



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:33 PM UTC

PDB ID : 7MWC / pdb_00007mwc
Title : ERAP1 binds peptide C-terminus of a LPF sequence (AAAAFKARKF)
Authors : Guo, H.C.; Sui, L.
Deposited on : 2021-05-16
Resolution : 3.00 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

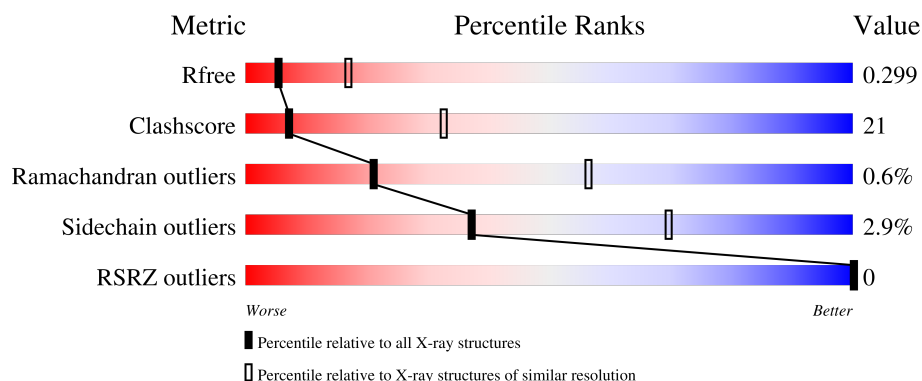
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	423	
1	B	423	
1	C	423	
1	D	423	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13007 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 Endoplasmic reticulum aminopeptidase 1,LPF sequence.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3183	2048	541	579	15			
1	B	400	Total	C	N	O	S	29	0	0
			3252	2092	553	592	15			
1	C	399	Total	C	N	O	S	29	0	0
			3236	2082	552	587	15			
1	D	398	Total	C	N	O	S	13	0	0
			3215	2067	547	586	15			

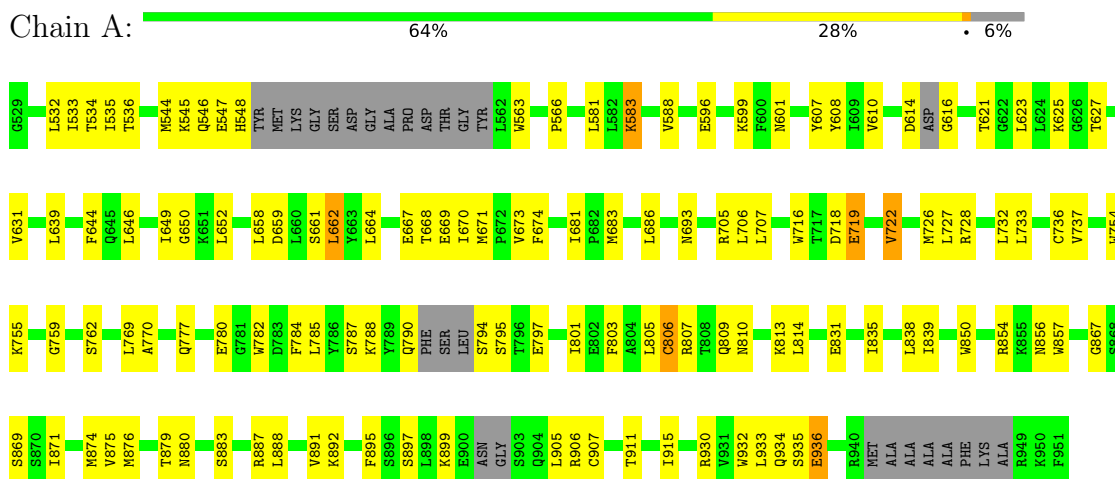
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	32	Total	O	0	0
			32	32		
2	B	27	Total	O	0	0
			27	27		
2	C	26	Total	O	0	0
			26	26		
2	D	36	Total	O	0	0
			36	36		

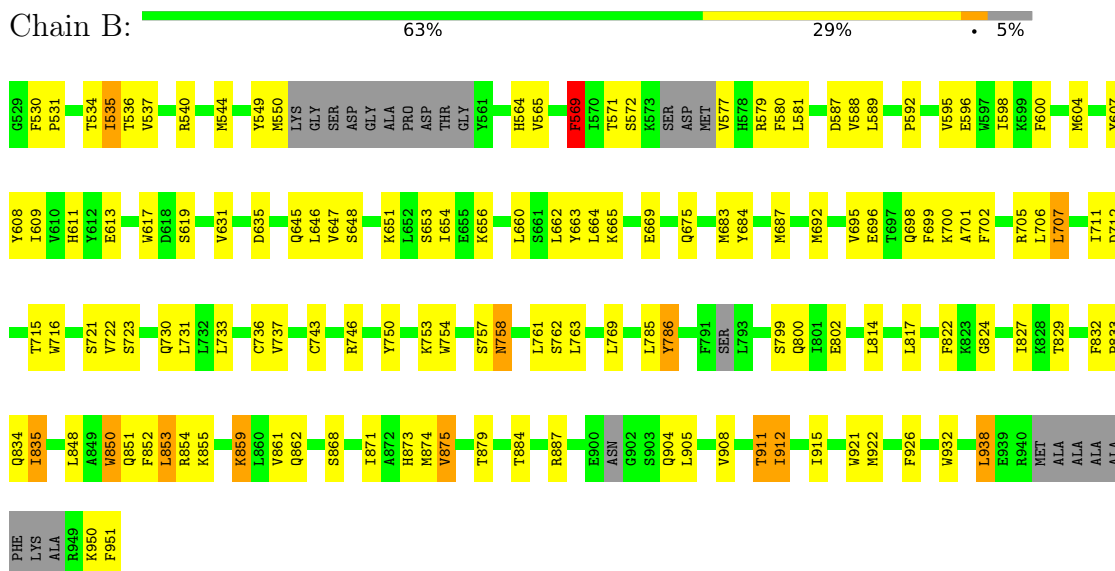
3 Residue-property plots

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: Endoplasmic reticulum aminopeptidase 1,LPF sequence

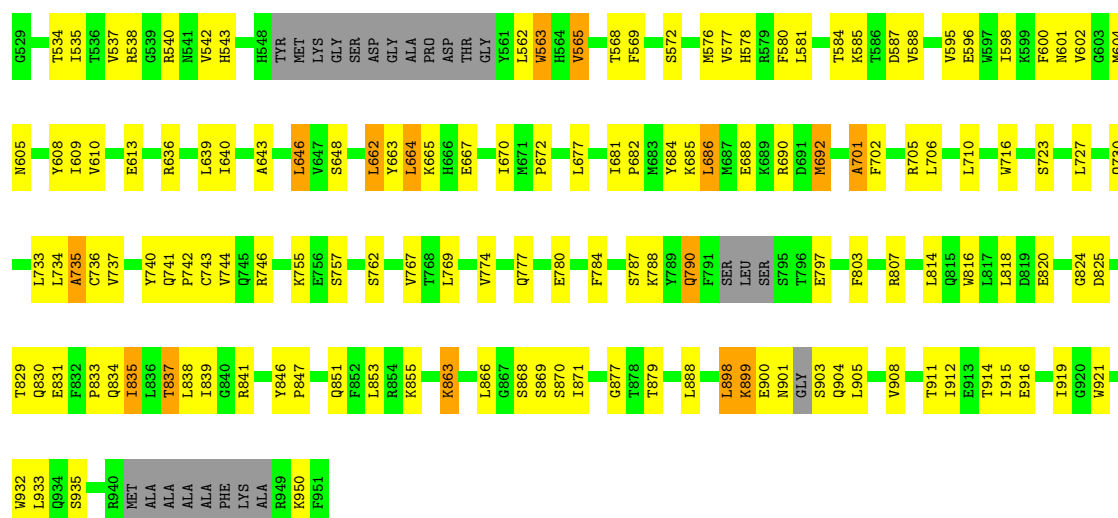


- Molecule 1: Endoplasmic reticulum aminopeptidase 1,LPF sequence



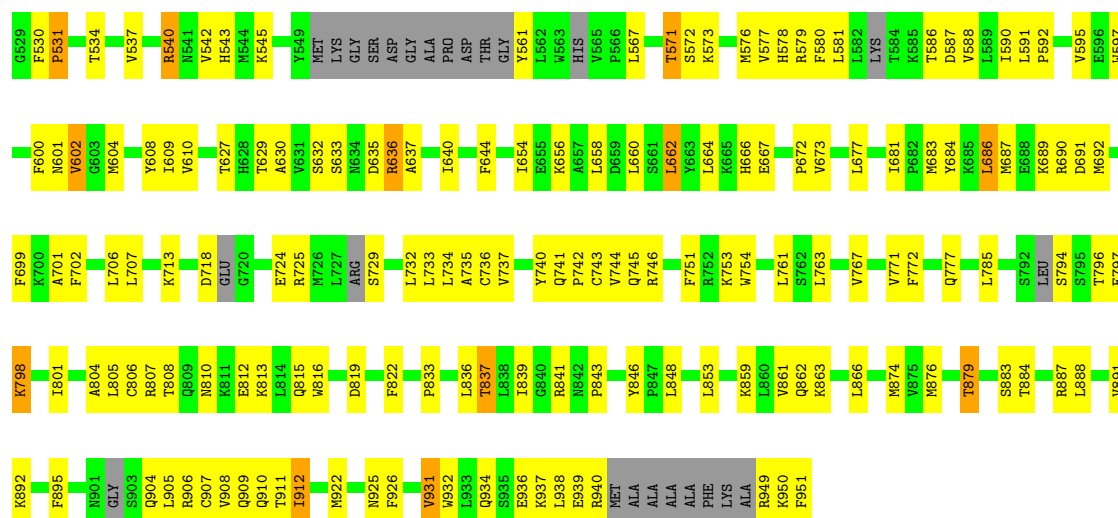
- Molecule 1: Endoplasmic reticulum aminopeptidase 1,LPF sequence





• Molecule 1: Endoplasmic reticulum aminopeptidase 1, LPF sequence

Chain D: 56% 35% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.03Å 66.68Å 121.71Å 90.07° 101.81° 90.05°	Depositor
Resolution (Å)	55.12 – 3.00 55.12 – 3.00	Depositor EDS
% Data completeness (in resolution range)	86.9 (55.12-3.00) 81.5 (55.12-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.238 , 0.298 0.242 , 0.299	Depositor DCC
R_{free} test set	1725 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 21.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-h-l 0.418 for -h,k,-l 0.024 for -h,-k,h+l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13007	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.81	0/3248	1.12	6/4386 (0.1%)
1	B	0.82	1/3320 (0.0%)	1.25	24/4476 (0.5%)
1	C	0.80	2/3303 (0.1%)	1.20	24/4454 (0.5%)
1	D	0.84	1/3278 (0.0%)	1.25	24/4416 (0.5%)
All	All	0.82	4/13149 (0.0%)	1.21	78/17732 (0.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	790	GLN	C-N	5.26	1.40	1.33
1	B	950	LYS	N-CA	5.23	1.49	1.46
1	D	636	ARG	CA-C	5.17	1.59	1.52
1	C	950	LYS	N-CA	5.10	1.49	1.46

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	786	TYR	N-CA-C	10.54	123.83	111.71
1	B	723	SER	N-CA-C	10.38	122.18	111.07
1	B	855	LYS	N-CA-C	10.29	122.19	110.97
1	C	790	GLN	N-CA-C	9.27	123.05	112.57
1	D	637	ALA	N-CA-C	9.03	121.94	111.11
1	A	662	LEU	N-CA-C	8.25	120.27	111.28
1	B	915	ILE	N-CA-C	7.94	117.99	110.53
1	A	806	CYS	N-CA-C	-7.82	103.72	113.18
1	B	712	ASP	N-CA-C	7.75	121.99	112.54
1	D	804	ALA	N-CA-C	7.71	121.62	111.75
1	C	853	LEU	N-CA-C	-7.69	102.23	111.69
1	B	859	LYS	N-CA-C	7.50	119.46	111.28
1	D	579	ARG	N-CA-C	7.24	121.20	109.40
1	B	698	GLN	N-CA-C	-6.96	103.69	111.28
1	C	877	GLY	N-CA-C	6.93	121.05	112.73
1	C	664	LEU	N-CA-C	-6.86	103.42	112.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	763	LEU	N-CA-C	-6.81	100.30	110.24
1	D	740	TYR	N-CA-C	-6.72	99.95	109.96
1	C	684	TYR	N-CA-C	6.70	120.71	112.54
1	C	565	VAL	N-CA-C	6.70	114.52	107.76
