	0
2	A	24	0	36	3	0
2	B	16	0	24	1	0
2	C	16	0	24	2	0
2	D	8	0	12	1	0
2	E	24	0	36	0	0
2	F	8	0	12	1	0
3	A	295	0	0	3	0
3	B	208	0	0	2	0
3	C	234	0	0	2	0
3	D	267	0	0	4	0
3	E	243	0	0	2	0
3	F	191	0	0	1	0
All	All	38890	0	35748	378	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 5.

All (378) 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:F:274:THR:HG22	1:F:276:SER:H	1.08	1.11
1:B:32:MET:HE2	1:B:94:ILE:HG23	1.28	1.10
1:F:274:THR:HG21	1:F:540:HIS:ND1	1.67	1.06
1:E:668:LEU:HD21	1:E:714:LEU:HD12	1.33	1.06
1:F:32:MET:HE2	1:F:94:ILE:HG23	1.08	1.05
1:F:32:MET:CE	1:F:94:ILE:HG23	1.99	0.92
1:E:669:LEU:HD23	1:E:671:LEU:HD11	1.56	0.86
1:D:212:HIS:HE1	1:D:238:GLU:H	1.21	0.86
1:B:579:ARG:HH11	1:B:579:ARG:HB2	1.41	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:MET:HE2	1:C:94:ILE:HG23	1.57	0.84
1:E:32:MET:HE3	1:E:94:ILE:HG23	1.58	0.82
1:F:274:THR:CG2	1:F:276:SER:H	1.91	0.82
1:D:657:LEU:HD21	3:D:2206:HOH:O	1.79	0.81
1:B:300:LEU:HD13	1:B:340:LEU:HD21	1.62	0.81
1:A:300:LEU:HD13	1:A:340:LEU:HD21	1.62	0.81
1:D:695:ASP:OD1	1:D:719:THR:O	1.99	0.81
1:B:332:ILE:HD13	1:B:408:MET:O	1.81	0.80
1:D:723:ILE:HG23	1:D:770:ILE:HB	1.64	0.79
1:C:32:MET:HE3	1:C:103:PHE:HB2	1.63	0.79
1:B:332:ILE:CD1	1:B:408:MET:O	2.31	0.78
1:C:246:THR:HG22	1:C:249:ALA:H	1.47	0.78
1:B:525:LYS:HG2	1:B:558:VAL:HG21	1.66	0.78
1:D:212:HIS:CE1	1:D:238:GLU:H	2.02	0.78
1:F:274:THR:HG22	1:F:276:SER:N	1.92	0.77
1:D:764:GLN:HA	1:D:764:GLN:HE21	1.49	0.77
1:C:525:LYS:HG2	1:C:558:VAL:HG21	1.65	0.77
1:C:332:ILE:HD11	1:C:409:GLY:HA3	1.66	0.76
1:E:638:LEU:O	1:E:739:ARG:NH2	2.18	0.76
1:F:32:MET:HE1	1:F:102:GLU:O	1.86	0.76
1:F:668:LEU:HD21	1:F:714:LEU:HD22	1.67	0.75
1:F:273:LEU:HB2	1:F:300:LEU:HD21	1.69	0.75
1:E:201:MET:HE1	1:E:247:PRO:HB3	1.68	0.74
1:B:300:LEU:CD1	1:B:340:LEU:HD21	2.16	0.74
1:C:32:MET:HE1	1:C:102:GLU:C	2.13	0.73
1:A:332:ILE:HD11	1:A:409:GLY:HA3	1.69	0.73
1:D:723:ILE:HD13	1:D:723:ILE:C	2.13	0.73
1:F:13:GLY:O	1:F:143:THR:HB	1.88	0.72
1:D:32:MET:CE	1:D:101:ALA:HB1	2.20	0.72
1:B:695:ASP:HA	1:B:718:ARG:HG2	1.72	0.71
1:F:290:ILE:HD13	1:F:340:LEU:HD11	1.71	0.71
1:D:565:LEU:HG	1:D:569:MET:HE2	1.72	0.70
1:C:764:GLN:HA	1:C:764:GLN:HE21	1.56	0.69
1:F:548:PRO:HG3	1:F:559:VAL:HG21	1.73	0.69
1:D:32:MET:HE2	1:D:101:ALA:HB1	1.75	0.69
1:F:668:LEU:CD2	1:F:714:LEU:HD22	2.21	0.69
1:B:290:ILE:CD1	1:B:335:LEU:HD22	2.22	0.68
1:B:32:MET:HE1	1:B:102:GLU:O	1.94	0.67
1:A:744:VAL:HG21	1:A:770:ILE:HG23	1.76	0.67
1:D:201:MET:HE1	1:D:247:PRO:HA	1.74	0.67
1:C:174:ARG:O	1:C:177:GLN:HG3	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ASN:ND2	3:B:2201:HOH:O	2.19	0.65
1:F:124:ARG:NH2	1:F:243:ASP:OD1	2.29	0.65
1:E:750:GLY:HA2	1:E:764:GLN:HG2	1.78	0.65
1:F:32:MET:HE1	1:F:102:GLU:C	2.21	0.65
1:D:657:LEU:N	1:D:657:LEU:HD22	2.13	0.64
1:A:744:VAL:HG22	1:A:771:THR:O	1.97	0.64
1:C:459:GLU:CD	1:C:459:GLU:H	2.03	0.64
1:E:744:VAL:HG22	1:E:771:THR:O	1.98	0.64
1:F:560:ARG:HG3	1:F:560:ARG:HH11	1.63	0.64
1:B:32:MET:HE1	1:B:102:GLU:C	2.23	0.64
1:C:185:ASP:OD2	2:C:2006:TRS:H31	1.98	0.64
1:D:124:ARG:NH2	1:D:243:ASP:OD1	2.28	0.63
1:D:723:ILE:CG2	1:D:770:ILE:HB	2.29	0.63
1:E:668:LEU:HD21	1:E:714:LEU:CD1	2.19	0.63
1:D:764:GLN:HA	1:D:764:GLN:NE2	2.12	0.63
1:F:290:ILE:HD13	1:F:340:LEU:CD1	2.27	0.63
1:B:459:GLU:CD	1:B:459:GLU:H	2.07	0.62
1:B:579:ARG:HB2	1:B:579:ARG:NH1	2.14	0.62
1:E:174:ARG:HB3	1:E:220:VAL:HG11	1.80	0.62
1:E:459:GLU:CD	1:E:459:GLU:H	2.07	0.61
1:B:463:LEU:O	1:B:477:VAL:HB	2.00	0.60
1:D:693:LEU:HD13	1:D:718:ARG:HB2	1.82	0.60
1:C:341:LYS:C	1:C:342:ILE:HD12	2.26	0.59
1:E:630:LEU:O	1:E:647:SER:N	2.35	0.59
1:C:70:GLU:HG3	3:C:2154:HOH:O	2.02	0.59
