



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:40 PM UTC

PDB ID : 3JVZ / pdb_00003jvz
Title : E2 Ubiquitin-HECT
Authors : Souphron, J.; Kamadurai, H.B.; Schulman, B.A.
Deposited on : 2009-09-17
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

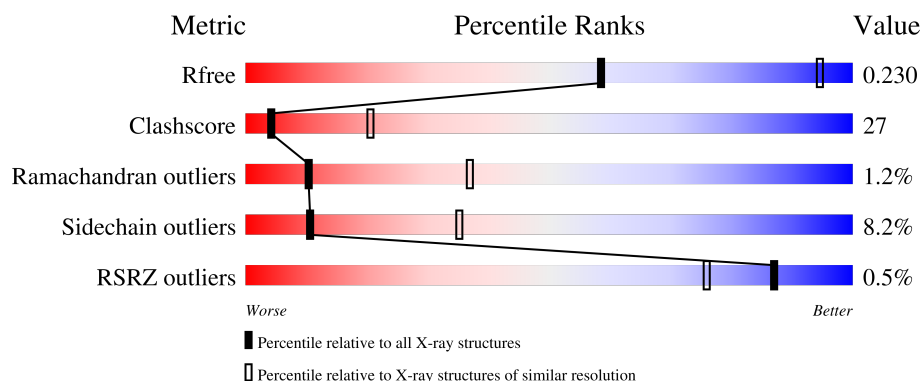
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

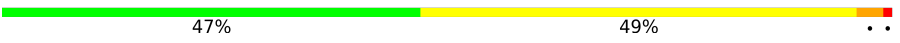
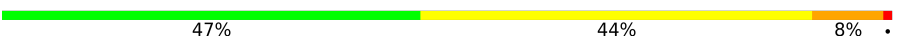
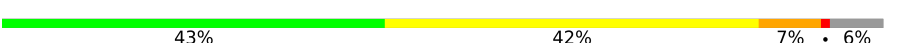
The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	146	
1	B	146	
2	C	385	
2	D	385	
3	X	81	

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Mol	Chain	Length	Quality of chain
3	Y	81	 A horizontal bar chart showing the quality of chain Y. The bar is divided into three segments: green (43%), yellow (48%), and red (6%). The percentages are labeled below the bar segments. The red segment is very small and is preceded by a dot.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9814 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 Ubiquitin-conjugating enzyme E2 D2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	0	0	0
			1170	749	202	213	6			
1	B	146	Total	C	N	O	S	0	0	0
			1170	749	202	213	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	SER	LEU	engineered mutation	UNP P62837
A	85	SER	CYS	engineered mutation	UNP P62837
A	98	LYS	THR	engineered mutation	UNP P62837
B	3	SER	LEU	engineered mutation	UNP P62837
B	85	SER	CYS	engineered mutation	UNP P62837
B	98	LYS	THR	engineered mutation	UNP P62837

- Molecule 2 is a protein called E3 ubiquitin-protein ligase NEDD4-like.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	377	Total	C	N	O	S	0	0	0
			3148	2037	520	574	17			
2	D	374	Total	C	N	O	S	0	0	0
			3124	2021	517	569	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	571	GLY	-	expression tag	UNP Q96PU5
C	572	SER	-	expression tag	UNP Q96PU5
C	573	PRO	-	expression tag	UNP Q96PU5
C	574	GLU	-	expression tag	UNP Q96PU5
C	575	PHE	-	expression tag	UNP Q96PU5
C	922	ALA	CYS	engineered mutation	UNP Q96PU5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	571	GLY	-	expression tag	UNP Q96PU5
D	572	SER	-	expression tag	UNP Q96PU5
D	573	PRO	-	expression tag	UNP Q96PU5
D	574	GLU	-	expression tag	UNP Q96PU5
D	575	PHE	-	expression tag	UNP Q96PU5
D	922	ALA	CYS	engineered mutation	UNP Q96PU5

- Molecule 3 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	76	Total 601	C 378	N 105	O 117	S 1	0	0	0
3	Y	76	Total 601	C 378	N 105	O 117	S 1	0	0	0

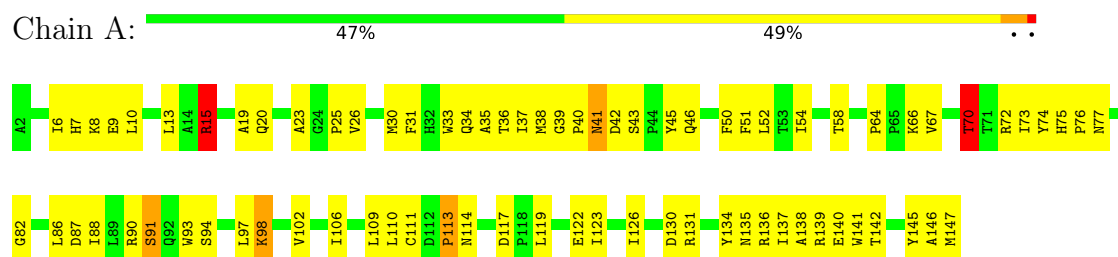
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	-4	GLY	-	expression tag	UNP P62988
X	-3	SER	-	expression tag	UNP P62988
X	-2	GLY	-	expression tag	UNP P62988
X	-1	GLY	-	expression tag	UNP P62988
X	0	SER	-	expression tag	UNP P62988
Y	-4	GLY	-	expression tag	UNP P62988
Y	-3	SER	-	expression tag	UNP P62988
Y	-2	GLY	-	expression tag	UNP P62988
Y	-1	GLY	-	expression tag	UNP P62988
Y	0	SER	-	expression tag	UNP P62988

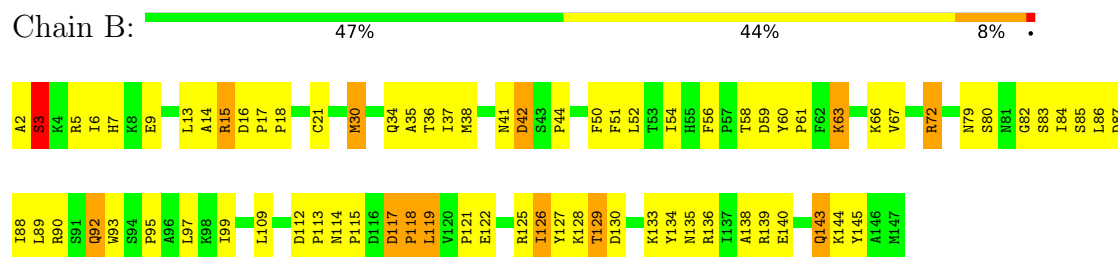
3 Residue-property plots

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.

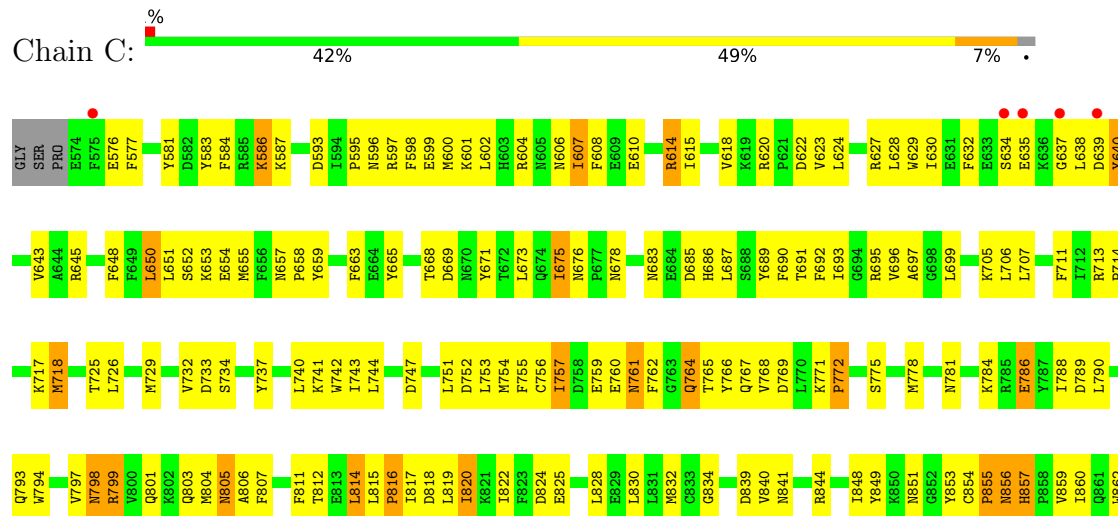
• Molecule 1: Ubiquitin-conjugating enzyme E2 D2