1	C	577	VAL	N-CA-C	6.63	123.14	109.34
1	B	873	HIS	N-CA-C	6.62	118.15	111.07
1	B	675	GLN	N-CA-C	-6.50	103.47	111.40
1	A	936	GLU	N-CA-C	-6.49	104.13	111.07
1	B	662	LEU	N-CA-C	6.41	124.44	110.80
1	D	701	ALA	N-CA-C	-6.31	104.32	111.07
1	B	875	VAL	N-CA-CB	6.28	118.61	110.57
1	D	931	VAL	N-CA-C	6.24	117.02	110.72
1	B	565	VAL	N-CA-C	6.17	113.66	107.55
1	B	853	LEU	N-CA-C	-6.13	103.92	112.45
1	D	925	ASN	N-CA-C	6.12	120.75	113.28
1	D	910	GLN	N-CA-CB	6.10	119.19	110.16
1	B	664	LEU	N-CA-C	-6.04	105.62	112.87
1	B	850	TRP	N-CA-C	6.01	117.83	111.28
1	D	578	HIS	N-CA-C	5.93	118.89	109.81
1	B	730	GLN	N-CA-C	5.91	118.95	111.69
1	D	588	VAL	N-CA-C	-5.88	99.32	108.44
1	D	879	THR	N-CA-C	5.84	123.24	110.80
1	C	540	ARG	N-CA-C	-5.83	106.79	114.31
1	C	686	LEU	N-CA-C	-5.80	104.33	111.40
1	B	861	VAL	N-CA-C	-5.74	103.91	111.09
1	B	938	LEU	N-CA-C	-5.74	104.93	111.07
1	D	635	ASP	N-CA-C	-5.74	104.63	111.69
1	B	763	LEU	N-CA-CB	-5.73	102.30	110.04
1	D	530	PHE	CA-C-O	-5.70	116.01	121.08
1	D	862	GLN	N-CA-C	-5.66	105.11	111.28
1	B	875	VAL	N-CA-C	-5.64	105.23	110.53
1	C	900	GLU	N-CA-C	-5.63	106.40	113.72
1	B	569	PHE	CA-CB-CG	5.60	119.40	113.80
1	C	710	LEU	N-CA-C	-5.59	104.81	111.69
1	A	693	ASN	N-CA-C	5.58	117.05	111.07
1	D	686	LEU	N-CA-C	-5.55	105.31	111.36
1	D	931	VAL	CB-CA-C	-5.46	104.69	112.22
1	D	879	THR	CB-CA-C	-5.42	99.63	110.42
1	A	722	VAL	CA-C-O	-5.41	116.02	121.59
1	C	692	MET	N-CA-C	5.40	118.20	109.83
1	D	686	LEU	N-CA-CB	5.40	118.15	110.16
1	C	576	MET	N-CA-C	5.40	117.29	108.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	662	LEU	N-CA-C	5.29	122.07	110.80
1	D	839	ILE	N-CA-CB	5.26	118.47	110.58
1	C	866	LEU	N-CA-C	5.26	116.70	110.97
1	C	563	TRP	N-CA-C	5.25	115.28	107.88
1	C	818	LEU	N-CA-C	-5.25	105.25	110.97
1	C	898	LEU	CA-C-O	-5.25	116.18	122.27
1	D	806	CYS	N-CA-C	-5.22	106.91	113.28
1	C	578	HIS	N-CA-CB	5.22	117.75	109.71
1	B	835	ILE	N-CA-C	5.21	115.42	110.42
1	C	735	ALA	N-CA-C	-5.21	104.86	111.11
1	C	701	ALA	N-CA-C	-5.21	105.50	111.07
1	D	940	ARG	N-CA-CB	-5.20	101.66	110.50
1	D	540	ARG	N-CA-C	-5.13	106.33	112.59
1	C	879	THR	N-CA-C	5.12	120.18	113.88
1	C	835	ILE	N-CA-C	5.11	115.83	110.62
1	C	831	GLU	N-CA-C	5.09	119.48	113.16
1	B	669	GLU	N-CA-C	5.07	117.87	109.46
1	A	809	GLN	N-CA-C	-5.06	107.13	113.15
1	C	797	GLU	N-CA-C	5.06	117.19	111.02
1	D	531	PRO	CB-CA-C	-5.04	103.25	111.56

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	3183	0	3130	134	0
1	B	3252	0	3230	146	0
1	C	3236	0	3225	109	0
1	D	3215	0	3185	163	0
2	A	32	0	0	11	0
2	B	27	0	0	7	0
2	C	26	0	0	2	0
2	D	36	0	0	7	0
All	All	13007	0	12770	531	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 21.

All (531) 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:B:687:MET:HA	1:B:692:MET:SD	1.67	1.33
1:D:667:GLU:OE2	1:D:672:PRO:HG2	1.32	1.22
1:A:806:CYS:HB2	1:A:838:LEU:CD2	1.74	1.17
1:A:581:LEU:HD23	1:A:583:LYS:NZ	1.63	1.14
1:A:806:CYS:HB2	1:A:838:LEU:HD22	1.20	1.14
1:A:806:CYS:CB	1:A:838:LEU:HD22	1.77	1.14
1:B:692:MET:HE1	1:B:922:MET:HE1	1.30	1.09
1:C:755:LYS:HG3	1:C:784:PHE:CD2	1.87	1.09
1:A:581:LEU:HD23	1:A:583:LYS:CE	1.85	1.05
1:A:813:LYS:HB2	2:A:1001:HOH:O	1.55	1.05
1:A:737:VAL:HG13	1:A:807:ARG:HE	1.17	1.05
1:A:867:GLY:HA2	1:A:905:LEU:HD21	1.09	1.03
1:B:692:MET:HE1	1:B:922:MET:CE	1.87	1.03
1:A:867:GLY:CA	1:A:905:LEU:HD21	1.88	1.03
1:D:807:ARG:HH22	1:D:843:PRO:CD	1.71	1.02
1:B:611:HIS:HE1	1:B:651:LYS:HB3	1.24	1.01
1:D:629:THR:HA	1:D:636:ARG:NH2	1.75	1.01