1:B:638:LEU:O	1:B:739:ARG:NH2	2.36	0.58
1:D:352:GLN:HA	1:D:357:PHE:CD2	2.38	0.58
1:A:576:GLU:OE2	1:A:579:ARG:NH1	2.36	0.58
1:E:735:THR:HG23	1:E:760:VAL:HG13	1.86	0.58
1:E:246:THR:HG22	1:E:249:ALA:H	1.69	0.58
1:F:744:VAL:HG22	1:F:771:THR:O	2.04	0.57
1:C:763:PRO:CB	1:C:768:LEU:HD21	2.35	0.57
1:D:533:LEU:CD1	1:D:569:MET:HE1	2.35	0.56
1:E:671:LEU:N	1:E:671:LEU:HD12	2.20	0.56
1:F:417:PHE:HA	1:F:419:GLU:OE2	2.06	0.56
1:B:31:GLU:OE1	1:B:56:ARG:HD3	2.05	0.56
1:A:124:ARG:HD3	1:A:243:ASP:OD1	2.05	0.56
1:E:289:PHE:HZ	1:E:545:TYR:CD1	2.24	0.56
1:F:744:VAL:HG21	1:F:770:ILE:HG23	1.88	0.56
1:A:174:ARG:HB3	1:A:220:VAL:HG11	1.88	0.56
1:B:579:ARG:HH11	1:B:579:ARG:CB	2.18	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:PHE:HA	1:C:419:GLU:OE2	2.06	0.55
1:F:220:VAL:HG13	1:F:228:VAL:HG22	1.88	0.55
1:F:293:MET:HE2	1:F:300:LEU:HD23	1.88	0.55
1:A:652:GLN:NE2	1:A:654:HIS:NE2	2.55	0.55
1:C:342:ILE:HD12	1:C:342:ILE:N	2.22	0.55
1:A:352:GLN:HA	1:A:357:PHE:CD2	2.42	0.55
1:C:447:LEU:C	1:C:447:LEU:HD23	2.32	0.54
1:A:123:LEU:HD12	1:A:128:ARG:HA	1.87	0.54
1:B:763:PRO:HB3	1:B:768:LEU:HD21	1.89	0.54
1:C:32:MET:HE1	1:C:102:GLU:O	2.07	0.54
1:C:336:LYS:HE2	1:C:342:ILE:HD13	1.89	0.54
2:A:2008:TRS:H32	1:D:185:ASP:OD2	2.07	0.54
1:A:750:GLY:HA2	1:A:764:GLN:HG2	1.89	0.54
1:D:336:LYS:HD2	1:D:342:ILE:HD13	1.90	0.53
1:C:576:GLU:HG3	1:C:611:GLY:HA3	1.91	0.53
1:C:764:GLN:HA	1:C:764:GLN:NE2	2.22	0.53
1:A:515:PHE:CZ	2:A:2001:TRS:H22	2.44	0.53
1:B:485:ALA:HB1	1:B:519:ALA:HB2	1.91	0.53
1:E:583:ARG:NH1	3:E:2111:HOH:O	2.42	0.53
1:D:324:THR:HG21	3:D:2074:HOH:O	2.08	0.53
1:E:748:GLN:O	1:E:749:ASP:HB2	2.09	0.53
1:A:165:LEU:HA	1:A:197:ILE:O	2.09	0.53
1:B:560:ARG:HG3	1:B:560:ARG:HH11	1.74	0.53
1:A:336:LYS:HD2	1:A:342:ILE:HD13	1.90	0.52
1:C:260:ARG:HG3	1:C:581:ASN:O	2.09	0.52
1:C:65:VAL:HG12	1:C:108:LEU:HD21	1.90	0.52
1:C:65:VAL:HG12	1:C:108:LEU:CD2	2.40	0.52
1:D:566:LYS:HA	1:D:569:MET:HE3	1.91	0.52
1:A:183:ASN:HB3	1:A:419:GLU:HB3	1.92	0.52
1:C:308:PHE:CZ	1:D:44:ARG:HB3	2.44	0.52
1:E:273:LEU:HD13	1:E:274:THR:N	2.24	0.52
1:F:248:LYS:NZ	1:F:594:GLU:OE1	2.34	0.52
1:D:723:ILE:HD13	1:D:724:THR:N	2.25	0.52
1:C:634:ARG:HD3	1:C:643:GLU:OE2	2.10	0.52
1:F:300:LEU:HD12	1:F:340:LEU:HD21	1.92	0.51
1:F:447:LEU:C	1:F:447:LEU:HD23	2.35	0.51
1:D:183:ASN:HB3	1:D:419:GLU:HB3	1.91	0.51
1:B:572:TYR:CD1	1:B:669:LEU:HD11	2.45	0.51
1:A:185:ASP:OD2	2:A:2002:TRS:H32	2.11	0.51
1:C:298:LEU:CD2	1:C:560:ARG:HB2	2.41	0.51
1:C:328:PRO:O	1:C:332:ILE:HG23	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:201:MET:CE	1:E:247:PRO:HB3	2.38	0.51
1:F:652:GLN:NE2	1:F:654:HIS:NE2	2.58	0.51
1:C:352:GLN:HA	1:C:357:PHE:CD2	2.45	0.51
1:E:695:ASP:HA	1:E:718:ARG:HG2	1.91	0.51
1:F:429:ASP:OD1	1:F:431:SER:OG	2.23	0.51
1:A:31:GLU:OE1	1:A:56:ARG:HD3	2.11	0.51
1:B:187:GLY:HA2	1:B:194:TYR:OH	2.11	0.50
1:E:163:TYR:HB3	1:E:502:LEU:HD13	1.92	0.50
1:F:668:LEU:O	1:F:701:CYS:HB2	2.11	0.50
1:C:32:MET:CE	1:C:103:PHE:HB2	2.39	0.50
1:D:725:VAL:HB	1:D:768:LEU:HB2	1.92	0.50
1:E:289:PHE:CZ	1:E:545:TYR:CD1	3.00	0.50
1:F:515:PHE:CZ	2:F:2011:TRS:H22	2.47	0.50
1:E:592:MET:HE2	1:E:592:MET:O	2.11	0.50
1:B:32:MET:HE3	1:B:103:PHE:HB2	1.94	0.50
1:F:630:LEU:O	1:F:647:SER:N	2.43	0.50
1:E:137:ASN:HB3	1:E:152:GLU:OE1	2.11	0.50
1:B:352:GLN:HA	1:B:357:PHE:CD2	2.47	0.49
1:E:557:ASP:OD1	1:E:560:ARG:NH2	2.45	0.49
1:E:533:LEU:CD1	1:E:569:MET:HE1	2.41	0.49
1:B:70:GLU:HG3	3:B:2120:HOH:O	2.12	0.49
1:B:749:ASP:HB2	1:B:768:LEU:HA	1.94	0.49
1:F:690:LEU:HD21	1:F:693:LEU:HD12	1.94	0.49
1:B:226:SER:O	1:B:227:LYS:HG3	2.13	0.49
1:D:447:LEU:C	1:D:447:LEU:HD23	2.37	0.49