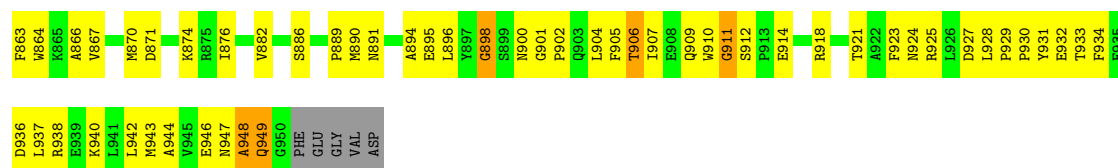


• Molecule 1: Ubiquitin-conjugating enzyme E2 D2



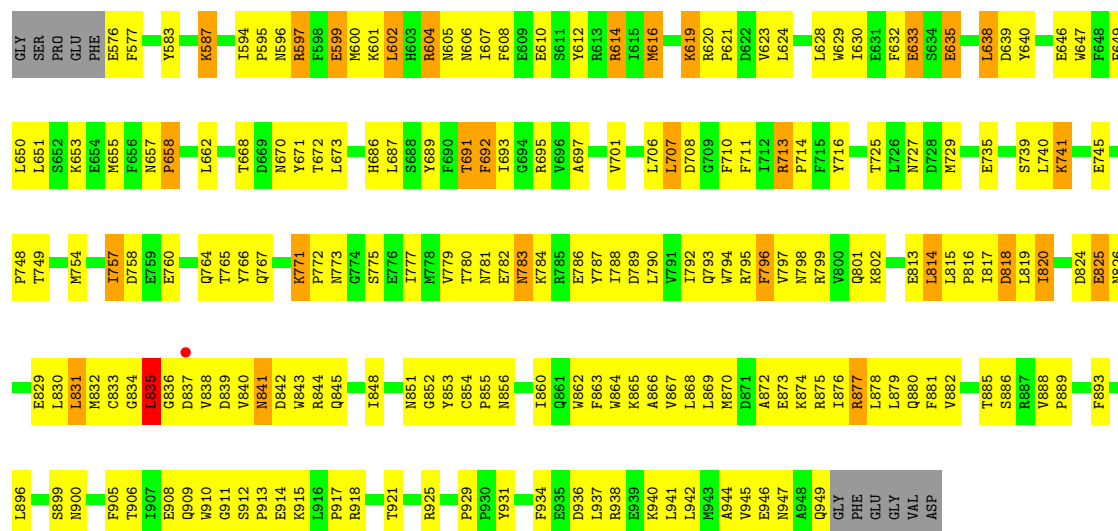
• Molecule 2: E3 ubiquitin-protein ligase NEDD4-like





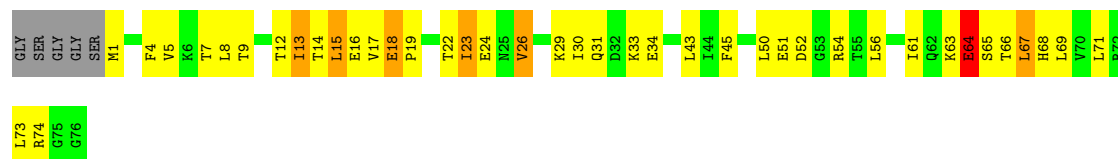
• Molecule 2: E3 ubiquitin-protein ligase NEDD4-like

Chain D: 44% 45% 7%



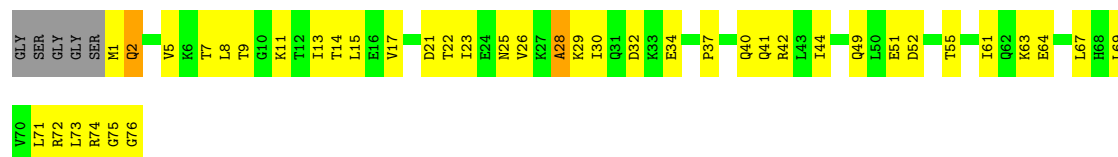
• Molecule 3: Ubiquitin

Chain X: 43% 42% 7% 6%



• Molecule 3: Ubiquitin

Chain Y: 43% 48% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	173.98Å 199.89Å 109.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 50.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	87.5 (50.00-3.30) 87.4 (50.00-3.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 3.33Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.267 0.220 , 0.230	Depositor DCC
R_{free} test set	1288 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å ²)	74.2	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9814	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.53	0/1206	1.09	12/1642 (0.7%)
1	B	0.50	0/1206	1.01	10/1642 (0.6%)
2	C	0.56	1/3232 (0.0%)	1.03	13/4366 (0.3%)
2	D	0.59	0/3207	1.08	19/4333 (0.4%)
3	X	0.55	0/607	1.13	8/816 (1.0%)
3	Y	0.47	0/607	0.93	3/816 (0.4%)
All	All	0.55	1/10065 (0.0%)	1.05	65/13615 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	639	ASP	CG-OD1	5.29	1.35	1.25

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	764	GLN	N-CA-C	-8.87	94.94	109.40
2	D	638	LEU	N-CA-C	8.13	121.08	110.43
1	A	119	LEU	N-CA-C	-8.07	104.03	114.04
1	B	84	ILE	N-CA-C	7.94	119.35	107.75
2	D	599	GLU	N-CA-C	7.61	121.07	108.96
2	D	707	LEU	N-CA-C	-7.38	99.59	110.52
2	C	799	ARG	N-CA-C	7.37	121.92	113.15
1	B	30	MET	N-CA-C	7.16	121.11	112.38
2	D	797	VAL	N-CA-C	6.92	123.74	109.34
3	Y	28	ALA	N-CA-C	-6.87	105.43	113.88
3	X	64	GLU	N-CA-C	6.78	122.98	113.56
3	X	15	LEU	N-CA-C	6.30	118.34	108.96
2	C	882	VAL	N-CA-C	6.29	117.22	111.81
1	B	114	ASN	CA-C-N	6.18	125.91	119.05
1	B	114	ASN	C-N-CA	6.18	125.91	119.05
2	D	672	THR	N-CA-C	-6.18	99.64	109.59
2	C	607	ILE	N-CA-C	6.16	116.94	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	ASP	CA-C-N	6.13	126.48	119.92
1	B	112	ASP	C-N-CA	6.13	126.48	119.92
3	X	26	VAL	N-CA-C	-5.93	103.68	111.09
1	A	87	ASP	N-CA-C	5.92	117.74	111.28
1	A	70	THR	N-CA-C	-5.83	106.20	113.55
2	C	732	VAL	N-CA-C	5.79	115.97	110.53
1	A	114	ASN	CA-C-N	5.72	125.43	119.82
1	A	114	ASN	C-N-CA	5.72	125.43	119.82
1	A	91	SER	N-CA-C	5.72	117.52	111.28
3	X	18	GLU	N-CA-C	-5.67	102.47	110.29
2	C	911	GLY	N-CA-C	5.65	121.65	112.61
1	A	43	SER	N-CA-C	-5.62	100.38	109.82
2	D	934	PHE	N-CA-C	-5.59	106.81	113.97
2	C	948	ALA	N-CA-C	5.55	117.06	109.18
2	C	639	ASP	N-CA-C	-5.53	99.01	110.80
3	X	13	ILE	N-CA-C	5.53	115.22	106.32
2	C	857	HIS	CA-C-N	5.52	126.74	119.84
2	C	857	HIS	C-N-CA	5.52	126.74	119.84
2	D	936	ASP	N-CA-C	-5.51	105.35	112.68
3	Y	9	THR	N-CA-C	-5.51	103.11	110.55
2	D	708	ASP	N-CA-C	5.50	117.63	107.73
1	B	119	LEU	N-CA-C	-5.49	99.11	110.80
3	X	71	LEU	N-CA-C	5.48	117.05	109.15
1	B	117	ASP	CA-C-N	5.41	125.41	120.21
1	B	117	ASP	C-N-CA	5.41	125.41	120.21
2	D	799	ARG	N-CA-C	5.40	119.74	113.20
1	A	117	ASP	CA-C-N	5.40	125.37	120.03
1	A	117	ASP	C-N-CA	5.40	125.37	120.03
2	C	816	PRO	N-CA-C	-5.33	102.13	110.50
2	C	814	LEU	N-CA-C	-5.32	108.56	114.62
2	D	605	ASN	N-CA-C	5.25	119.31	113.01
2	D	912	SER	N-CA-C	-5.25	104.01	110.31
2	D	616	MET	N-CA-C	5.24	119.29	113.01
2	C	898	GLY	N-CA-C	-5.23	104.31	112.58
2	C	855	PRO	N-CA-C	5.18	123.14	112.47
2	D	760	GLU	N-CA-C	5.17	117.05	108.20
2	D	692	PHE	N-CA-C	-5.17	105.09	111.40
3	X	12	THR	N-CA-C	5.16	117.81	109.40
2	D	796	PHE	N-CA-C	5.13	120.39	113.72
2	D	835	LEU	N-CA-C	-5.11	103.78	110.53
2	D	852	GLY	N-CA-C	5.10	122.14	115.36
2	D	777	ILE	N-CA-C	5.10	115.62	108.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	ARG	N-CA-C	5.08	116.50	111.07
1	A	15	ARG	N-CA-C	-5.06	106.45	113.18
1	A	82	GLY	N-CA-C	-5.05	107.84	115.32
3	X	66	THR	N-CA-C	5.05	116.99	108.96
1	B	90	ARG	N-CA-C	5.04	121.54	110.80
3	Y	11	LYS	N-CA-C	5.02	117.61	110.24

There are no chirality outliers.