1:D:573:LYS:HB2	2:D:1008:HOH:O	1.60	1.00
1:A:810:ASN:HB3	2:A:1001:HOH:O	1.61	1.00
1:C:604:MET:HE2	1:C:608:TYR:HB3	1.39	1.00
1:B:884:THR:HG23	1:B:887:ARG:H	1.27	0.98
1:C:851:GLN:OE1	1:C:855:LYS:HE3	1.63	0.97
1:A:581:LEU:CD2	1:A:583:LYS:HE3	1.95	0.97
1:C:762:SER:HB2	2:C:1010:HOH:O	1.64	0.96
1:A:737:VAL:HG13	1:A:807:ARG:NE	1.82	0.95
1:D:807:ARG:NH2	1:D:843:PRO:CD	2.30	0.94
1:C:790:GLN:O	1:C:790:GLN:HG2	1.63	0.94
1:D:543:HIS:CE1	1:D:586:THR:CG2	2.52	0.92
1:C:898:LEU:HB3	1:C:901:ASN:OD1	1.68	0.92
1:D:735:ALA:HB1	1:D:743:CYS:SG	2.10	0.92
1:B:687:MET:CA	1:B:692:MET:SD	2.56	0.92
1:A:566:PRO:HG2	1:D:741:GLN:NE2	1.84	0.91
1:B:817:LEU:CD2	1:B:835:ILE:HG21	1.99	0.91
1:A:867:GLY:HA2	1:A:905:LEU:CD2	1.99	0.91
1:A:670:ILE:HD12	1:A:727:LEU:HD13	1.51	0.91
1:B:884:THR:CG2	1:B:887:ARG:H	1.85	0.89
1:B:611:HIS:CE1	1:B:651:LYS:HB3	2.07	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:707:LEU:HD22	1:B:731:LEU:HD22	1.54	0.89
1:A:755:LYS:NZ	1:A:780:GLU:HB3	1.88	0.88
1:B:904:GLN:O	1:B:905:LEU:HG	1.73	0.87
1:A:754:TRP:CZ3	1:A:784:PHE:CE2	2.63	0.87
1:D:543:HIS:CE1	1:D:586:THR:HG23	2.10	0.87
1:D:543:HIS:HE1	1:D:586:THR:HG21	1.39	0.87
1:B:687:MET:HG2	1:B:692:MET:HE2	1.57	0.86
1:B:753:LYS:O	1:B:761:LEU:HD22	1.74	0.86
1:B:822:PHE:CD1	1:B:852:PHE:HZ	1.94	0.86
1:B:951:PHE:CE1	1:C:803:PHE:CZ	2.65	0.85
1:C:829:THR:HG21	1:C:863:LYS:HD3	1.59	0.85
1:D:692:MET:HE3	1:D:926:PHE:CE1	2.12	0.85
1:D:736:CYS:SG	1:D:743:CYS:HB3	2.15	0.85
1:D:687:MET:HG2	1:D:692:MET:HE1	1.60	0.84
1:C:733:LEU:O	1:C:737:VAL:HG23	1.76	0.84
1:A:621:THR:CG2	1:A:625:LYS:HE2	2.06	0.83
1:B:687:MET:HG2	1:B:692:MET:CE	2.07	0.83
1:C:730:GLN:O	1:C:734:LEU:HD13	1.78	0.83
1:A:806:CYS:CB	1:A:838:LEU:CD2	2.46	0.83
1:B:700:LYS:HE2	2:B:1014:HOH:O	1.79	0.82
1:A:581:LEU:HD23	1:A:583:LYS:HE3	1.55	0.82
1:A:803:PHE:HD1	1:A:838:LEU:HD11	1.45	0.82
1:D:751:PHE:HE1	1:D:785:LEU:HD21	1.44	0.81
1:D:543:HIS:CE1	1:D:586:THR:HG21	2.13	0.80
1:D:879:THR:OG1	1:D:911:THR:HG21	1.82	0.80
1:D:687:MET:HG2	1:D:692:MET:CE	2.12	0.80
1:D:807:ARG:NH2	1:D:843:PRO:HD2	1.97	0.80
1:C:665:LYS:HG2	1:C:706:LEU:HD23	1.64	0.79
1:B:769:LEU:CD2	1:B:800:GLN:HG2	2.13	0.79
1:C:534:THR:O	1:C:535:ILE:HD13	1.83	0.79
1:B:832:PHE:CZ	1:B:852:PHE:HE2	2.02	0.78
1:B:665:LYS:HG3	1:B:706:LEU:HD12	1.66	0.78
1:D:629:THR:HA	1:D:636:ARG:HH21	1.45	0.78
1:A:621:THR:HG23	1:A:625:LYS:HE2	1.66	0.77
1:A:581:LEU:HD21	1:A:583:LYS:HE3	1.65	0.77
1:B:769:LEU:HD21	1:B:800:GLN:HG2	1.65	0.77
1:B:884:THR:HG22	1:B:887:ARG:HG2	1.66	0.77
1:C:790:GLN:O	1:C:790:GLN:CG	2.32	0.77
1:B:868:SER:OG	1:B:871:ILE:HG12	1.85	0.77
1:B:850:TRP:CE2	1:B:854:ARG:HD2	2.20	0.76
1:D:735:ALA:CB	1:D:743:CYS:SG	2.73	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:817:LEU:CD2	1:B:835:ILE:CG2	2.63	0.76
1:D:692:MET:HE3	1:D:926:PHE:CD1	2.21	0.76
1:C:667:GLU:OE2	1:C:672:PRO:HG2	1.86	0.76
1:B:832:PHE:CD1	1:B:874:MET:HE2	2.21	0.75
1:B:884:THR:HG23	1:B:887:ARG:N	2.02	0.75
1:A:581:LEU:HD23	1:A:583:LYS:HZ2	1.53	0.74
1:B:716:TRP:NE1	1:B:746:ARG:NH1	2.36	0.74
1:D:807:ARG:HH22	1:D:843:PRO:HD3	1.51	0.74
1:C:604:MET:HG2	1:C:605:ASN:N	2.02	0.74
1:D:753:LYS:HB3	1:D:761:LEU:HD11	1.69	0.73
1:D:807:ARG:HH22	1:D:843:PRO:CG	2.01	0.73
1:D:543:HIS:HE1	1:D:586:THR:CG2	1.95	0.73
1:D:949:ARG:HD2	2:D:1018:HOH:O	1.89	0.73
1:B:580:PHE:HZ	1:B:587:ASP:OD2	1.71	0.72
1:D:567:LEU:CD2	1:D:602:VAL:HG22	2.19	0.72
1:A:532:LEU:HD23	1:A:547:GLU:OE1	1.89	0.72
1:A:532:LEU:CD2	1:A:547:GLU:OE1	2.37	0.72
1:D:746:ARG:HD2	2:D:1014:HOH:O	1.89	0.72