1:E:506:GLY:HA2	1:E:586:PRO:HA	1.94	0.49
1:D:533:LEU:HD12	1:D:569:MET:HE1	1.94	0.49
1:E:449:TRP:CH2	1:E:476:PRO:HD2	2.48	0.49
1:A:201:MET:HE1	1:A:250:VAL:HB	1.94	0.49
1:A:273:LEU:HB2	1:A:300:LEU:HD21	1.95	0.49
1:B:768:LEU:N	1:B:768:LEU:CD1	2.76	0.49
1:D:736:LEU:HD11	1:D:738:LEU:HD23	1.95	0.49
1:E:273:LEU:HD13	1:E:273:LEU:C	2.38	0.49
1:B:479:TRP:CD1	1:B:481:GLY:H	2.31	0.48
1:B:735:THR:HG23	1:B:760:VAL:HG13	1.95	0.48
1:B:490:MET:HE2	1:B:620:PHE:CD1	2.48	0.48
1:F:463:LEU:O	1:F:477:VAL:HB	2.13	0.48
1:C:516:GLU:O	1:C:517:ASN:HB2	2.13	0.48
1:C:718:ARG:HA	1:C:723:ILE:HG22	1.96	0.48
1:B:332:ILE:HD11	1:B:408:MET:O	2.12	0.48
1:A:744:VAL:HG21	1:A:770:ILE:CG2	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:572:TYR:CD1	1:B:669:LEU:CD1	2.97	0.48
1:D:631:PRO:O	1:D:646:GLY:HA3	2.14	0.48
1:B:736:LEU:CD1	1:B:738:LEU:HD21	2.44	0.48
1:C:579:ARG:NH1	1:C:579:ARG:HG3	2.28	0.48
1:C:745:ASN:HB2	1:C:773:HIS:HA	1.96	0.48
1:F:763:PRO:HB2	1:F:765:GLY:O	2.14	0.48
1:A:336:LYS:HD2	1:A:342:ILE:CD1	2.43	0.48
1:C:652:GLN:NE2	1:C:654:HIS:NE2	2.61	0.48
1:D:479:TRP:CD1	1:D:481:GLY:H	2.32	0.48
1:E:747:LEU:HD22	1:E:750:GLY:O	2.14	0.47
1:F:560:ARG:HG3	1:F:560:ARG:NH1	2.29	0.47
1:A:201:MET:HE2	3:A:2235:HOH:O	2.14	0.47
1:E:401:LYS:HE3	3:E:2183:HOH:O	2.14	0.47
1:F:300:LEU:HD12	1:F:340:LEU:CD2	2.44	0.47
1:F:668:LEU:HD23	1:F:701:CYS:HB3	1.96	0.47
1:D:698:GLU:OE1	1:D:715:LYS:HD3	2.14	0.47
1:F:459:GLU:H	1:F:459:GLU:CD	2.21	0.47
1:D:566:LYS:HA	1:D:569:MET:CE	2.44	0.47
1:A:736:LEU:CD1	1:A:738:LEU:CD2	2.93	0.47
1:D:431:SER:HB3	1:D:436:MET:HG2	1.95	0.47
1:A:201:MET:CE	1:A:250:VAL:HB	2.45	0.47
1:A:443:ILE:HD11	3:A:2165:HOH:O	2.14	0.47
1:A:569:MET:HB3	1:A:573:LEU:HD22	1.97	0.47
1:C:346:ILE:HD11	1:C:415:THR:HG22	1.96	0.47
1:B:261:PRO:HA	1:B:473:GLN:O	2.15	0.47
1:F:526:ARG:HD2	1:F:619:VAL:HB	1.97	0.47
1:A:136:ASN:HB3	1:A:153:ARG:HB2	1.97	0.47
1:C:748:GLN:O	1:C:749:ASP:HB2	2.15	0.47
1:D:174:ARG:O	1:D:177:GLN:HG2	2.14	0.47
1:A:736:LEU:HD11	1:A:738:LEU:CD2	2.45	0.46
1:B:414:LYS:HE3	1:B:479:TRP:CH2	2.50	0.46
1:C:763:PRO:HB3	1:C:768:LEU:HD21	1.97	0.46
1:D:356:VAL:HG11	1:D:397:TRP:CZ2	2.50	0.46
1:E:165:LEU:HA	1:E:197:ILE:O	2.15	0.46
1:E:498:LEU:HD21	1:E:608:TYR:HB3	1.97	0.46
1:B:719:THR:HG22	1:B:722:THR:HB	1.97	0.46
1:D:657:LEU:CD2	3:D:2206:HOH:O	2.53	0.46
1:E:246:THR:CG2	1:E:249:ALA:H	2.28	0.46
1:F:200:TYR:CZ	1:F:208:VAL:HG13	2.50	0.46
1:F:246:THR:HG22	1:F:249:ALA:H	1.81	0.46
1:A:736:LEU:CD1	1:A:738:LEU:HD23	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:11:GLN:HA	1:E:12:PRO:HD3	1.81	0.46
1:A:479:TRP:CD1	1:A:481:GLY:H	2.34	0.46
1:C:463:LEU:O	1:C:477:VAL:HB	2.16	0.46
1:F:165:LEU:HA	1:F:197:ILE:O	2.16	0.46
1:B:273:LEU:HB2	1:B:300:LEU:HD21	1.98	0.46
1:C:631:PRO:O	1:C:646:GLY:HA3	2.16	0.46
1:E:336:LYS:HE3	1:E:411:ASP:OD2	2.16	0.46
1:A:332:ILE:HD12	1:A:336:LYS:HD3	1.97	0.46
1:B:568:ARG:CG	1:B:675:ASP:HB3	2.46	0.46
1:C:515:PHE:CZ	2:C:2005:TRS:H22	2.51	0.46
1:F:490:MET:HE3	1:F:620:PHE:CD1	2.51	0.46
1:A:736:LEU:HD13	1:A:736:LEU:C	2.41	0.45
1:D:174:ARG:HB3	1:D:220:VAL:HG11	1.98	0.45
1:A:498:LEU:HD21	1:A:608:TYR:HB3	1.97	0.45
1:C:246:THR:HG23	3:C:2209:HOH:O	2.16	0.45
1:D:723:ILE:C	1:D:723:ILE:CD1	2.84	0.45
1:D:537:SER:HA	3:D:2245:HOH:O	2.16	0.45
1:B:82:TYR:HB3	1:B:84:LEU:HD13	1.98	0.45
1:D:736:LEU:HD13	1:D:736:LEU:C	2.42	0.45
1:B:631:PRO:HD2	1:B:635:TRP:CZ2	2.52	0.45
1:C:44:ARG:HB3	1:E:308:PHE:CZ	2.51	0.45
1:E:652:GLN:NE2	1:E:654:HIS:NE2	2.64	0.45
1:F:290:ILE:HD12	1:F:335:LEU:HD22	1.99	0.45
1:A:44:ARG:HB3	1:F:308:PHE:CZ	2.52	0.45
1:B:414:LYS:NZ	1:B:538:ARG:HH12	2.15	0.45
1:F:18:HIS:O	1:F:38:PRO:HA	2.17	0.45