There are no planarity outliers.

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	1170	0	1152	65	0
1	B	1170	0	1152	62	0
2	C	3148	0	3063	185	0
2	D	3124	0	3045	162	0
3	X	601	0	629	42	0
3	Y	601	0	629	41	0
All	All	9814	0	9670	529	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 27.

All (529) 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)
2:D:597:ARG:HG3	2:D:597:ARG:HH11	1.25	1.00
2:C:817:ILE:O	2:C:820:ILE:HG22	1.61	1.00
2:C:675:ILE:HD12	2:C:675:ILE:H	1.26	0.97
2:C:848:ILE:HG13	2:C:906:THR:HG23	1.49	0.95
2:C:944:ALA:O	2:C:948:ALA:HB2	1.69	0.92
3:X:7:THR:HG22	3:X:69:LEU:HD23	1.54	0.89
3:Y:41:GLN:HB2	3:Y:69:LEU:HD11	1.56	0.86
2:C:817:ILE:O	2:C:820:ILE:CG2	2.23	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:1:MET:SD	3:X:19:PRO:HG3	2.17	0.84
1:A:147:MET:HE2	2:D:856:ASN:HB3	1.60	0.82
3:X:5:VAL:HB	3:X:13:ILE:HB	1.60	0.82
2:C:618:VAL:HG11	2:C:624:LEU:HD21	1.61	0.82
3:X:13:ILE:HA	3:X:33:LYS:HZ1	1.45	0.82
1:A:51:PHE:CE2	2:D:868:LEU:HD11	2.16	0.81
2:D:779:VAL:HG23	2:D:779:VAL:O	1.83	0.79
2:C:910:TRP:CH2	2:C:918:ARG:HD2	2.17	0.79
3:Y:25:ASN:O	3:Y:29:LYS:HG2	1.81	0.79
2:D:619:LYS:CE	2:D:619:LYS:H	1.96	0.78
1:A:40:PRO:HD3	1:A:110:LEU:HD23	1.63	0.78
1:B:125:ARG:NH1	1:B:125:ARG:HB3	1.98	0.78
3:X:4:PHE:CD1	3:X:14:THR:HG22	2.18	0.78
2:D:794:TRP:HA	2:D:798:ASN:HD22	1.48	0.77
2:D:740:LEU:HD13	2:D:792:ILE:HD11	1.68	0.76
3:X:13:ILE:HG23	3:X:33:LYS:HD3	1.68	0.76
2:C:871:ASP:OD1	2:C:874:LYS:HD3	1.86	0.76
2:C:876:ILE:HG22	2:C:886:SER:HB2	1.68	0.75
3:X:45:PHE:HB3	3:X:50:LEU:HD21	1.66	0.75
2:D:729:MET:HE2	2:D:795:ARG:HD2	1.68	0.75
2:D:599:GLU:HB2	2:D:629:TRP:CE3	2.22	0.73
2:D:837:ASP:OD1	2:D:872:ALA:HB1	1.88	0.73
2:D:597:ARG:HG3	2:D:597:ARG:NH1	2.01	0.73
3:X:13:ILE:HA	3:X:33:LYS:NZ	2.03	0.73
1:B:44:PRO:HB2	1:B:138:ALA:HB3	1.71	0.73
2:D:619:LYS:H	2:D:619:LYS:HE3	1.52	0.73
1:A:102:VAL:O	1:A:106:ILE:HG13	1.88	0.73
2:D:794:TRP:HA	2:D:798:ASN:ND2	2.03	0.73
2:C:764:GLN:HE21	2:C:764:GLN:N	1.87	0.73
1:B:125:ARG:HB3	1:B:125:ARG:HH11	1.54	0.72
2:C:876:ILE:CG2	2:C:886:SER:HB2	2.20	0.72
2:D:646:GLU:HG3	2:D:650:LEU:HD13	1.71	0.71
3:X:4:PHE:CE1	3:X:14:THR:HG22	2.26	0.71
3:X:15:LEU:HD22	3:X:29:LYS:HE3	1.73	0.71
2:D:815:LEU:HD23	2:D:820:ILE:HD13	1.74	0.70
1:A:135:ASN:HB3	1:A:139:ARG:HH12	1.57	0.70
2:D:686:HIS:CD2	2:D:687:LEU:H	2.10	0.69
2:D:780:THR:OG1	2:D:782:GLU:HG2	1.93	0.69
1:A:7:HIS:HD2	1:A:30:MET:HE2	1.58	0.69
2:C:706:LEU:HD13	2:C:834:GLY:HA3	1.75	0.68
2:C:844:ARG:HG3	2:C:864:TRP:CE2	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ASP:OD2	1:B:133:LYS:HB2	1.94	0.67
2:D:630:ILE:HG12	2:D:647:TRP:HB2	1.75	0.67
2:C:675:ILE:HD12	2:C:675:ILE:N	2.07	0.67
2:D:713:ARG:NH2	2:D:825:GLU:HG3	2.09	0.67
2:C:675:ILE:H	2:C:675:ILE:CD1	1.95	0.67
3:X:67:LEU:HD12	3:X:67:LEU:H	1.60	0.67
2:D:740:LEU:HD13	2:D:792:ILE:CD1	2.24	0.67
2:C:729:MET:O	2:C:729:MET:HG3	1.93	0.66
2:D:862:TRP:O	2:D:865:LYS:HB3	1.95	0.66
1:A:122:GLU:O	1:A:126:ILE:HD13	1.95	0.66
1:A:136:ARG:HG2	1:A:140:GLU:OE2	1.96	0.66
2:C:604:ARG:HH22	2:C:635:GLU:HB2	1.59	0.66
1:A:90:ARG:HG2	1:A:90:ARG:HH11	1.61	0.66
2:C:761:ASN:N	2:C:761:ASN:HD22	1.93	0.66
3:Y:1:MET:HG2	3:Y:2:GLN:H	1.59	0.66
2:C:848:ILE:CG1	2:C:906:THR:HG23	2.25	0.65
2:D:853:TYR:CD2	2:D:860:ILE:HD11	2.32	0.65
3:Y:17:VAL:HG12	3:Y:29:LYS:HZ2	1.60	0.65
2:C:931:TYR:CE1	2:C:940:LYS:HG3	2.31	0.65
1:B:6:ILE:HG22	1:B:30:MET:HE3	1.78	0.65
2:D:921:THR:HG23	3:Y:74:ARG:HD2	1.78	0.65
3:Y:7:THR:HG22	3:Y:69:LEU:HB3	1.78	0.65
1:B:9:GLU:OE1	1:B:99:ILE:N	2.25	0.65
1:A:10:LEU:HD22	1:A:30:MET:HE1	1.77	0.65
2:C:645:ARG:NH1	2:C:705:LYS:HE2	2.12	0.65
3:Y:63:LYS:HG3	3:Y:64:GLU:OE1	1.97	0.64
2:D:600:MET:HE2	2:D:602:LEU:CD2	2.27	0.64
2:C:794:TRP:HA	2:C:798:ASN:HD22	1.61	0.64
1:B:144:LYS:HD3	1:B:145:TYR:CZ	2.33	0.63
1:A:7:HIS:CD2	1:A:30:MET:HE2	2.33	0.63
1:A:76:PRO:HG3	1:A:123:ILE:HG22	1.80	0.63
1:B:113:PRO:O	1:B:115:PRO:HD3	1.98	0.63
2:D:877:ARG:NH1	2:D:877:ARG:HB3	2.14	0.63
2:D:947:ASN:HB2	3:Y:71:LEU:HD12	1.80	0.63
1:A:15:ARG:HG2	1:A:15:ARG:HH21	1.63	0.63
2:C:615:ILE:O	2:C:618:VAL:HG22	1.98	0.63
2:C:933:THR:OG1	2:C:936:ASP:HB2	1.99	0.63
2:D:918:ARG:HD2	3:Y:40:GLN:NE2	2.14	0.63
2:D:844:ARG:HA	2:D:864:TRP:CZ2	2.34	0.62
3:X:31:GLN:O	3:X:31:GLN:HG2	1.99	0.62
1:B:14:ALA:O	1:B:17:PRO:HD3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:665:TYR:CD1	2:C:671:TYR:HA	2.34	0.62
2:D:813:GLU:C	2:D:814:LEU:HD12	2.25	0.62
3:X:63:LYS:HE3	3:X:64:GLU:OE1	2.00	0.62
1:B:2:ALA:HB1	1:B:5:ARG:HB3	1.80	0.62
2:D:915:LYS:HA	3:Y:37:PRO:HG2	1.80	0.62
3:X:50:LEU:HD13	3:X:61:ILE:HD11	1.82	0.62
2:C:608:PHE:HE1	2:C:655:MET:HA	1.64	0.62
2:D:649:PHE:HD2	2:D:650:LEU:HD12	1.65	0.62
1:A:26:VAL:HG21	1:A:34:GLN:CD	2.25	0.61
1:A:31:PHE:CE2	2:C:765:THR:HG21	2.36	0.61
3:X:45:PHE:CZ	3:X:65:SER:HB3	2.34	0.61
3:X:18:GLU:O	3:X:56:LEU:HD12	2.00	0.61
2:C:695:ARG:O	2:C:814:LEU:HD11	2.00	0.61
1:B:144:LYS:HD3	1:B:145:TYR:CE1	2.36	0.60
2:C:784:LYS:O	2:C:788:ILE:HG13	2.00	0.60
2:D:602:LEU:HD13	2:D:607:ILE:HG13	1.83	0.60
2:D:877:ARG:HB3	2:D:877:ARG:HH11	1.65	0.60
2:C:581:TYR:O	2:C:584:PHE:HB3	2.01	0.60
3:X:45:PHE:HB2	3:X:50:LEU:HD11	1.82	0.60
1:B:63:LYS:NZ	1:B:63:LYS:HB3	2.16	0.60
2:C:757:ILE:HD12	2:C:768:VAL:HG13	1.82	0.60
3:Y:22:THR:O	3:Y:26:VAL:HG23	2.02	0.60
2:D:842:ASP:OD2	2:D:893:PHE:HB2	2.02	0.59
1:B:18:PRO:HG2	1:B:21:CYS:HB2	1.84	0.59
2:C:856:ASN:N	2:C:856:ASN:HD22	2.00	0.59
2:C:855:PRO:C	2:C:856:ASN:HD22	2.10	0.59
2:D:687:LEU:O	2:D:691:THR:HG23	2.02	0.59
1:A:135:ASN:HB3	1:A:139:ARG:NH1	2.17	0.59
2:C:898:GLY:C	2:C:900:ASN:H	2.10	0.59
2:C:910:TRP:CZ2	2:C:918:ARG:HD2	2.38	0.59
2:C:762:PHE:O	2:C:764:GLN:NE2	2.36	0.59
2:C:844:ARG:HA	2:C:864:TRP:CZ2	2.38	0.59
2:C:755:PHE:CD1	2:C:771:LYS:HE2	2.38	0.58
2:D:765:THR:HG23	2:D:765:THR:O	2.03	0.58
2:C:657:ASN:ND2	2:C:890:MET:HE1	2.18	0.58
2:C:849:TYR:HE1	2:C:907:ILE:HD12	1.68	0.58