1:A:581:LEU:CD2	1:A:583:LYS:CE	2.57	0.72
1:B:853:LEU:HD11	1:B:874:MET:HB3	1.72	0.72
1:D:627:THR:O	1:D:627:THR:HG22	1.88	0.72
1:C:716:TRP:CE2	1:C:746:ARG:HD2	2.25	0.72
1:B:716:TRP:NE1	1:B:746:ARG:HH11	1.86	0.71
1:B:817:LEU:HD21	1:B:835:ILE:HG21	1.72	0.71
1:D:934:GLN:O	1:D:934:GLN:HG2	1.91	0.70
1:B:707:LEU:HD22	1:B:731:LEU:CD2	2.22	0.69
1:A:806:CYS:HB2	1:A:838:LEU:HD21	1.73	0.69
1:B:665:LYS:CG	1:B:706:LEU:HD12	2.22	0.69
1:B:832:PHE:HZ	1:B:852:PHE:HE2	1.38	0.69
1:B:577:VAL:HG12	2:B:1018:HOH:O	1.92	0.69
1:D:534:THR:HB	1:D:545:LYS:HB2	1.73	0.69
1:A:581:LEU:HD23	1:A:583:LYS:HZ1	1.58	0.69
1:A:733:LEU:O	1:A:737:VAL:HG23	1.92	0.69
1:B:832:PHE:CZ	1:B:852:PHE:CE2	2.80	0.69
1:D:664:LEU:HD12	1:D:706:LEU:HD21	1.73	0.69
1:A:737:VAL:CG1	1:A:807:ARG:HE	2.02	0.69
1:A:867:GLY:CA	1:A:905:LEU:CD2	2.66	0.69
1:B:580:PHE:CZ	1:B:587:ASP:OD2	2.46	0.69
1:A:566:PRO:HG2	1:D:741:GLN:HE21	1.57	0.68
1:B:832:PHE:HZ	1:B:852:PHE:CE2	2.12	0.68
1:B:544:MET:HE1	1:B:589:LEU:HD23	1.74	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:684:TYR:CD1	1:B:700:LYS:HE3	2.29	0.68
1:B:884:THR:CG2	1:B:887:ARG:HG2	2.23	0.68
1:C:667:GLU:OE2	1:C:672:PRO:CG	2.42	0.68
1:A:755:LYS:HZ1	1:A:780:GLU:HB3	1.58	0.67
1:B:611:HIS:CE1	1:B:651:LYS:CB	2.77	0.67
1:B:611:HIS:CD2	1:B:617:TRP:HE1	2.12	0.67
1:D:754:TRP:HZ3	1:D:785:LEU:HD23	1.60	0.67
1:B:609:ILE:HG21	1:B:646:LEU:HD21	1.77	0.66
1:C:677:LEU:HD22	1:C:681:ILE:HD11	1.75	0.66
1:C:685:LYS:HA	1:C:688:GLU:OE1	1.96	0.66
1:C:834:GLN:O	1:C:838:LEU:HG	1.96	0.66
1:A:755:LYS:HZ2	1:A:780:GLU:HB3	1.60	0.66
1:B:611:HIS:HE1	1:B:651:LYS:CB	2.03	0.66
1:B:716:TRP:HE1	1:B:746:ARG:NH1	1.94	0.66
1:A:681:ILE:HG21	1:D:949:ARG:O	1.95	0.65
1:A:722:VAL:HG11	1:D:934:GLN:O	1.96	0.65
1:A:581:LEU:HG	1:A:583:LYS:HG3	1.78	0.65
1:D:644:PHE:CE1	1:D:683:MET:HE1	2.32	0.65
1:A:907:CYS:O	1:A:911:THR:HG23	1.97	0.65
1:B:692:MET:HG2	2:B:1015:HOH:O	1.97	0.64
1:D:636:ARG:HD3	1:D:667:GLU:OE1	1.96	0.64
1:C:636:ARG:NH1	1:C:667:GLU:OE2	2.30	0.64
1:D:567:LEU:HD23	1:D:602:VAL:HG22	1.80	0.64
1:D:576:MET:HG2	1:D:577:VAL:H	1.62	0.64
1:D:602:VAL:HG12	1:D:604:MET:H	1.62	0.64
1:B:817:LEU:HD23	1:B:835:ILE:HG21	1.80	0.64
1:A:599:LYS:CD	1:A:639:LEU:HD21	2.29	0.63
1:C:755:LYS:HG3	1:C:784:PHE:CE2	2.32	0.63
1:C:824:GLY:O	1:C:825:ASP:OD1	2.16	0.63
1:D:836:LEU:HD23	1:D:874:MET:HG2	1.80	0.63
1:B:832:PHE:CE1	1:B:874:MET:HE2	2.32	0.63
1:A:599:LYS:HD2	1:A:639:LEU:HD21	1.81	0.63
1:A:726:MET:HE3	1:D:938:LEU:HB3	1.80	0.63
1:B:904:GLN:O	1:B:905:LEU:CG	2.46	0.63
1:C:735:ALA:HB1	1:C:740:TYR:HB3	1.81	0.63
1:A:566:PRO:HG2	1:D:741:GLN:HE22	1.62	0.62
1:B:611:HIS:HD2	1:B:617:TRP:HE1	1.47	0.62
1:B:951:PHE:CE1	1:C:807:ARG:HB2	2.35	0.62
1:D:667:GLU:CD	1:D:672:PRO:HG2	2.20	0.62
1:D:807:ARG:NH2	1:D:843:PRO:HD3	2.10	0.62
1:B:951:PHE:CD1	1:C:807:ARG:HD3	2.35	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:718:ASP:HB3	1:D:725:ARG:HE	1.66	0.61
1:B:817:LEU:HD21	1:B:835:ILE:CG2	2.29	0.61
1:B:951:PHE:CE1	1:C:807:ARG:HD3	2.36	0.61
1:D:576:MET:HG2	1:D:577:VAL:N	2.16	0.61
1:D:542:VAL:HG21	1:D:591:LEU:HD11	1.83	0.60
1:A:726:MET:HE3	1:D:938:LEU:CB	2.31	0.60
1:B:832:PHE:HD1	1:B:874:MET:HE2	1.66	0.60
1:C:604:MET:CG	1:C:605:ASN:N	2.64	0.60
1:B:540:ARG:NH2	1:B:592:PRO:HA	2.16	0.60
1:C:736:CYS:SG	1:C:743:CYS:HB3	2.41	0.60
1:A:794:SER:HB2	1:A:797:GLU:HB2	1.83	0.60
1:B:848:LEU:HD13	1:B:851:GLN:NE2	2.17	0.60
1:C:665:LYS:CG	1:C:706:LEU:HD23	2.31	0.60
1:D:777:GLN:NE2	1:D:807:ARG:O	2.33	0.59
1:D:819:ASP:O	1:D:822:PHE:HB3	2.02	0.59