1:F:735:THR:HG23	1:F:760:VAL:HG13	1.98	0.45
1:A:736:LEU:HD11	1:A:738:LEU:HD23	1.99	0.44
1:B:376:GLN:HA	1:B:384:LEU:O	2.18	0.44
1:F:134:VAL:O	1:F:135:LYS:HB2	2.17	0.44
1:C:290:ILE:CD1	1:C:335:LEU:HD22	2.48	0.44
1:E:325:PHE:CD1	1:E:331:MET:HE1	2.53	0.44
1:A:747:LEU:C	1:A:747:LEU:CD2	2.91	0.44
1:B:576:GLU:HG3	1:B:611:GLY:HA3	1.99	0.44
1:D:515:PHE:CZ	2:D:2007:TRS:H22	2.52	0.44
1:D:736:LEU:CD1	1:D:738:LEU:HD23	2.47	0.44
1:F:487:TYR:HD1	1:F:490:MET:HE2	1.83	0.44
1:F:588:MET:HG3	1:F:608:TYR:CD1	2.51	0.44
1:A:447:LEU:C	1:A:447:LEU:HD23	2.42	0.44
1:B:184:ARG:HD3	1:B:192:GLN:CD	2.43	0.44
1:D:18:HIS:O	1:D:38:PRO:HA	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:414:LYS:HE3	1:F:479:TRP:CH2	2.53	0.44
1:D:201:MET:CE	1:D:247:PRO:HA	2.45	0.44
1:A:187:GLY:HA2	1:A:194:TYR:OH	2.18	0.44
1:D:764:GLN:NE2	1:D:764:GLN:CA	2.80	0.44
1:E:447:LEU:HD23	1:E:447:LEU:C	2.43	0.44
1:B:768:LEU:N	1:B:768:LEU:HD12	2.33	0.44
1:C:526:ARG:HD2	1:C:619:VAL:HB	1.99	0.44
1:E:516:GLU:O	1:E:517:ASN:HB2	2.18	0.44
1:F:444:TYR:O	1:F:448:VAL:HG23	2.18	0.44
1:C:61:GLN:HB2	1:C:64:ILE:HD12	1.99	0.43
1:F:84:LEU:HB3	1:F:86:ILE:HD11	2.00	0.43
1:F:598:ASP:HA	1:F:599:PRO:HD2	1.91	0.43
1:A:431:SER:HB3	1:A:436:MET:HG2	2.00	0.43
1:C:200:TYR:CZ	1:C:208:VAL:HG13	2.53	0.43
1:F:352:GLN:HA	1:F:357:PHE:CD2	2.53	0.43
1:A:205:GLY:HA3	1:A:245:PRO:O	2.17	0.43
1:B:285:THR:O	1:B:288:SER:HB3	2.19	0.43
1:B:690:LEU:O	1:B:739:ARG:HB2	2.17	0.43
1:D:498:LEU:HD21	1:D:608:TYR:HB3	2.01	0.43
1:A:414:LYS:HE3	1:A:479:TRP:CH2	2.53	0.43
1:C:18:HIS:O	1:C:38:PRO:HA	2.18	0.43
1:E:635:TRP:O	1:E:643:GLU:HA	2.19	0.43
1:F:576:GLU:HG3	1:F:611:GLY:HA3	2.00	0.43
1:C:82:TYR:HB3	1:C:84:LEU:HD13	2.00	0.43
1:F:273:LEU:HD22	1:F:274:THR:H	1.81	0.43
1:C:595:PHE:CE1	1:C:631:PRO:HG2	2.52	0.43
1:B:133:GLN:O	1:B:136:ASN:HB2	2.19	0.43
1:E:419:GLU:HG3	1:E:467:SER:HB3	2.00	0.43
1:E:479:TRP:CD1	1:E:481:GLY:H	2.37	0.43
1:E:736:LEU:C	1:E:736:LEU:HD13	2.44	0.43
1:A:646:GLY:O	1:A:647:SER:HB2	2.19	0.43
1:B:296:ARG:O	1:B:560:ARG:NH1	2.37	0.43
1:E:261:PRO:HA	1:E:473:GLN:O	2.18	0.43
1:B:18:HIS:O	1:B:38:PRO:HA	2.19	0.43
1:B:321:ASP:HA	1:B:322:PRO:HD3	1.91	0.43
1:B:768:LEU:CD1	1:B:768:LEU:H	2.31	0.43
1:C:267:TRP:CE3	1:C:341:LYS:HG3	2.54	0.43
1:C:274:THR:HG22	1:C:304:HIS:HB3	2.01	0.43
1:C:630:LEU:O	1:C:647:SER:N	2.51	0.43
1:F:635:TRP:CH2	1:F:664:ARG:HB3	2.54	0.43
1:E:32:MET:HE1	1:E:102:GLU:N	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:ALA:O	1:A:732:LYS:HD2	2.18	0.42
1:F:498:LEU:HD21	1:F:608:TYR:HB3	2.01	0.42
1:C:579:ARG:HG3	1:C:579:ARG:HH11	1.83	0.42
1:E:187:GLY:HA2	1:E:194:TYR:OH	2.19	0.42
1:E:290:ILE:HD13	1:E:340:LEU:CD1	2.48	0.42
1:F:80:PRO:HD3	1:F:431:SER:HB3	2.01	0.42
1:A:267:TRP:CE3	1:A:341:LYS:HG3	2.54	0.42
1:F:184:ARG:HD3	1:F:192:GLN:CD	2.43	0.42
1:C:449:TRP:CH2	1:C:476:PRO:HD2	2.54	0.42
1:D:31:GLU:OE1	1:D:56:ARG:HD3	2.19	0.42
1:F:500:ILE:HG12	1:F:505:PHE:HB2	2.00	0.42
1:C:744:VAL:HG22	1:C:771:THR:O	2.18	0.42
1:D:201:MET:HE3	1:D:201:MET:HB2	1.80	0.42
1:E:246:THR:HG22	1:E:249:ALA:CB	2.50	0.42
1:E:267:TRP:CE3	1:E:341:LYS:HG3	2.54	0.42
1:E:671:LEU:N	1:E:671:LEU:CD1	2.82	0.42
1:A:300:LEU:CD1	1:A:340:LEU:HD21	2.38	0.42
1:B:515:PHE:CZ	2:B:2003:TRS:H22	2.55	0.42
1:D:657:LEU:N	1:D:657:LEU:CD2	2.81	0.42
1:A:289:PHE:HZ	1:A:545:TYR:CD1	2.37	0.42
1:D:635:TRP:O	1:D:643:GLU:HA	2.20	0.42
1:E:297:ASN:O	1:E:560:ARG:CD	2.68	0.42
1:E:669:LEU:HD23	1:E:671:LEU:CD1	2.40	0.42
1:B:332:ILE:HD12	1:B:333:ARG:N	2.35	0.42
1:E:744:VAL:HG21	1:E:770:ILE:CG2	2.49	0.42
1:B:76:LEU:HD23	1:B:76:LEU:HA	1.84	0.42
1:B:572:TYR:CG	1:B:669:LEU:HD11	2.55	0.42