2:C:630:ILE:O	2:C:643:VAL:HG21	2.03	0.58
2:D:839:ASP:OD2	2:D:842:ASP:HB2	2.04	0.58
1:A:147:MET:CE	2:D:856:ASN:HB3	2.31	0.58
2:D:671:TYR:CZ	2:D:889:PRO:HG3	2.38	0.58
2:D:783:ASN:HD22	2:D:783:ASN:C	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:686:HIS:CD2	2:C:687:LEU:H	2.21	0.58
2:C:707:LEU:HD12	2:C:832:MET:HE3	1.85	0.58
2:D:918:ARG:HD2	3:Y:40:GLN:HE22	1.69	0.58
2:D:851:ASN:O	2:D:909:GLN:HB3	2.03	0.57
2:D:882:VAL:HG11	2:D:905:PHE:CE1	2.38	0.57
1:A:54:ILE:HG12	1:A:67:VAL:HG22	1.85	0.57
2:C:583:TYR:CZ	2:C:587:LYS:HD2	2.39	0.57
2:D:689:TYR:O	2:D:692:PHE:HB3	2.04	0.57
2:C:743:ILE:O	2:C:784:LYS:HD2	2.05	0.57
2:D:599:GLU:HB2	2:D:629:TRP:HE3	1.66	0.57
2:D:783:ASN:C	2:D:783:ASN:ND2	2.62	0.57
2:D:840:VAL:CG2	2:D:875:ARG:HD3	2.35	0.57
1:B:115:PRO:HG2	1:B:128:LYS:HE2	1.86	0.57
2:D:779:VAL:O	2:D:779:VAL:CG2	2.52	0.57
2:C:658:PRO:HG2	2:C:665:TYR:CE2	2.39	0.57
2:D:942:LEU:C	2:D:944:ALA:H	2.12	0.57
3:Y:17:VAL:HG12	3:Y:29:LYS:NZ	2.20	0.57
1:B:13:LEU:HD23	1:B:18:PRO:HD3	1.86	0.56
2:C:938:ARG:HG2	2:C:942:LEU:HD12	1.87	0.56
2:C:947:ASN:ND2	3:X:9:THR:OG1	2.39	0.56
2:D:606:ASN:ND2	2:D:610:GLU:HG3	2.21	0.56
3:Y:61:ILE:HG21	3:Y:67:LEU:HD11	1.87	0.56
1:A:23:ALA:HB2	1:A:35:ALA:HB2	1.88	0.56
2:C:794:TRP:HA	2:C:798:ASN:ND2	2.20	0.56
2:C:870:MET:HB3	2:C:874:LYS:HB2	1.87	0.56
1:B:125:ARG:HH11	1:B:125:ARG:CB	2.16	0.56
2:D:848:ILE:HG13	2:D:906:THR:HG23	1.88	0.56
3:X:43:LEU:HA	3:X:68:HIS:O	2.05	0.56
2:C:812:THR:HG22	2:C:817:ILE:HB	1.89	0.55
2:C:801:GLN:O	2:C:805:ASN:HB2	2.05	0.55
2:C:844:ARG:HA	2:C:864:TRP:CH2	2.41	0.55
2:D:689:TYR:O	2:D:693:ILE:HG12	2.06	0.55
1:A:75:HIS:ND1	1:A:76:PRO:HD2	2.22	0.55
2:C:608:PHE:CE1	2:C:655:MET:HA	2.41	0.55
1:B:41:ASN:O	1:B:42:ASP:HB2	2.06	0.55
1:B:126:ILE:HD12	1:B:133:LYS:NZ	2.22	0.55
2:D:651:LEU:O	2:D:655:MET:HG3	2.07	0.55
3:Y:15:LEU:HD11	3:Y:30:ILE:HG12	1.89	0.54
3:X:26:VAL:O	3:X:30:ILE:HG13	2.08	0.54
2:D:814:LEU:HD12	2:D:814:LEU:N	2.22	0.54
3:X:50:LEU:HD12	3:X:67:LEU:HD23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ALA:CB	1:A:35:ALA:HB2	2.37	0.54
2:C:600:MET:O	2:C:630:ILE:HA	2.08	0.54
1:B:36:THR:HG22	1:B:51:PHE:HD2	1.73	0.54
3:Y:42:ARG:NH1	3:Y:72:ARG:HH21	2.06	0.54
2:D:931:TYR:CE1	2:D:940:LYS:HG2	2.43	0.54
1:A:40:PRO:CD	1:A:110:LEU:HD23	2.36	0.53
2:C:599:GLU:O	2:C:614:ARG:NH1	2.40	0.53
2:C:906:THR:HB	2:C:925:ARG:HG3	1.90	0.53
2:D:729:MET:O	2:D:729:MET:HG2	2.08	0.53
2:D:874:LYS:HD3	2:D:946:GLU:OE2	2.08	0.53
2:C:849:TYR:CE1	2:C:907:ILE:HD12	2.44	0.53
3:Y:1:MET:HB3	3:Y:17:VAL:O	2.08	0.53
2:C:584:PHE:CE1	2:C:819:LEU:HG	2.44	0.53
2:C:769:ASP:HB3	2:C:771:LYS:O	2.07	0.53
2:C:623:VAL:HG23	2:C:624:LEU:HD23	1.89	0.53
2:C:665:TYR:CE1	2:C:671:TYR:HA	2.44	0.53
2:C:910:TRP:HB3	2:C:927:ASP:HB3	1.91	0.53
1:A:94:SER:HB3	1:A:97:LEU:HG	1.91	0.53
1:A:72:ARG:HB2	1:A:145:TYR:CD2	2.44	0.53
1:A:142:THR:O	1:A:146:ALA:HB3	2.08	0.53
2:D:706:LEU:HD22	2:D:834:GLY:N	2.23	0.53
3:X:67:LEU:HD12	3:X:67:LEU:N	2.23	0.53
2:C:786:GLU:O	2:C:790:LEU:HG	2.09	0.52
2:D:687:LEU:O	2:D:691:THR:CG2	2.57	0.52
2:D:813:GLU:HB3	2:D:814:LEU:HD12	1.91	0.52
3:X:4:PHE:HD1	3:X:14:THR:HG22	1.74	0.52
1:A:86:LEU:HD13	1:A:109:LEU:HD22	1.91	0.52
2:D:729:MET:CE	2:D:795:ARG:HD2	2.38	0.52
1:B:129:THR:OG1	1:B:130:ASP:N	2.42	0.52
2:C:853:TYR:CD2	2:C:860:ILE:HD11	2.44	0.52
2:D:838:VAL:HG11	2:D:843:TRP:CE3	2.45	0.52
2:D:741:LYS:O	2:D:745:GLU:HG2	2.09	0.52
1:B:86:LEU:HD13	1:B:109:LEU:HD22	1.91	0.52
2:C:632:PHE:C	2:C:634:SER:H	2.17	0.52
2:C:659:TYR:CG	2:D:597:ARG:HD3	2.45	0.52
1:A:70:THR:HG22	2:D:841:ASN:OD1	2.09	0.51
2:C:671:TYR:CZ	2:C:889:PRO:HG3	2.44	0.51
2:D:619:LYS:H	2:D:619:LYS:HE2	1.74	0.51
2:D:813:GLU:HB3	2:D:814:LEU:CD1	2.41	0.51
1:A:111:CYS:C	1:A:113:PRO:HD3	2.36	0.51
1:B:36:THR:HG22	1:B:51:PHE:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:830:LEU:HD23	2:C:830:LEU:O	2.11	0.51
3:X:15:LEU:HD13	3:X:29:LYS:HD3	1.92	0.51
1:B:119:LEU:O	2:D:925:ARG:NH2	2.43	0.51
2:C:857:HIS:HE1	2:C:859:VAL:HG23	1.75	0.51
2:C:863:PHE:O	2:C:867:VAL:HG23	2.11	0.51
2:D:686:HIS:CD2	2:D:687:LEU:N	2.76	0.51
2:D:729:MET:HG3	2:D:796:PHE:HZ	1.75	0.51
2:D:740:LEU:CD1	2:D:792:ILE:HD11	2.38	0.51
2:C:761:ASN:O	2:C:761:ASN:ND2	2.43	0.51
2:C:804:MET:HE3	2:C:804:MET:O	2.11	0.51
2:C:937:LEU:C	2:C:937:LEU:HD23	2.35	0.51
3:X:16:GLU:O	3:X:17:VAL:HG13	2.11	0.51
2:C:794:TRP:CD1	2:C:799:ARG:HD2	2.46	0.51
3:Y:1:MET:O	3:Y:2:GLN:HB2	2.11	0.51
2:C:640:TYR:HD2	2:C:640:TYR:N	2.09	0.51
2:C:676:ASN:OD1	2:C:678:ASN:N	2.43	0.51
2:C:747:ASP:CG	2:C:781:ASN:HD22	2.19	0.51
2:C:740:LEU:HD22	2:C:788:ILE:HG23	1.93	0.50
2:D:606:ASN:HD22	2:D:610:GLU:HG3	1.76	0.50
2:D:914:GLU:HA	2:D:914:GLU:OE2	2.11	0.50
2:C:584:PHE:HE1	2:C:819:LEU:HG	1.75	0.50
3:Y:13:ILE:HG21	3:Y:34:GLU:OE2	2.11	0.50
1:B:122:GLU:O	1:B:126:ILE:HG12	2.11	0.50
2:C:714:PRO:O	2:C:718:MET:HE3	2.11	0.50
2:D:817:ILE:HG23	2:D:818:ASP:N	2.25	0.50
1:A:41:ASN:ND2	1:A:46:GLN:OE1	2.45	0.50
2:C:683:ASN:C	2:C:685:ASP:H	2.20	0.50
1:A:10:LEU:CD2	1:A:30:MET:HE1	2.41	0.50
1:A:15:ARG:HG2	1:A:15:ARG:NH2	2.26	0.50
2:D:748:PRO:O	2:D:749:THR:C	2.55	0.50
2:D:786:GLU:O	2:D:790:LEU:HG	2.12	0.50
3:Y:26:VAL:O	3:Y:30:ILE:HG13	2.11	0.50
2:D:620:ARG:O	2:D:623:VAL:HG22	2.12	0.49
2:D:830:LEU:O	2:D:834:GLY:HA2	2.12	0.49
2:C:757:ILE:HD12	2:C:757:ILE:H	1.77	0.49
1:A:7:HIS:O	1:A:10:LEU:HB3	2.12	0.49
2:C:671:TYR:CE1	2:C:889:PRO:HD3	2.46	0.49
2:D:882:VAL:HG11	2:D:905:PHE:CZ	2.47	0.49
3:X:7:THR:HA	3:X:69:LEU:HB3	1.94	0.49
2:C:929:PRO:HG2	2:C:931:TYR:CZ	2.47	0.49
1:A:75:HIS:HE1	1:A:77:ASN:OD1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:640:TYR:N	2:C:640:TYR:CD2	2.81	0.49
2:D:583:TYR:CE1	2:D:587:LYS:HG2	2.47	0.49
1:B:113:PRO:C	1:B:115:PRO:HD3	2.38	0.49
1:B:63:LYS:HB3	1:B:63:LYS:HZ2	1.76	0.49
2:C:807:PHE:CD2	2:C:807:PHE:C	2.91	0.49
2:C:583:TYR:O	2:C:587:LYS:HG3	2.12	0.49
2:C:949:GLN:O	2:C:949:GLN:HG2	2.13	0.49
2:D:880:GLN:O	2:D:881:PHE:C	2.56	0.49