1:A:876:MET:O	1:A:880:ASN:ND2	2.35	0.59
1:B:684:TYR:HB2	1:B:700:LYS:HZ1	1.67	0.59
1:D:754:TRP:N	1:D:761:LEU:HD12	2.17	0.59
1:A:623:LEU:HD21	1:A:631:VAL:CG2	2.33	0.59
1:A:754:TRP:CE3	1:A:784:PHE:HE2	2.20	0.59
1:D:754:TRP:HA	1:D:761:LEU:HD12	1.83	0.59
1:A:754:TRP:CZ3	1:A:784:PHE:HE2	2.14	0.59
1:C:662:LEU:HD21	1:C:932:TRP:CZ2	2.38	0.59
1:A:607:TYR:CE2	1:D:742:PRO:HG3	2.38	0.59
1:D:733:LEU:O	1:D:737:VAL:HG23	2.02	0.59
1:D:629:THR:HA	1:D:636:ARG:HH22	1.66	0.58
1:B:571:THR:HG22	1:B:598:ILE:HB	1.85	0.58
1:A:548:HIS:C	2:A:1011:HOH:O	2.45	0.58
1:A:596:GLU:HG3	2:A:1009:HOH:O	2.03	0.58
1:A:759:GLY:HA3	1:A:788:LYS:HE3	1.85	0.58
1:C:604:MET:HG2	1:C:605:ASN:H	1.67	0.58
1:C:905:LEU:HB2	1:C:908:VAL:HG12	1.85	0.58
1:D:636:ARG:HD3	1:D:667:GLU:CD	2.28	0.58
1:D:586:THR:HG22	1:D:587:ASP:N	2.18	0.58
1:A:670:ILE:CD1	1:A:727:LEU:HD13	2.30	0.58
1:C:535:ILE:HG21	1:C:600:PHE:CE2	2.38	0.57
1:B:684:TYR:CD1	1:B:700:LYS:CE	2.87	0.57
1:D:904:GLN:O	1:D:904:GLN:HG2	2.04	0.57
1:D:640:ILE:CD1	1:D:664:LEU:HD21	2.35	0.57
1:C:777:GLN:NE2	1:C:807:ARG:NH1	2.53	0.57
1:C:777:GLN:NE2	1:C:807:ARG:HH12	2.02	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:604:MET:CG	1:C:605:ASN:H	2.17	0.57
1:D:754:TRP:CA	1:D:761:LEU:HD12	2.34	0.57
1:D:754:TRP:CZ3	1:D:785:LEU:HD23	2.38	0.57
1:A:532:LEU:HG	1:A:547:GLU:OE1	2.05	0.56
1:A:803:PHE:CD1	1:A:838:LEU:HD11	2.35	0.56
1:B:716:TRP:CE2	1:B:746:ARG:HD2	2.40	0.56
1:C:648:SER:HG	1:C:921:TRP:CD1	2.23	0.56
1:D:576:MET:CG	1:D:577:VAL:H	2.18	0.56
1:B:822:PHE:CD1	1:B:852:PHE:CZ	2.85	0.56
1:B:544:MET:HE1	1:B:589:LEU:CD2	2.36	0.56
1:B:587:ASP:CG	1:B:588:VAL:H	2.14	0.56
1:C:682:PRO:O	1:C:686:LEU:HD13	2.05	0.56
1:C:777:GLN:HE22	1:C:807:ARG:NH1	2.04	0.56
1:D:632:SER:O	1:D:636:ARG:HG3	2.06	0.56
1:B:611:HIS:HD2	1:B:617:TRP:NE1	2.04	0.56
1:B:577:VAL:HG12	1:B:577:VAL:O	2.06	0.55
1:C:604:MET:CE	1:C:608:TYR:HB3	2.25	0.55
1:D:673:VAL:HG13	1:D:707:LEU:HD21	1.88	0.55
1:A:599:LYS:CD	1:A:639:LEU:HD11	2.36	0.55
1:D:742:PRO:O	1:D:746:ARG:CZ	2.55	0.55
1:A:850:TRP:CZ2	1:A:854:ARG:HD3	2.42	0.55
1:A:616:GLY:N	2:A:1002:HOH:O	2.40	0.55
1:A:856:ASN:C	2:A:1004:HOH:O	2.48	0.55
1:B:701:ALA:HB1	1:B:705:ARG:HH22	1.72	0.55
1:B:871:ILE:O	1:B:875:VAL:HG23	2.06	0.55
1:D:892:LYS:HG3	1:D:912:ILE:HD13	1.89	0.55
1:C:851:GLN:CD	1:C:855:LYS:HE3	2.31	0.55
1:B:587:ASP:CG	1:B:588:VAL:N	2.65	0.54
1:D:687:MET:HA	1:D:692:MET:SD	2.48	0.54
1:D:542:VAL:CG2	1:D:591:LEU:HD11	2.37	0.54
1:A:532:LEU:CG	1:A:547:GLU:OE1	2.55	0.54
1:D:754:TRP:HZ3	1:D:785:LEU:CD2	2.20	0.54
1:D:662:LEU:CD2	1:D:702:PHE:HZ	2.21	0.54
1:C:915:ILE:O	1:C:919:ILE:HG13	2.08	0.54
1:D:934:GLN:O	1:D:934:GLN:CG	2.55	0.54
1:B:692:MET:CG	2:B:1015:HOH:O	2.53	0.54
1:A:719:GLU:HG3	1:A:719:GLU:O	2.07	0.54
1:C:835:ILE:O	1:C:839:ILE:HD13	2.08	0.54
1:D:627:THR:HG22	1:D:630:ALA:HB2	1.90	0.54
1:B:692:MET:HE3	2:B:1015:HOH:O	2.07	0.53
1:B:951:PHE:HA	1:C:737:VAL:HG11	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:861:VAL:HB	1:D:866:LEU:HD23	1.90	0.53
1:C:888:LEU:HD13	1:C:919:ILE:HD12	1.91	0.53
1:B:702:PHE:CZ	1:B:932:TRP:HH2	2.27	0.53
1:D:763:LEU:CD1	1:D:771:VAL:HG11	2.38	0.53
1:D:938:LEU:O	1:D:939:GLU:HB3	2.08	0.53
1:A:801:ILE:O	1:A:805:LEU:HG	2.09	0.53
1:B:537:VAL:HG23	1:B:537:VAL:O	2.08	0.53
1:D:725:ARG:O	1:D:729:SER:HB3	2.08	0.53
1:D:689:LYS:HE3	1:D:846:TYR:HB2	1.91	0.53
1:D:692:MET:CE	1:D:922:MET:HE1	2.39	0.53
1:B:799:SER:HA	1:B:802:GLU:HB3	1.92	0.52
1:C:888:LEU:HD11	1:C:916:GLU:CG	2.39	0.52