1:F:179:VAL:HG22	1:F:218:PHE:HB2	2.00	0.42
1:B:278:THR:HG21	1:F:45:THR:HA	2.01	0.41
1:C:592:MET:HE2	1:C:592:MET:HB2	1.88	0.41
1:E:77:ASN:O	1:E:77:ASN:ND2	2.50	0.41
1:A:685:GLY:HA2	1:A:733:ASN:O	2.21	0.41
1:A:747:LEU:C	1:A:747:LEU:HD23	2.44	0.41
1:B:525:LYS:CG	1:B:558:VAL:HG21	2.45	0.41
1:C:485:ALA:HB1	1:C:519:ALA:HB2	2.02	0.41
1:F:246:THR:CG2	1:F:249:ALA:H	2.33	0.41
1:B:449:TRP:CH2	1:B:476:PRO:HD2	2.55	0.41
1:C:447:LEU:HD23	1:C:447:LEU:O	2.21	0.41
1:E:315:TRP:O	1:E:350:ILE:HA	2.20	0.41
1:F:274:THR:HB	1:F:539:LEU:O	2.20	0.41
1:F:277:PHE:CD2	1:F:278:THR:HG23	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ARG:HD2	3:A:2032:HOH:O	2.19	0.41
1:A:300:LEU:HD13	1:A:340:LEU:CD2	2.42	0.41
1:A:336:LYS:CD	1:A:342:ILE:HD13	2.49	0.41
1:E:191:GLU:HB3	1:F:222:SER:O	2.20	0.41
1:F:592:MET:HE2	1:F:592:MET:HB2	1.97	0.41
1:C:267:TRP:CD2	1:C:341:LYS:HG3	2.55	0.41
1:C:719:THR:CG2	1:C:722:THR:HB	2.50	0.41
1:D:136:ASN:HB3	1:D:153:ARG:HB2	2.02	0.41
1:D:200:TYR:CZ	1:D:208:VAL:HG13	2.55	0.41
1:E:273:LEU:HD13	1:E:274:THR:O	2.21	0.41
1:E:689:HIS:ND1	1:E:739:ARG:NH1	2.64	0.41
1:C:298:LEU:HD23	1:C:560:ARG:HB2	2.01	0.41
1:B:226:SER:C	1:B:227:LYS:HG3	2.45	0.41
1:B:592:MET:HE2	1:B:592:MET:HB2	1.80	0.41
1:C:300:LEU:HG	1:C:340:LEU:HD21	2.02	0.41
1:C:594:GLU:HG2	1:C:609:MET:HG3	2.02	0.41
1:C:201:MET:HE2	1:C:502:LEU:HD23	2.03	0.41
1:D:275:THR:O	1:D:276:SER:HB2	2.20	0.41
1:E:414:LYS:NZ	1:E:538:ARG:HH12	2.19	0.41
1:F:208:VAL:HA	1:F:240:PHE:O	2.21	0.41
1:A:82:TYR:HB3	1:A:84:LEU:HD13	2.02	0.41
1:D:191:GLU:OE1	1:D:191:GLU:N	2.50	0.41
1:D:652:GLN:NE2	1:D:654:HIS:NE2	2.68	0.41
1:F:315:TRP:O	1:F:350:ILE:HA	2.21	0.41
1:F:163:TYR:HB3	1:F:502:LEU:HD13	2.03	0.41
1:F:174:ARG:NH2	3:F:2078:HOH:O	2.33	0.41
1:B:569:MET:HB3	1:B:573:LEU:HD22	2.02	0.40
1:D:594:GLU:HG2	1:D:609:MET:HG3	2.02	0.40
1:A:748:GLN:HB3	1:A:769:THR:HG23	2.02	0.40
1:A:630:LEU:HG	1:A:635:TRP:CD1	2.57	0.40
1:A:700:VAL:HG22	1:A:715:LYS:HG2	2.04	0.40
1:C:534:SER:O	1:C:535:SER:C	2.64	0.40
1:E:402:LEU:HD12	1:E:451:VAL:HG21	2.03	0.40
1:B:617:ALA:O	1:B:660:PRO:HD2	2.22	0.40
1:B:718:ARG:HA	1:B:723:ILE:HG22	2.03	0.40
1:C:717:ALA:O	1:C:723:ILE:HA	2.21	0.40
1:A:417:PHE:HA	1:A:419:GLU:OE2	2.22	0.40
1:B:684:GLU:HG2	1:B:732:LYS:HB2	2.03	0.40
1:E:84:LEU:HD12	1:E:258:THR:HG22	2.03	0.40
1:E:352:GLN:HA	1:E:357:PHE:CD2	2.55	0.40
1:F:635:TRP:O	1:F:643:GLU:HA	2.21	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	771/778 (99%)	742 (96%)	25 (3%)	4 (0%)	24	22
1	B	771/778 (99%)	746 (97%)	24 (3%)	1 (0%)	48	50
1	C	771/778 (99%)	745 (97%)	24 (3%)	2 (0%)	36	36
1	D	771/778 (99%)	741 (96%)	28 (4%)	2 (0%)	36	36
1	E	771/778 (99%)	738 (96%)	27 (4%)	6 (1%)	16	12
1	F	771/778 (99%)	737 (96%)	29 (4%)	5 (1%)	21	18
All	All	4626/4668 (99%)	4449 (96%)	157 (3%)	20 (0%)	30	28

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	477	VAL
1	E	766	ASN
1	F	749	ASP
1	C	749	ASP
1	A	338	LYS
1	E	316	CYS
1	E	477	VAL
1	F	77	ASN
1	A	477	VAL
1	A	692	ASN
1	B	477	VAL
1	D	338	LYS
1	E	720	GLY
1	F	477	VAL
1	F	692	ASN
1	C	477	VAL
1	A	348	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	765	GLY
1	E	681	VAL
1	F	348	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	659/665 (99%)	625 (95%)	34 (5%)	21	20
1	B	659/665 (99%)	620 (94%)	39 (6%)	18	16
1	C	659/665 (99%)	618 (94%)	41 (6%)	16	14
1	D	659/665 (99%)	624 (95%)	35 (5%)	20	19
1	E	659/665 (99%)	621 (94%)	38 (6%)	18	16
1	F	659/665 (99%)	613 (93%)	46 (7%)	14	11
All	All	3954/3990 (99%)	3721 (94%)	233 (6%)	18	16

All (233) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	52	LEU
1	A	70	GLU
1	A	84	LEU
1	A	91	LYS
1	A	93	THR
1	A	120	LEU
1	A	123	LEU