1:B:117:ASP:O	3:Y:76:GLY:O	2.31	0.49
2:D:604:ARG:HG2	2:D:604:ARG:HH11	1.78	0.49
1:A:45:TYR:CE2	1:A:138:ALA:HB1	2.48	0.49
2:D:601:LYS:NZ	2:D:633:GLU:HG2	2.28	0.49
1:A:74:TYR:HB2	1:A:141:TRP:CD2	2.48	0.48
2:C:671:TYR:CE2	2:C:889:PRO:HG3	2.47	0.48
2:C:761:ASN:O	2:C:764:GLN:HB2	2.13	0.48
2:D:787:TYR:O	2:D:790:LEU:N	2.46	0.48
3:Y:44:ILE:HD13	3:Y:49:GLN:HA	1.95	0.48
2:C:699:LEU:N	2:C:814:LEU:HD13	2.28	0.48
2:D:754:MET:HE3	2:D:775:SER:O	2.13	0.48
1:B:121:PRO:HG2	1:B:122:GLU:H	1.78	0.48
2:C:756:CYS:SG	2:C:775:SER:HA	2.54	0.48
1:B:136:ARG:O	1:B:140:GLU:HG3	2.14	0.48
2:C:699:LEU:CA	2:C:814:LEU:HD13	2.42	0.48
3:Y:23:ILE:HB	3:Y:51:GLU:O	2.13	0.48
1:B:13:LEU:CD2	1:B:18:PRO:HD3	2.43	0.48
2:C:760:GLU:HA	2:C:764:GLN:O	2.13	0.48
3:X:54:ARG:HG2	3:X:54:ARG:HH11	1.77	0.48
2:D:899:SER:C	2:D:900:ASN:HD22	2.22	0.48
2:C:923:PHE:O	2:C:924:ASN:C	2.57	0.48
2:D:697:ALA:HA	2:D:707:LEU:HD21	1.95	0.48
3:X:13:ILE:HD11	3:X:34:GLU:HG3	1.96	0.48
1:A:19:ALA:HB1	1:A:20:GLN:HE21	1.79	0.48
2:C:695:ARG:O	2:C:814:LEU:CD1	2.61	0.48
2:D:888:VAL:HG13	2:D:889:PRO:HD2	1.95	0.48
1:A:25:PRO:HA	1:A:33:TRP:HA	1.96	0.47
2:C:737:TYR:CZ	2:C:741:LYS:HD3	2.49	0.47
2:C:812:THR:CG2	2:C:817:ILE:HB	2.44	0.47
2:D:701:VAL:HG13	2:D:831:LEU:HD11	1.96	0.47
2:C:743:ILE:CD1	2:C:751:LEU:CD1	2.93	0.47
2:D:941:LEU:O	2:D:945:VAL:HG23	2.15	0.47
2:C:918:ARG:HG2	2:C:918:ARG:HH11	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:928:LEU:HD12	2:C:929:PRO:HD2	1.97	0.47
2:D:710:PHE:CE1	2:D:833:CYS:HB2	2.50	0.47
2:C:638:LEU:HG	2:C:638:LEU:O	2.14	0.47
2:C:820:ILE:HD11	2:C:828:LEU:CD1	2.44	0.47
2:D:757:ILE:HD13	2:D:758:ASP:H	1.80	0.47
3:X:15:LEU:HD22	3:X:29:LYS:CE	2.43	0.47
2:C:597:ARG:HA	2:C:627:ARG:H	1.80	0.47
2:C:637:GLY:O	2:C:640:TYR:HE2	1.97	0.47
2:C:686:HIS:CD2	2:C:687:LEU:HG	2.50	0.47
2:C:863:PHE:O	2:C:866:ALA:HB3	2.15	0.47
2:C:918:ARG:HG2	2:C:918:ARG:NH1	2.30	0.47
2:D:942:LEU:C	2:D:944:ALA:N	2.73	0.47
2:C:762:PHE:C	2:C:764:GLN:H	2.23	0.47
1:B:88:ILE:O	1:B:93:TRP:HB2	2.15	0.47
2:C:606:ASN:O	2:C:610:GLU:HG3	2.15	0.47
2:D:601:LYS:HZ3	2:D:639:ASP:CB	2.28	0.47
3:Y:42:ARG:NH2	3:Y:49:GLN:OE1	2.48	0.47
2:D:854:CYS:HB2	2:D:855:PRO:HD2	1.97	0.47
1:B:54:ILE:HG12	1:B:67:VAL:HG22	1.98	0.46
2:D:729:MET:HG3	2:D:796:PHE:CZ	2.50	0.46
3:X:13:ILE:HG23	3:X:33:LYS:CD	2.43	0.46
3:X:45:PHE:CE1	3:X:65:SER:HB3	2.51	0.46
2:C:576:GLU:O	2:C:577:PHE:C	2.58	0.46
2:C:604:ARG:NH2	2:C:635:GLU:HB2	2.29	0.46
2:C:898:GLY:C	2:C:900:ASN:N	2.71	0.46
3:X:24:GLU:HB2	3:X:52:ASP:HB3	1.96	0.46
1:B:95:PRO:HG3	2:D:739:SER:HB3	1.97	0.46
2:C:686:HIS:CD2	2:C:687:LEU:N	2.82	0.46
2:D:771:LYS:NZ	2:D:786:GLU:OE2	2.49	0.46
1:A:147:MET:O	2:D:844:ARG:HD2	2.15	0.46
1:B:15:ARG:HD3	1:B:15:ARG:C	2.40	0.46
2:C:597:ARG:HD2	2:C:629:TRP:CE3	2.50	0.46
2:D:671:TYR:CE2	2:D:889:PRO:HG3	2.50	0.46
2:D:757:ILE:HD13	2:D:758:ASP:N	2.30	0.46
3:X:54:ARG:HG2	3:X:54:ARG:NH1	2.31	0.46
1:A:8:LYS:HE2	2:C:752:ASP:HB2	1.97	0.46
2:C:741:LYS:O	2:C:744:LEU:HB3	2.16	0.46
3:X:50:LEU:CD1	3:X:67:LEU:HD23	2.45	0.46
1:B:134:TYR:O	1:B:135:ASN:C	2.59	0.46
2:D:793:GLN:NE2	2:D:798:ASN:OD1	2.48	0.46
1:A:19:ALA:O	1:A:20:GLN:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:PRO:HB3	1:A:93:TRP:CG	2.50	0.46
2:D:583:TYR:O	2:D:587:LYS:HB2	2.16	0.46
3:X:22:THR:O	3:X:23:ILE:C	2.59	0.46
1:B:66:LYS:C	1:B:66:LYS:HD2	2.41	0.46
1:A:72:ARG:HB2	1:A:145:TYR:CG	2.50	0.46
1:B:60:TYR:CD1	1:B:61:PRO:HA	2.50	0.46
1:B:72:ARG:HG3	1:B:72:ARG:NH1	2.31	0.46
2:D:597:ARG:NH1	2:D:597:ARG:CG	2.74	0.46
2:D:697:ALA:CB	2:D:707:LEU:HD11	2.47	0.46
2:C:685:ASP:N	2:C:685:ASP:OD1	2.48	0.45
2:C:948:ALA:O	2:C:949:GLN:HB3	2.17	0.45
2:D:781:ASN:O	2:D:781:ASN:ND2	2.49	0.45
1:B:37:ILE:HD12	1:B:52:LEU:HD11	1.99	0.45
2:C:620:ARG:HH11	2:C:620:ARG:HB2	1.82	0.45
2:D:917:PRO:O	3:Y:73:LEU:HD22	2.16	0.45
2:D:814:LEU:N	2:D:814:LEU:CD1	2.79	0.45
2:C:891:ASN:HB2	2:C:895:GLU:HG3	1.98	0.45
2:D:716:TYR:CZ	2:D:829:GLU:HG3	2.52	0.45
2:C:690:PHE:CE2	2:C:803:GLN:HG2	2.52	0.45
2:C:820:ILE:O	2:C:820:ILE:HG12	2.16	0.45
1:A:6:ILE:HG22	1:A:30:MET:HE3	1.99	0.45
1:A:37:ILE:HG13	1:A:52:LEU:HD11	1.98	0.45
2:C:747:ASP:HA	2:C:781:ASN:ND2	2.32	0.45
2:D:673:LEU:O	2:D:711:PHE:HA	2.17	0.45
3:X:13:ILE:HG22	3:X:15:LEU:HG	1.98	0.45
2:C:697:ALA:HA	2:C:707:LEU:HD11	1.98	0.45
2:D:653:LYS:O	2:D:657:ASN:HB2	2.17	0.45
1:B:117:ASP:N	1:B:118:PRO:CD	2.78	0.45
2:C:608:PHE:HE2	2:C:689:TYR:CE2	2.35	0.45
2:D:836:GLY:O	2:D:876:ILE:HD11	2.16	0.45
2:D:888:VAL:CG1	2:D:889:PRO:HD2	2.47	0.45
2:D:937:LEU:C	2:D:937:LEU:HD23	2.42	0.45
1:A:88:ILE:O	1:A:93:TRP:HB2	2.16	0.45
2:D:601:LYS:NZ	2:D:639:ASP:HB3	2.32	0.45
3:Y:17:VAL:CG1	3:Y:29:LYS:NZ	2.80	0.45
1:A:51:PHE:CD2	2:D:868:LEU:HD11	2.51	0.45
1:A:75:HIS:ND1	1:A:76:PRO:N	2.65	0.45
1:B:35:ALA:O	1:B:51:PHE:HA	2.17	0.45
1:A:9:GLU:OE1	1:A:98:LYS:HA	2.16	0.44
2:D:918:ARG:HH22	3:Y:75:GLY:HA3	1.82	0.44
1:A:50:PHE:CE1	1:A:73:ILE:HD12	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ASN:ND2	1:B:83:SER:HB2	2.33	0.44
3:X:73:LEU:O	3:X:74:ARG:C	2.58	0.44
2:C:586:LYS:HZ2	2:C:586:LYS:HA	1.81	0.44
2:C:675:ILE:N	2:C:675:ILE:CD1	2.74	0.44
2:C:824:ASP:O	2:C:825:GLU:C	2.60	0.44
2:D:869:LEU:HD13	2:D:938:ARG:NH1	2.33	0.44
2:C:764:GLN:HE21	2:C:764:GLN:CA	2.27	0.44
3:X:16:GLU:H	3:X:29:LYS:HE2	1.83	0.44
1:A:75:HIS:ND1	1:A:76:PRO:CD	2.80	0.44
2:C:645:ARG:HH11	2:C:705:LYS:CD	2.31	0.44
2:C:696:VAL:O	2:C:699:LEU:HB3	2.18	0.44
1:B:125:ARG:C	1:B:127:TYR:N	2.75	0.44
1:B:126:ILE:HD12	1:B:133:LYS:HZ2	1.80	0.44
2:C:759:GLU:HB2	2:C:766:TYR:CE1	2.53	0.44
2:D:835:LEU:HD23	2:D:836:GLY:H	1.82	0.44
1:B:36:THR:HA	1:B:50:PHE:O	2.18	0.44
2:D:601:LYS:HZ3	2:D:639:ASP:HB3	1.83	0.44
1:A:6:ILE:HG23	1:A:33:TRP:CZ2	2.53	0.44
1:B:117:ASP:N	1:B:118:PRO:HD3	2.33	0.44
2:C:648:PHE:CE2	2:C:705:LYS:HG3	2.53	0.44
2:C:756:CYS:HB2	2:C:768:VAL:O	2.18	0.44
2:D:612:TYR:CE1	2:D:616:MET:HG3	2.53	0.44