1:B:753:LYS:O	1:B:761:LEU:CD2	2.52	0.52
1:C:837:THR:HG23	1:C:841:ARG:HH12	1.75	0.52
1:C:837:THR:HG23	1:C:841:ARG:NH1	2.24	0.52
1:A:838:LEU:HD23	1:A:838:LEU:O	2.09	0.52
1:D:807:ARG:HH21	1:D:843:PRO:HD2	1.74	0.52
1:D:662:LEU:HD11	1:D:932:TRP:HH2	1.74	0.52
1:D:837:THR:O	1:D:841:ARG:HG2	2.10	0.52
1:C:604:MET:HE2	1:C:608:TYR:CB	2.26	0.52
1:D:690:ARG:HD2	1:D:883:SER:HB2	1.92	0.51
1:B:868:SER:HG	1:B:871:ILE:HG12	1.76	0.51
1:B:884:THR:HG22	1:B:887:ARG:CG	2.38	0.51
1:D:636:ARG:HB2	1:D:672:PRO:HG3	1.92	0.51
1:A:736:CYS:SG	1:A:770:ALA:HB1	2.50	0.51
1:C:609:ILE:HG22	1:C:646:LEU:HD11	1.93	0.51
1:C:662:LEU:HD21	1:C:932:TRP:CH2	2.45	0.51
1:D:540:ARG:HB2	1:D:591:LEU:HB2	1.92	0.51
1:D:644:PHE:HE1	1:D:683:MET:HE1	1.75	0.51
1:A:782:TRP:CE3	1:A:813:LYS:HD3	2.46	0.51
1:A:787:SER:HA	1:A:790:GLN:HE21	1.75	0.51
1:A:887:ARG:O	1:A:891:VAL:HG23	2.10	0.51
1:B:540:ARG:NE	1:B:592:PRO:O	2.44	0.51
1:B:683:MET:HE2	1:B:921:TRP:HZ2	1.74	0.51
1:A:785:LEU:HB3	1:A:801:ILE:HG23	1.93	0.51
1:B:648:SER:HG	1:B:921:TRP:CD1	2.29	0.51
1:B:684:TYR:CE1	1:B:700:LYS:HE3	2.46	0.51
1:B:699:PHE:O	1:B:702:PHE:HB3	2.10	0.51
1:D:691:ASP:O	1:D:692:MET:HG3	2.11	0.51
1:C:534:THR:CG2	1:C:613:GLU:OE2	2.59	0.50
1:D:576:MET:CG	1:D:577:VAL:N	2.75	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:876:MET:HE3	1:D:907:CYS:HA	1.92	0.50
1:C:777:GLN:HE22	1:C:807:ARG:HH12	1.57	0.50
1:D:662:LEU:CD2	1:D:702:PHE:CZ	2.94	0.50
1:B:577:VAL:HG13	2:B:1001:HOH:O	2.10	0.50
1:D:677:LEU:HD22	1:D:734:LEU:HD11	1.92	0.50
1:D:794:SER:HA	2:D:1030:HOH:O	2.12	0.50
1:D:905:LEU:HD23	1:D:907:CYS:SG	2.52	0.50
1:B:653:SER:OG	1:B:656:LYS:HG2	2.12	0.50
1:D:807:ARG:O	1:D:807:ARG:HG3	2.11	0.50
1:A:536:THR:CG2	1:A:614:ASP:OD2	2.59	0.50
1:A:806:CYS:HB3	1:A:838:LEU:CD2	2.40	0.50
1:D:744:VAL:HG12	1:D:744:VAL:O	2.12	0.50
1:A:607:TYR:O	1:A:607:TYR:CD1	2.65	0.50
1:A:621:THR:CG2	1:A:625:LYS:CE	2.86	0.50
1:A:668:THR:O	1:A:669:GLU:OE2	2.29	0.50
1:D:537:VAL:HG13	1:D:542:VAL:HG22	1.93	0.50
1:D:662:LEU:HD21	1:D:932:TRP:CH2	2.46	0.50
1:B:733:LEU:HD12	1:B:769:LEU:HB3	1.94	0.49
1:A:795:SER:HB3	2:A:1022:HOH:O	2.10	0.49
1:A:814:LEU:HD22	1:A:839:ILE:CD1	2.41	0.49
1:B:684:TYR:HB2	1:B:700:LYS:NZ	2.27	0.49
1:D:531:PRO:O	1:D:609:ILE:HB	2.12	0.49
1:B:951:PHE:CZ	1:C:803:PHE:CZ	3.00	0.49
1:D:686:LEU:HD22	1:D:883:SER:OG	2.12	0.49
1:B:757:SER:HB3	1:B:761:LEU:HD13	1.94	0.49
1:C:833:PRO:O	1:C:834:GLN:C	2.56	0.49
1:D:810:ASN:OD1	1:D:812:GLU:HB3	2.13	0.49
1:D:813:LYS:O	1:D:816:TRP:HB3	2.12	0.49
1:B:696:GLU:O	1:B:699:PHE:HB3	2.13	0.49
1:C:730:GLN:O	1:C:734:LEU:CD1	2.58	0.49
1:A:777:GLN:CD	1:A:807:ARG:NH2	2.71	0.49
1:A:806:CYS:SG	1:A:838:LEU:HD22	2.53	0.49
1:B:530:PHE:HB2	1:B:531:PRO:HD2	1.95	0.49
1:B:631:VAL:CG1	1:B:635:ASP:HB3	2.43	0.48
1:B:692:MET:HE3	1:B:926:PHE:CD1	2.48	0.48
1:C:868:SER:OG	1:C:871:ILE:HD13	2.13	0.48
1:B:536:THR:HG22	1:B:537:VAL:N	2.28	0.48
1:B:951:PHE:CE1	1:C:803:PHE:HZ	2.24	0.48
1:C:733:LEU:HD12	1:C:769:LEU:HB3	1.94	0.48
1:D:690:ARG:CD	1:D:883:SER:HB2	2.43	0.48
1:B:534:THR:CG2	1:B:613:GLU:OE2	2.61	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:665:LYS:HG3	1:B:706:LEU:CD1	2.38	0.48
1:D:662:LEU:HD21	1:D:932:TRP:HH2	1.78	0.48
1:B:607:TYR:OH	1:B:645:GLN:HG3	2.12	0.48
1:B:736:CYS:SG	1:B:743:CYS:O	2.72	0.48
1:B:833:PRO:O	1:B:834:GLN:C	2.54	0.48
1:D:833:PRO:HG3	1:D:874:MET:HE2	1.96	0.48
1:D:905:LEU:HG	1:D:906:ARG:N	2.28	0.48
1:D:937:LYS:O	1:D:937:LYS:HG2	2.13	0.48
1:A:869:SER:HB2	1:D:666:HIS:HB3	1.95	0.48