1	A	127	GLU
1	A	174	ARG
1	A	178	THR
1	A	180	GLU
1	A	273	LEU
1	A	300	LEU
1	A	306	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	316	CYS
1	A	332	ILE
1	A	336	LYS
1	A	379	LYS
1	A	419	GLU
1	A	452	LEU
1	A	464	PHE
1	A	500	ILE
1	A	573	LEU
1	A	592	MET
1	A	614	VAL
1	A	616	VAL
1	A	630	LEU
1	A	657	LEU
1	A	719	THR
1	A	732	LYS
1	A	747	LEU
1	A	756	GLU
1	A	769	THR
1	B	48	LEU
1	B	69	ILE
1	B	84	LEU
1	B	91	LYS
1	B	99	ARG
1	B	120	LEU
1	B	123	LEU
1	B	174	ARG
1	B	208	VAL
1	B	273	LEU
1	B	281	TYR
1	B	300	LEU
1	B	316	CYS
1	B	324	THR
1	B	334	ARG
1	B	336	LYS
1	B	338	LYS
1	B	408	MET
1	B	452	LEU
1	B	464	PHE
1	B	479	TRP
1	B	532	LEU
1	B	533	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	573	LEU
1	B	579	ARG
1	B	583	ARG
1	B	614	VAL
1	B	616	VAL
1	B	630	LEU
1	B	671	LEU
1	B	693	LEU
1	B	714	LEU
1	B	723	ILE
1	B	735	THR
1	B	739	ARG
1	B	744	VAL
1	B	766	ASN
1	B	768	LEU
1	B	769	THR
1	C	26	GLU
1	C	27	GLN
1	C	48	LEU
1	C	52	LEU
1	C	70	GLU
1	C	84	LEU
1	C	91	LYS
1	C	93	THR
1	C	99	ARG
1	C	120	LEU
1	C	123	LEU
1	C	124	ARG
1	C	177	GLN
1	C	180	GLU
1	C	208	VAL
1	C	246	THR
1	C	260	ARG
1	C	316	CYS
1	C	332	ILE
1	C	333	ARG
1	C	336	LYS
1	C	356	VAL
1	C	408	MET
1	C	419	GLU
1	C	452	LEU
1	C	459	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	464	PHE
1	C	500	ILE
1	C	573	LEU
1	C	592	MET
1	C	616	VAL
1	C	630	LEU
1	C	657	LEU
1	C	693	LEU
1	C	723	ILE
1	C	732	LYS
1	C	744	VAL
1	C	748	GLN
1	C	754	GLU
1	C	768	LEU
1	C	769	THR
1	D	48	LEU
1	D	52	LEU
1	D	84	LEU
1	D	99	ARG
1	D	116	GLU
1	D	120	LEU
1	D	123	LEU
1	D	146	GLN
1	D	174	ARG
1	D	177	GLN
1	D	208	VAL
1	D	273	LEU
1	D	281	TYR
1	D	316	CYS
1	D	329	GLU
1	D	336	LYS
1	D	379	LYS
1	D	419	GLU
1	D	452	LEU
1	D	453	LYS
1	D	459	GLU
1	D	464	PHE
1	D	467	SER
1	D	533	LEU
1	D	614	VAL
1	D	630	LEU
1	D	671	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	693	LEU
1	D	723	ILE
1	D	743	LYS
1	D	747	LEU
1	D	748	GLN
1	D	759	LEU
1	D	764	GLN
1	D	769	THR
1	E	48	LEU
1	E	77	ASN
1	E	84	LEU
1	E	120	LEU
1	E	174	ARG
1	E	179	VAL
1	E	208	VAL
1	E	246	THR
1	E	300	LEU
1	E	316	CYS
1	E	336	LYS
1	E	342	ILE
1	E	447	LEU
1	E	452	LEU
1	E	459	GLU
1	E	464	PHE
1	E	479	TRP
1	E	533	LEU
1	E	573	LEU
1	E	592	MET
1	E	614	VAL
1	E	616	VAL
1	E	630	LEU
1	E	647	SER
1	E	669	LEU
1	E	733	ASN
1	E	735	THR
1	E	736	LEU
1	E	739	ARG
1	E	742	VAL
1	E	744	VAL
1	E	745	ASN
1	E	747	LEU
1	E	748	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	749	ASP
1	E	757	GLN
1	E	764	GLN
1	E	769	THR
1	F	48	LEU
1	F	52	LEU
1	F	84	LEU
1	F	91	LYS
1	F	95	GLU
1	F	99	ARG
1	F	120	LEU
1	F	123	LEU
1	F	143	THR
1	F	174	ARG
1	F	179	VAL
1	F	208	VAL
1	F	246	THR
1	F	260	ARG
1	F	273	LEU
1	F	274	THR
1	F	300	LEU
1	F	316	CYS
1	F	336	LYS
1	F	408	MET
1	F	419	GLU
1	F	452	LEU
1	F	453	LYS
1	F	459	GLU
1	F	464	PHE
1	F	479	TRP
1	F	532	LEU
1	F	533	LEU
1	F	573	LEU
1	F	579	ARG
1	F	614	VAL
1	F	630	LEU
1	F	651	LYS
1	F	657	LEU
1	F	664	ARG
1	F	669	LEU
1	F	693	LEU
1	F	711	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	735	THR
1	F	736	LEU
1	F	742	VAL
1	F	756	GLU
1	F	759	LEU
1	F	768	LEU
1	F	769	THR
1	F	772	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	47	GLN
1	A	73	GLN
1	A	107	ASN
1	A	133	GLN
1	A	280	ASN
1	A	517	ASN
1	A	564	GLN
1	A	613	ASN
1	A	652	GLN
1	A	653	GLN
1	A	752	GLN
1	B	15	ASN
1	B	27	GLN
1	B	47	GLN
1	B	107	ASN
1	B	125	ASN
1	B	133	GLN
1	B	141	GLN
1	B	146	GLN
1	B	280	ASN
1	B	517	ASN
1	B	564	GLN
1	B	653	GLN
1	B	692	ASN
1	C	15	ASN
1	C	27	GLN
1	C	47	GLN
1	C	133	GLN
1	C	141	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	146	GLN
1	C	177	GLN
1	C	211	ASN
1	C	517	ASN
1	C	564	GLN
1	C	652	GLN
1	C	653	GLN
1	C	666	ASN
1	C	692	ASN
1	C	694	GLN