2:D:635:GLU:H	2:D:635:GLU:HG3	1.61	0.43
1:A:111:CYS:O	1:A:113:PRO:HD3	2.18	0.43
2:C:669:ASP:OD1	2:C:669:ASP:N	2.51	0.43
2:C:911:GLY:O	2:C:930:PRO:HD2	2.18	0.43
2:C:912:SER:OG	2:C:914:GLU:CG	2.66	0.43
2:D:949:GLN:OE1	2:D:949:GLN:N	2.39	0.43
1:A:58:THR:HG21	2:C:760:GLU:HG3	2.00	0.43
2:C:598:PHE:N	2:C:627:ARG:O	2.44	0.43
3:Y:41:GLN:HB2	3:Y:69:LEU:CD1	2.38	0.43
1:B:80:SER:C	1:B:82:GLY:H	2.26	0.43
2:D:817:ILE:C	2:D:819:LEU:H	2.25	0.43
2:D:662:LEU:HA	2:D:662:LEU:HD23	1.86	0.43
2:D:921:THR:HG23	3:Y:74:ARG:CD	2.48	0.43
1:A:90:ARG:HG2	1:A:90:ARG:NH1	2.31	0.43
2:C:651:LEU:O	2:C:655:MET:HG3	2.19	0.43
2:D:863:PHE:O	2:D:867:VAL:HG23	2.19	0.43
2:D:876:ILE:CG2	2:D:886:SER:HB2	2.49	0.43
1:A:137:ILE:O	1:A:138:ALA:C	2.60	0.43
2:C:811:PHE:C	2:C:811:PHE:CD2	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:929:PRO:HG2	2:C:931:TYR:CE2	2.53	0.43
2:D:632:PHE:O	2:D:639:ASP:HA	2.18	0.43
1:A:74:TYR:HB2	1:A:141:TRP:CE3	2.54	0.43
2:C:620:ARG:NH1	2:C:620:ARG:CB	2.82	0.43
2:C:658:PRO:HA	2:C:663:PHE:O	2.19	0.43
1:A:37:ILE:HG13	1:A:52:LEU:CD1	2.49	0.43
1:A:74:TYR:CE1	1:A:123:ILE:HG23	2.54	0.43
2:C:857:HIS:CE1	2:C:859:VAL:HG23	2.53	0.43
2:C:901:GLY:O	2:C:902:PRO:C	2.61	0.43
2:C:948:ALA:O	3:X:8:LEU:HD23	2.19	0.43
2:D:947:ASN:HA	3:Y:8:LEU:HD23	2.00	0.43
3:Y:22:THR:HA	3:Y:55:THR:HA	2.00	0.43
2:C:733:ASP:O	2:C:734:SER:C	2.61	0.42
2:C:789:ASP:O	2:C:793:GLN:HB2	2.19	0.42
2:C:862:TRP:O	2:C:863:PHE:C	2.62	0.42
2:D:947:ASN:CB	3:Y:71:LEU:HD12	2.45	0.42
1:B:87:ASP:HB3	1:B:92:GLN:HB2	2.00	0.42
1:B:5:ARG:NH1	1:B:97:LEU:O	2.53	0.42
1:B:139:ARG:O	1:B:143:GLN:HB2	2.20	0.42
2:C:607:ILE:HD13	2:C:650:LEU:HB3	2.01	0.42
2:D:816:PRO:HG2	2:D:819:LEU:HB2	2.01	0.42
2:D:910:TRP:CG	2:D:911:GLY:N	2.87	0.42
2:C:713:ARG:HH21	2:C:717:LYS:HD2	1.84	0.42
2:C:729:MET:HE3	2:C:740:LEU:HD12	2.01	0.42
2:C:754:MET:HE1	2:C:778:MET:HG2	2.02	0.42
2:C:839:ASP:OD1	2:C:839:ASP:C	2.62	0.42
2:D:716:TYR:CE2	2:D:829:GLU:HG3	2.54	0.42
1:A:38:MET:O	1:A:39:GLY:C	2.62	0.42
1:B:72:ARG:HG3	1:B:72:ARG:HH11	1.84	0.42
1:B:87:ASP:C	1:B:89:LEU:N	2.77	0.42
2:D:844:ARG:O	2:D:845:GLN:C	2.61	0.42
2:D:910:TRP:CD2	2:D:910:TRP:C	2.97	0.42
2:D:784:LYS:O	2:D:788:ILE:HG13	2.20	0.42
3:Y:28:ALA:O	3:Y:32:ASP:OD1	2.38	0.42
3:Y:49:GLN:O	3:Y:49:GLN:HG3	2.19	0.42
2:D:600:MET:HG2	2:D:614:ARG:HG2	2.02	0.42
2:C:942:LEU:O	2:C:946:GLU:HG2	2.20	0.42
1:A:134:TYR:CD1	1:A:134:TYR:C	2.98	0.42
2:C:638:LEU:C	2:C:638:LEU:HD12	2.45	0.42
2:D:758:ASP:OD2	2:D:767:GLN:HG3	2.19	0.42
2:D:817:ILE:C	2:D:819:LEU:N	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:880:GLN:HA	2:D:885:THR:O	2.20	0.42
2:C:673:LEU:O	2:C:711:PHE:HA	2.19	0.42
2:C:851:ASN:ND2	2:C:909:GLN:O	2.53	0.41
2:C:921:THR:HG21	3:X:74:ARG:NH1	2.35	0.41
2:D:604:ARG:HH11	2:D:604:ARG:CG	2.32	0.41
2:D:910:TRP:O	2:D:929:PRO:HA	2.20	0.41
1:B:3:SER:O	1:B:7:HIS:HB2	2.20	0.41
2:C:725:THR:O	2:C:726:LEU:C	2.64	0.41
2:C:797:VAL:O	2:C:798:ASN:C	2.63	0.41
2:C:904:LEU:O	2:C:905:PHE:C	2.62	0.41
3:Y:63:LYS:O	3:Y:64:GLU:HB2	2.21	0.41
2:D:607:ILE:HG23	2:D:608:PHE:N	2.35	0.41
1:A:26:VAL:HG23	1:A:34:GLN:HG2	2.01	0.41
2:C:620:ARG:HH11	2:C:623:VAL:HG13	1.85	0.41
2:D:616:MET:HE1	2:D:691:THR:OG1	2.20	0.41
2:D:866:ALA:O	2:D:870:MET:HG2	2.20	0.41
2:D:670:ASN:O	2:D:671:TYR:HB2	2.20	0.41
2:C:757:ILE:H	2:C:757:ILE:CD1	2.33	0.41
2:C:818:ASP:C	2:C:820:ILE:N	2.78	0.41
2:C:854:CYS:HB2	2:C:855:PRO:HD2	2.03	0.41
2:D:596:ASN:HD22	2:D:596:ASN:HA	1.62	0.41
2:D:621:PRO:O	2:D:624:LEU:HD12	2.21	0.41
3:Y:14:THR:HG22	3:Y:15:LEU:N	2.35	0.41
3:Y:42:ARG:NH2	3:Y:49:GLN:CD	2.78	0.41
1:A:13:LEU:C	1:A:15:ARG:H	2.29	0.41
1:B:59:ASP:HB2	1:B:63:LYS:HG3	2.02	0.41
2:C:814:LEU:HB2	2:C:815:LEU:HD12	2.03	0.41
1:A:42:ASP:HA	1:A:46:GLN:NE2	2.35	0.41
1:B:5:ARG:HG2	1:B:61:PRO:HG3	2.03	0.41
1:B:128:LYS:HA	1:B:128:LYS:HD3	1.71	0.41
2:C:653:LYS:HD3	2:C:890:MET:HG3	2.03	0.41
2:C:742:TRP:O	2:C:743:ILE:C	2.62	0.41
2:C:815:LEU:HA	2:C:816:PRO:HD3	1.80	0.41
2:C:894:ALA:HB1	2:D:640:TYR:HA	2.03	0.41
2:C:933:THR:OG1	2:C:936:ASP:CB	2.67	0.41
2:D:713:ARG:O	2:D:714:PRO:C	2.64	0.41
3:Y:72:ARG:O	3:Y:72:ARG:HG3	2.20	0.41
1:A:126:ILE:O	1:A:130:ASP:O	2.39	0.41
2:C:771:LYS:HB2	2:C:772:PRO:HD2	2.03	0.41
2:D:619:LYS:HE3	2:D:619:LYS:N	2.29	0.41
2:D:937:LEU:HD23	2:D:938:ARG:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:PRO:HB3	1:A:33:TRP:CD1	2.56	0.40
2:C:608:PHE:CE1	2:C:655:MET:HG2	2.56	0.40
2:C:921:THR:CG2	3:X:74:ARG:HH11	2.34	0.40
2:D:914:GLU:OE2	2:D:914:GLU:CA	2.69	0.40
1:B:79:ASN:HD21	1:B:83:SER:HB2	1.85	0.40
2:C:740:LEU:HA	2:C:740:LEU:HD23	1.89	0.40
2:D:576:GLU:O	2:D:577:PHE:C	2.65	0.40
2:D:766:TYR:N	2:D:766:TYR:CD1	2.89	0.40
2:D:789:ASP:O	2:D:793:GLN:HB2	2.22	0.40
3:X:45:PHE:CB	3:X:50:LEU:HD21	2.45	0.40
1:B:121:PRO:O	1:B:122:GLU:C	2.63	0.40
1:B:126:ILE:O	1:B:130:ASP:O	2.39	0.40
2:C:691:THR:HA	2:C:806:ALA:O	2.21	0.40
2:C:692:PHE:O	2:C:693:ILE:C	2.65	0.40
2:C:753:LEU:O	2:C:754:MET:HE2	2.21	0.40
2:C:934:PHE:CD2	2:C:934:PHE:C	2.96	0.40
2:D:878:LEU:O	2:D:879:LEU:C	2.65	0.40
2:C:652:SER:C	2:C:654:GLU:N	2.77	0.40
2:C:692:PHE:O	2:C:695:ARG:N	2.55	0.40
2:D:670:ASN:O	2:D:671:TYR:CB	2.69	0.40
2:D:824:ASP:C	2:D:826:ASN:H	2.29	0.40
3:Y:5:VAL:HA	3:Y:67:LEU:O	2.20	0.40
3:Y:7:THR:CG2	3:Y:69:LEU:HD23	2.52	0.40
1:B:15:ARG:HD3	1:B:16:ASP:HB2	2.03	0.40
1:B:56:PHE:HZ	1:B:99:ILE:HG13	1.87	0.40
1:B:89:LEU:HD23	1:B:89:LEU:HA	1.88	0.40
2:D:594:ILE:HB	2:D:595:PRO:HD2	2.04	0.40
2:D:601:LYS:HZ2	2:D:633:GLU:HG2	1.85	0.40
3:Y:1:MET:C	3:Y:63:LYS:HZ2	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	144/146 (99%)	133 (92%)	10 (7%)	1 (1%)	18	49
1	B	144/146 (99%)	124 (86%)	17 (12%)	3 (2%)	5	26
2	C	375/385 (97%)	321 (86%)	50 (13%)	4 (1%)	11	39
2	D	372/385 (97%)	328 (88%)	42 (11%)	2 (0%)	24	55
3	X	74/81 (91%)	64 (86%)	8 (11%)	2 (3%)	4	22
3	Y	74/81 (91%)	63 (85%)	9 (12%)	2 (3%)	4	22
All	All	1183/1224 (97%)	1033 (87%)	136 (12%)	14 (1%)	10	37