1:C:670:ILE:HD12	1:C:723:SER:O	2.14	0.48
1:D:767:VAL:HG12	1:D:771:VAL:HG23	1.95	0.48
1:D:567:LEU:HD12	1:D:580:PHE:CD2	2.48	0.48
1:D:595:VAL:HG12	2:D:1008:HOH:O	2.14	0.48
1:A:546:GLN:OE1	1:A:563:TRP:HB2	2.14	0.48
1:B:577:VAL:CG1	2:B:1018:HOH:O	2.55	0.48
1:D:884:THR:OG1	1:D:887:ARG:HG2	2.14	0.48
1:A:599:LYS:HD2	1:A:639:LEU:CD2	2.44	0.47
1:C:888:LEU:HD11	1:C:916:GLU:HG2	1.95	0.47
1:A:658:LEU:O	1:A:661:SER:OG	2.30	0.47
1:D:662:LEU:HD11	1:D:932:TRP:CH2	2.50	0.47
1:A:876:MET:O	1:A:880:ASN:CG	2.57	0.47
1:C:851:GLN:OE1	1:C:855:LYS:CE	2.50	0.47
1:A:668:THR:O	1:A:668:THR:HG23	2.14	0.47
1:C:587:ASP:CG	1:C:588:VAL:H	2.22	0.47
1:A:599:LYS:HD3	1:A:639:LEU:HD11	1.96	0.47
1:A:625:LYS:NZ	1:A:659:ASP:OD1	2.46	0.47
1:D:542:VAL:HG23	1:D:591:LEU:HG	1.97	0.47
1:A:716:TRP:CZ2	1:A:732:LEU:HD22	2.50	0.47
1:C:580:PHE:CZ	1:C:587:ASP:OD2	2.68	0.47
1:D:796:THR:HG23	1:D:797:GLU:N	2.30	0.47
1:D:807:ARG:HH22	1:D:843:PRO:HG3	1.79	0.47
1:A:673:VAL:HG13	1:A:707:LEU:HD21	1.96	0.47
1:B:564:HIS:HB3	1:B:581:LEU:HD21	1.97	0.47
1:C:755:LYS:C	1:C:757:SER:H	2.23	0.47
1:B:571:THR:HG22	1:B:598:ILE:CB	2.44	0.47
1:C:716:TRP:NE1	1:C:746:ARG:HD2	2.29	0.47
1:B:850:TRP:NE1	1:B:854:ARG:HD2	2.30	0.47
1:B:832:PHE:CD1	1:B:874:MET:CE	2.97	0.46
1:D:571:THR:HB	1:D:595:VAL:HG21	1.97	0.46
1:A:610:VAL:O	1:A:646:LEU:HD11	2.15	0.46
1:D:692:MET:HE1	1:D:922:MET:HE1	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:LEU:HD22	1:A:883:SER:HB3	1.98	0.46
1:A:754:TRP:HZ3	1:A:784:PHE:CE2	2.31	0.46
1:C:572:SER:HB3	1:C:596:GLU:HB2	1.97	0.46
1:D:586:THR:CG2	1:D:587:ASP:N	2.78	0.46
1:A:813:LYS:CB	2:A:1001:HOH:O	2.33	0.46
1:B:786:TYR:O	1:B:786:TYR:CD1	2.69	0.46
1:D:691:ASP:C	1:D:692:MET:HG3	2.40	0.46
1:D:754:TRP:CZ3	1:D:785:LEU:CD2	2.98	0.46
1:D:572:SER:HB3	1:D:597:TRP:H	1.81	0.46
1:D:658:LEU:C	1:D:660:LEU:H	2.24	0.46
1:B:580:PHE:CD2	1:B:589:LEU:HD23	2.51	0.45
1:B:701:ALA:HB1	1:B:705:ARG:NH2	2.30	0.45
1:C:663:TYR:C	1:C:665:LYS:N	2.74	0.45
1:C:580:PHE:HZ	1:C:587:ASP:OD2	1.99	0.45
1:A:718:ASP:O	1:A:719:GLU:C	2.60	0.45
1:B:736:CYS:SG	1:B:743:CYS:C	2.99	0.45
1:D:531:PRO:CG	1:D:604:MET:SD	3.05	0.45
1:D:713:LYS:HG3	1:D:713:LYS:O	2.15	0.45
1:A:838:LEU:HD23	1:A:838:LEU:C	2.42	0.45
1:B:859:LYS:O	1:B:862:GLN:HB2	2.17	0.45
1:D:580:PHE:CG	1:D:581:LEU:N	2.84	0.45
1:A:871:ILE:HD13	1:A:874:MET:HE2	1.99	0.45
1:B:824:GLY:HA2	1:B:827:ILE:O	2.16	0.45
1:D:600:PHE:HB2	1:D:610:VAL:HG11	1.99	0.45
1:A:769:LEU:HD22	1:A:803:PHE:CD2	2.52	0.45
1:B:660:LEU:O	1:B:663:TYR:HD1	2.00	0.45
1:A:534:THR:HB	1:A:545:LYS:HB3	1.99	0.45
1:C:901:ASN:C	1:C:903:SER:N	2.74	0.45
1:A:888:LEU:HD11	1:A:892:LYS:HE3	1.99	0.45
1:A:754:TRP:HH2	1:A:788:LYS:HG3	1.82	0.45
1:B:572:SER:HB3	1:B:596:GLU:HB3	1.98	0.44
1:A:601:ASN:HB2	1:A:608:TYR:CE2	2.52	0.44
1:D:636:ARG:HD3	1:D:667:GLU:OE2	2.17	0.44
1:D:699:PHE:O	1:D:702:PHE:HB3	2.16	0.44
1:A:664:LEU:HB2	1:A:706:LEU:HD11	2.00	0.44
1:D:654:ILE:HD11	1:D:683:MET:HE1	1.99	0.44
1:C:563:TRP:CE2	1:C:565:VAL:HG22	2.53	0.44
1:D:735:ALA:HB3	1:D:743:CYS:SG	2.57	0.44
1:D:763:LEU:HD11	1:D:771:VAL:HG11	2.00	0.44
1:A:533:ILE:HG22	1:A:535:ILE:HD11	1.99	0.44
1:C:535:ILE:HG21	1:C:600:PHE:CD2	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:543:HIS:CE1	2:C:1020:HOH:O	2.70	0.44
1:C:602:VAL:HB	1:C:608:TYR:CD1	2.53	0.44
1:A:670:ILE:HG23	1:A:671:MET:N	2.33	0.44
1:B:535:ILE:HD12	1:B:600:PHE:CG	2.52	0.44
1:C:824:GLY:HA3	1:C:829:THR:OG1	2.18	0.44
1:A:879:THR:O	1:A:915:ILE:HD11	2.18	0.44
1:D:815:GLN:OE1	1:D:848:LEU:HD12	2.17	0.44