1	C	748	GLN
1	C	764	GLN
1	D	27	GLN
1	D	47	GLN
1	D	73	GLN
1	D	133	GLN
1	D	146	GLN
1	D	177	GLN
1	D	211	ASN
1	D	212	HIS
1	D	280	ASN
1	D	564	GLN
1	D	652	GLN
1	D	764	GLN
1	D	766	ASN
1	E	27	GLN
1	E	47	GLN
1	E	73	GLN
1	E	77	ASN
1	E	107	ASN
1	E	125	ASN
1	E	133	GLN
1	E	144	ASN
1	E	280	ASN
1	E	287	ASN
1	E	517	ASN
1	E	564	GLN
1	E	613	ASN
1	E	652	GLN
1	E	692	ASN
1	E	745	ASN
1	E	748	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	764	GLN
1	E	766	ASN
1	F	15	ASN
1	F	27	GLN
1	F	47	GLN
1	F	73	GLN
1	F	81	HIS
1	F	107	ASN
1	F	125	ASN
1	F	141	GLN
1	F	146	GLN
1	F	192	GLN
1	F	280	ASN
1	F	517	ASN
1	F	564	GLN
1	F	652	GLN
1	F	653	GLN
1	F	748	GLN
1	F	752	GLN
1	F	766	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TRS	B	2004	-	7,7,7	0.37	0	9,9,9	0.96	0
2	TRS	E	2010	-	7,7,7	0.43	0	9,9,9	0.94	0
2	TRS	A	2002	-	7,7,7	0.55	0	9,9,9	1.53	2 (22%)
2	TRS	B	2003	-	7,7,7	0.52	0	9,9,9	1.52	2 (22%)
2	TRS	A	2001	-	7,7,7	0.51	0	9,9,9	0.66	0
2	TRS	C	2005	-	7,7,7	0.48	0	9,9,9	0.76	0
2	TRS	E	2012	-	7,7,7	0.53	0	9,9,9	0.87	0
2	TRS	A	2008	-	7,7,7	0.72	0	9,9,9	1.72	3 (33%)
2	TRS	F	2011	-	7,7,7	0.51	0	9,9,9	0.71	0
2	TRS	C	2006	-	7,7,7	0.62	0	9,9,9	1.07	1 (11%)
2	TRS	D	2007	-	7,7,7	0.30	0	9,9,9	0.86	0
2	TRS	E	2009	-	7,7,7	0.58	0	9,9,9	0.99	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRS	B	2004	-	-	7/9/9/9	-
2	TRS	E	2010	-	-	3/9/9/9	-
2	TRS	A	2002	-	-	8/9/9/9	-
2	TRS	B	2003	-	-	0/9/9/9	-
2	TRS	A	2001	-	-	3/9/9/9	-
2	TRS	C	2005	-	-	3/9/9/9	-
2	TRS	E	2012	-	-	6/9/9/9	-
2	TRS	A	2008	-	-	7/9/9/9	-
2	TRS	F	2011	-	-	2/9/9/9	-
2	TRS	C	2006	-	-	6/9/9/9	-
2	TRS	D	2007	-	-	3/9/9/9	-
2	TRS	E	2009	-	-	1/9/9/9	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2008	TRS	C3-C-C1	2.92	118.44	110.66
2	A	2002	TRS	C3-C-C1	2.90	118.39	110.66
2	A	2008	TRS	C3-C-N	-2.69	101.31	108.17
2	C	2006	TRS	C3-C-N	-2.64	101.44	108.17
2	A	2008	TRS	O2-C2-C	-2.33	104.37	110.88
2	B	2003	TRS	C3-C-C1	-2.20	104.80	110.66
2	B	2003	TRS	O2-C2-C	-2.01	105.27	110.88
2	A	2002	TRS	C3-C-C2	-2.00	105.33	110.66

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2002	TRS	N-C-C1-O1
2	A	2002	TRS	C1-C-C3-O3
2	A	2002	TRS	C2-C-C3-O3
2	A	2002	TRS	N-C-C3-O3
2	A	2008	TRS	C1-C-C3-O3
2	A	2008	TRS	C2-C-C3-O3
2	A	2008	TRS	N-C-C3-O3
2	B	2004	TRS	C1-C-C3-O3
2	B	2004	TRS	N-C-C3-O3
2	E	2010	TRS	C1-C-C3-O3
2	E	2010	TRS	N-C-C3-O3
2	E	2012	TRS	N-C-C3-O3
2	A	2008	TRS	C2-C-C1-O1
2	B	2004	TRS	C2-C-C1-O1
2	C	2006	TRS	C2-C-C1-O1
2	C	2006	TRS	C2-C-C3-O3
2	E	2012	TRS	C2-C-C1-O1
2	A	2001	TRS	N-C-C2-O2
2	A	2008	TRS	N-C-C1-O1
2	B	2004	TRS	N-C-C1-O1
2	B	2004	TRS	C2-C-C3-O3
2	C	2005	TRS	N-C-C2-O2
2	C	2006	TRS	N-C-C1-O1
2	C	2006	TRS	N-C-C3-O3
2	D	2007	TRS	N-C-C2-O2
2	E	2010	TRS	C2-C-C3-O3
2	E	2012	TRS	C3-C-C1-O1
2	E	2012	TRS	N-C-C1-O1
2	A	2008	TRS	C3-C-C1-O1
2	B	2004	TRS	C3-C-C1-O1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	2005	TRS	C1-C-C2-O2
2	C	2005	TRS	C3-C-C2-O2
2	C	2006	TRS	C3-C-C1-O1
2	C	2006	TRS	C1-C-C3-O3
2	D	2007	TRS	C1-C-C2-O2
2	D	2007	TRS	C3-C-C2-O2
2	E	2012	TRS	C2-C-C3-O3
2	A	2002	TRS	C2-C-C1-O1
2	A	2008	TRS	C3-C-C2-O2
2	E	2012	TRS	C1-C-C3-O3
2	A	2001	TRS	C3-C-C2-O2
2	A	2002	TRS	C1-C-C2-O2
2	B	2004	TRS	C3-C-C2-O2
2	E	2009	TRS	C3-C-C2-O2
2	F	2011	TRS	C3-C-C1-O1
2	F	2011	TRS	C3-C-C2-O2
2	A	2001	TRS	C1-C-C2-O2
2	A	2002	TRS	C3-C-C1-O1
2	A	2002	TRS	N-C-C2-O2

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2002	TRS	1	0
2	B	2003	TRS	1	0
2	A	2001	TRS	1	0
2	C	2005	TRS	1	0
2	A	2008	TRS	1	0
2	F	2011	TRS	1	0
2	C	2006	TRS	1	0
2	D	2007	TRS	1	0

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	773/778 (99%)	-0.30	10 (1%) 75 77	9, 18, 33, 43	0