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3	SER
2	D	825	GLU
1	B	129	THR
2	C	593	ASP
3	Y	2	GLN
3	Y	21	ASP
2	C	949	GLN
3	X	51	GLU
2	C	798	ASN
2	C	595	PRO
1	A	113	PRO
2	D	658	PRO
3	X	23	ILE
1	B	126	ILE

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	130/130 (100%)	123 (95%)	7 (5%)	20	49
1	B	130/130 (100%)	118 (91%)	12 (9%)	8	30
2	C	341/347 (98%)	313 (92%)	28 (8%)	10	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	339/347 (98%)	301 (89%)	38 (11%)	6	22
3	X	68/70 (97%)	66 (97%)	2 (3%)	37	62
3	Y	68/70 (97%)	67 (98%)	1 (2%)	57	72
All	All	1076/1094 (98%)	988 (92%)	88 (8%)	10	35

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	36	THR
1	A	41	ASN
1	A	66	LYS
1	A	70	THR
1	A	91	SER
1	A	98	LYS
1	B	3	SER
1	B	15	ARG
1	B	34	GLN
1	B	38	MET
1	B	42	ASP
1	B	58	THR
1	B	63	LYS
1	B	72	ARG
1	B	85	SER
1	B	92	GLN
1	B	118	PRO
1	B	143	GLN
2	C	586	LYS
2	C	596	ASN
2	C	601	LYS
2	C	602	LEU
2	C	614	ARG
2	C	622	ASP
2	C	628	LEU
2	C	640	TYR
2	C	650	LEU
2	C	668	THR
2	C	675	ILE
2	C	718	MET
2	C	757	ILE
2	C	761	ASN

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Mol	Chain	Res	Type
2	C	764	GLN
2	C	767	GLN
2	C	772	PRO
2	C	786	GLU
2	C	805	ASN
2	C	820	ILE
2	C	822	ILE
2	C	840	VAL
2	C	841	ASN
2	C	856	ASN
2	C	896	LEU
2	C	906	THR
2	C	932	GLU
2	C	943	MET
2	D	587	LYS
2	D	597	ARG
2	D	602	LEU
2	D	604	ARG
2	D	614	ARG
2	D	619	LYS
2	D	628	LEU
2	D	633	GLU
2	D	635	GLU
2	D	638	LEU
2	D	658	PRO
2	D	668	THR
2	D	691	THR
2	D	695	ARG
2	D	713	ARG
2	D	725	THR
2	D	727	ASN
2	D	735	GLU
2	D	741	LYS
2	D	757	ILE
2	D	771	LYS
2	D	772	PRO
2	D	773	ASN
2	D	783	ASN
2	D	801	GLN
2	D	802	LYS
2	D	814	LEU
2	D	818	ASP

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Mol	Chain	Res	Type
2	D	820	ILE
2	D	831	LEU
2	D	832	MET
2	D	835	LEU
2	D	841	ASN
2	D	873	GLU
2	D	877	ARG
2	D	896	LEU
2	D	908	GLU
2	D	913	PRO
3	X	64	GLU
3	X	67	LEU
3	Y	52	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	32	HIS
1	A	41	ASN
1	A	46	GLN
1	A	135	ASN
1	B	11	ASN
1	B	55	HIS
1	B	77	ASN
1	B	81	ASN
1	B	92	GLN
1	B	135	ASN
1	B	143	GLN
2	C	605	ASN
2	C	674	GLN
2	C	683	ASN
2	C	703	HIS
2	C	746	ASN
2	C	761	ASN
2	C	764	GLN
2	C	781	ASN
2	C	793	GLN
2	C	798	ASN
2	C	801	GLN
2	C	856	ASN
2	C	891	ASN

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Mol	Chain	Res	Type
2	C	909	GLN
2	C	947	ASN
2	D	579	GLN
2	D	596	ASN
2	D	606	ASN
2	D	670	ASN
2	D	674	GLN
2	D	727	ASN
2	D	767	GLN
2	D	783	ASN
2	D	793	GLN
2	D	798	ASN
2	D	801	GLN
2	D	900	ASN
2	D	909	GLN
3	X	2	GLN
3	X	25	ASN
3	X	62	GLN
3	Y	2	GLN
3	Y	25	ASN
3	Y	41	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	146/146 (100%)	-0.33	0	100	100	35, 80, 104, 114	0
1	B	146/146 (100%)	-0.26	0	100	100	52, 77, 99, 114	0
2	C	377/385 (97%)	-0.25	5 (1%)	75	56	45, 72, 112, 122	0
2	D	374/385 (97%)	-0.38	1 (0%)	90	82	38, 67, 96, 126	0
3	X	76/81 (93%)	0.41	0	100	100	93, 126, 127, 127	0
3	Y	76/81 (93%)	0.06	0	100	100	95, 125, 127, 127	0
All	All	1195/1224 (97%)	-0.24	6 (0%)	87	76	35, 75, 126, 127	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	639	ASP	4.2
2	D	837	ASP	2.8
2	C	634	SER	2.7
2	C	635	GLU	2.6
2	C	575	PHE	2.5
2	C	637	GLY	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.