1	B	773/778 (99%)	0.02	27 (3%) 47 49	12, 22, 48, 65	0
1	C	773/778 (99%)	-0.13	23 (2%) 52 55	11, 20, 41, 61	0
1	D	773/778 (99%)	-0.32	11 (1%) 73 75	9, 17, 32, 46	0
1	E	773/778 (99%)	-0.10	34 (4%) 39 41	9, 19, 45, 71	0
1	F	773/778 (99%)	0.11	43 (5%) 30 32	11, 23, 53, 71	0
All	All	4638/4668 (99%)	-0.12	148 (3%) 50 53	9, 20, 42, 71	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	765	GLY	6.8
1	E	767	ALA	5.9
1	E	773	HIS	5.6
1	F	768	LEU	5.5
1	C	773	HIS	5.0
1	F	773	HIS	4.7
1	B	767	ALA	4.7
1	F	767	ALA	4.7
1	F	719	THR	4.5
1	F	720	GLY	4.4
1	B	765	GLY	4.4
1	E	719	THR	4.2
1	F	746	GLY	4.0
1	B	768	LEU	3.9
1	D	719	THR	3.8
1	E	751	SER	3.7
1	E	747	LEU	3.6
1	E	765	GLY	3.6
1	F	723	ILE	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	719	THR	3.6
1	E	761	VAL	3.6
1	F	766	ASN	3.6
1	D	338	LYS	3.6
1	E	766	ASN	3.5
1	C	719	THR	3.5
1	E	744	VAL	3.5
1	C	766	ASN	3.4
1	E	753	ALA	3.3
1	E	764	GLN	3.3
1	F	747	LEU	3.3
1	E	733	ASN	3.2
1	E	763	PRO	3.2
1	E	742	VAL	3.1
1	B	773	HIS	3.1
1	F	731	ALA	3.1
1	B	323	LEU	3.1
1	B	332	ILE	3.1
1	C	720	GLY	3.1
1	E	771	THR	3.1
1	E	756	GLU	3.1
1	C	769	THR	3.0
1	B	742	VAL	3.0
1	C	337	ALA	3.0
1	F	725	VAL	3.0
1	C	768	LEU	3.0
1	F	750	GLY	2.9
1	D	77	ASN	2.9
1	C	747	LEU	2.9
1	E	772	LEU	2.9
1	B	338	LYS	2.9
1	D	88	GLN	2.8
1	B	720	GLY	2.8
1	C	749	ASP	2.8
1	F	722	THR	2.8
1	F	763	PRO	2.8
1	E	760	VAL	2.8
1	F	760	VAL	2.8
1	B	723	ILE	2.8
1	B	766	ASN	2.7
1	A	768	LEU	2.7
1	E	757	GLN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	77	ASN	2.7
1	F	323	LEU	2.7
1	E	722	THR	2.7
1	B	77	ASN	2.7
1	F	742	VAL	2.7
1	C	750	GLY	2.7
1	D	767	ALA	2.6
1	F	721	ASN	2.6
1	B	744	VAL	2.6
1	C	88	GLN	2.6
1	D	720	GLY	2.6
1	A	766	ASN	2.6
1	F	745	ASN	2.6
1	F	735	THR	2.6
1	D	764	GLN	2.5
1	F	769	THR	2.5
1	E	755	SER	2.5
1	E	770	ILE	2.5
1	E	748	GLN	2.5
1	C	98	GLU	2.5
1	B	729	GLY	2.5
1	D	29	ASP	2.5
1	F	749	ASP	2.5
1	C	756	GLU	2.5
1	F	717	ALA	2.4
1	B	750	GLY	2.4
1	E	759	LEU	2.4
1	C	696	GLY	2.4
1	E	750	GLY	2.4
1	F	477	VAL	2.4
1	B	753	ALA	2.4
1	F	726	THR	2.4
1	F	753	ALA	2.3
1	C	77	ASN	2.3
1	C	742	VAL	2.3
1	C	748	GLN	2.3
1	C	323	LEU	2.3
1	D	768	LEU	2.3
1	E	91	LYS	2.3
1	A	773	HIS	2.3
1	F	748	GLN	2.3
1	E	745	ASN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	743	LYS	2.3
1	B	759	LEU	2.3
1	F	734	TRP	2.3
1	F	764	GLN	2.2
1	A	744	VAL	2.2
1	F	728	ALA	2.2
1	F	759	LEU	2.2
1	B	329	GLU	2.2
1	B	337	ALA	2.2
1	F	757	GLN	2.2
1	A	29	ASP	2.2
1	F	770	ILE	2.2
1	F	741	VAL	2.2
1	D	765	GLY	2.2
1	E	768	LEU	2.2
1	C	732	LYS	2.2
1	E	726	THR	2.2
1	F	696	GLY	2.1
1	F	718	ARG	2.1
1	B	743	LYS	2.1
1	B	769	THR	2.1
1	E	720	GLY	2.1
1	A	323	LEU	2.1
1	F	743	LYS	2.1
1	B	98	GLU	2.1
1	B	730	GLU	2.1
1	B	745	ASN	2.1
1	E	752	GLN	2.1
1	B	770	ILE	2.1
1	B	700	VAL	2.1
1	A	753	ALA	2.1
1	D	30	ASN	2.1
1	E	769	THR	2.1
1	C	746	GLY	2.1
1	C	761	VAL	2.1
1	E	741	VAL	2.1
1	F	744	VAL	2.1
1	F	76	LEU	2.0
1	C	729	GLY	2.0
1	F	761	VAL	2.0
1	C	767	ALA	2.0
1	F	407	ALA	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	745	ASN	2.0
1	A	89	ASP	2.0
1	A	339	GLY	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TRS	A	2002	8/8	0.87	0.14	28,29,29,32	0
2	TRS	C	2006	8/8	0.87	0.11	29,31,32,33	0
2	TRS	E	2010	8/8	0.90	0.09	23,23,26,27	0
2	TRS	A	2008	8/8	0.91	0.10	25,26,26,27	0
2	TRS	C	2005	8/8	0.91	0.09	20,21,23,26	0
2	TRS	E	2012	8/8	0.91	0.11	26,27,30,30	0
2	TRS	E	2009	8/8	0.92	0.08	13,14,16,21	0
2	TRS	B	2003	8/8	0.92	0.09	18,18,19,24	0
2	TRS	B	2004	8/8	0.92	0.09	26,26,28,28	0
2	TRS	F	2011	8/8	0.93	0.08	18,21,22,25	0
2	TRS	A	2001	8/8	0.94	0.08	13,15,16,22	0
2	TRS	D	2007	8/8	0.94	0.09	14,16,17,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.