1:B:549:TYR:HE1	1:B:550:MET:SD	2.41	0.44
1:B:951:PHE:CZ	1:C:807:ARG:HB2	2.53	0.44
1:C:565:VAL:O	1:C:581:LEU:HA	2.18	0.44
1:D:692:MET:CE	1:D:926:PHE:CE1	2.94	0.44
1:A:905:LEU:HG	1:A:906:ARG:N	2.33	0.43
1:B:905:LEU:HB2	1:B:908:VAL:HG23	2.00	0.43
1:A:650:GLY:C	1:A:652:LEU:H	2.26	0.43
1:C:587:ASP:CG	1:C:588:VAL:N	2.77	0.43
1:C:911:THR:O	1:C:914:THR:N	2.51	0.43
1:A:737:VAL:HG11	1:D:951:PHE:HA	1.99	0.43
1:B:832:PHE:CE2	1:B:852:PHE:CE2	3.06	0.43
1:C:537:VAL:HG22	1:C:542:VAL:HG22	2.00	0.43
1:C:898:LEU:O	1:C:899:LYS:C	2.61	0.43
1:D:542:VAL:CG2	1:D:591:LEU:CD1	2.96	0.43
1:D:681:ILE:HA	1:D:684:TYR:CE2	2.54	0.43
1:D:736:CYS:O	1:D:737:VAL:C	2.61	0.43
1:D:763:LEU:HD13	1:D:771:VAL:HG11	1.99	0.43
1:C:601:ASN:ND2	1:C:602:VAL:O	2.51	0.43
1:A:532:LEU:HD22	1:A:649:ILE:CD1	2.48	0.43
1:C:870:SER:O	1:C:871:ILE:C	2.60	0.43
1:D:636:ARG:CD	1:D:667:GLU:OE2	2.66	0.43
1:C:534:THR:HG21	1:C:613:GLU:OE2	2.19	0.43
1:D:797:GLU:O	1:D:798:LYS:C	2.61	0.43
1:A:644:PHE:CE1	1:A:683:MET:HE1	2.53	0.43
1:A:897:SER:C	1:A:899:LYS:H	2.27	0.43
1:B:687:MET:HE1	1:B:699:PHE:CD2	2.54	0.43
1:A:857:TRP:N	2:A:1004:HOH:O	2.51	0.43
1:D:891:VAL:O	1:D:895:PHE:HD2	2.02	0.43
1:A:599:LYS:HD2	1:A:639:LEU:CG	2.49	0.42
1:A:905:LEU:HG	1:A:906:ARG:H	1.83	0.42
1:B:746:ARG:HD3	1:B:750:TYR:CE2	2.54	0.42
1:C:816:TRP:CE2	1:C:820:GLU:HG3	2.54	0.42
1:D:751:PHE:HE1	1:D:785:LEU:CD2	2.24	0.42
1:D:771:VAL:HG12	1:D:772:PHE:CD1	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:687:MET:HG2	1:B:692:MET:HE1	1.99	0.42
1:D:879:THR:OG1	1:D:911:THR:CG2	2.61	0.42
1:D:909:GLN:HG2	2:D:1036:HOH:O	2.18	0.42
1:A:668:THR:O	1:A:669:GLU:CD	2.63	0.42
1:B:549:TYR:CE1	1:B:550:MET:SD	3.13	0.42
1:A:769:LEU:HD22	1:A:803:PHE:HD2	1.85	0.42
1:C:769:LEU:HA	1:C:769:LEU:HD23	1.71	0.42
1:A:875:VAL:HG13	1:A:895:PHE:CZ	2.55	0.42
1:B:746:ARG:HD3	1:B:750:TYR:HE2	1.84	0.42
1:B:757:SER:O	1:B:758:ASN:C	2.63	0.42
1:A:933:LEU:C	1:A:935:SER:H	2.28	0.42
1:C:701:ALA:HB1	1:C:705:ARG:HH22	1.85	0.42
1:C:784:PHE:CD1	1:C:784:PHE:C	2.96	0.42
1:D:859:LYS:HG3	1:D:863:LYS:HE2	2.01	0.42
1:A:813:LYS:N	2:A:1001:HOH:O	2.52	0.42
1:A:875:VAL:HG12	1:A:911:THR:HG21	2.02	0.42
1:B:619:SER:O	1:C:830:GLN:NE2	2.52	0.42
1:B:665:LYS:HG2	1:B:706:LEU:HD12	2.00	0.42
1:B:684:TYR:CG	1:B:700:LYS:HE3	2.54	0.42
1:B:701:ALA:CB	1:B:705:ARG:HH12	2.32	0.42
1:B:879:THR:OG1	1:B:911:THR:HG21	2.20	0.42
1:C:734:LEU:O	1:C:735:ALA:C	2.62	0.42
1:D:640:ILE:HD11	1:D:664:LEU:HD21	2.01	0.42
1:A:536:THR:HG23	1:A:614:ASP:OD2	2.18	0.41
1:B:721:SER:O	1:B:722:VAL:C	2.62	0.41
1:C:568:THR:HG22	1:C:569:PHE:N	2.35	0.41
1:C:639:LEU:O	1:C:643:ALA:HB2	2.20	0.41
1:C:741:GLN:HB3	1:C:742:PRO:HD3	2.01	0.41
1:C:767:VAL:O	1:C:767:VAL:HG12	2.19	0.41
1:A:933:LEU:C	1:A:935:SER:N	2.78	0.41
1:B:701:ALA:O	1:B:705:ARG:HB2	2.21	0.41
1:B:951:PHE:CZ	1:C:803:PHE:CE1	3.08	0.41
1:C:787:SER:O	1:C:788:LYS:C	2.63	0.41
1:C:904:GLN:C	1:C:905:LEU:HG	2.45	0.41
1:B:711:ILE:HG12	1:B:731:LEU:HB3	2.02	0.41
1:D:658:LEU:C	1:D:660:LEU:N	2.79	0.41
1:D:687:MET:HG2	1:D:692:MET:HE2	1.96	0.41
1:A:728:ARG:HE	1:A:728:ARG:HB3	1.58	0.41
1:A:782:TRP:CZ3	1:A:813:LYS:HD3	2.54	0.41
1:C:662:LEU:HD21	1:C:932:TRP:HZ2	1.86	0.41
1:C:933:LEU:C	1:C:935:SER:H	2.29	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:567:LEU:HD12	1:D:580:PHE:HD2	1.83	0.41
1:D:853:LEU:C	1:D:853:LEU:HD23	2.45	0.41
1:A:667:GLU:OE2	1:A:668:THR:N	2.54	0.41
1:B:683:MET:HE2	1:B:921:TRP:CZ2	2.55	0.41
1:C:670:ILE:HD12	1:C:727:LEU:HB2	2.02	0.41
1:C:888:LEU:CD1	1:C:919:ILE:HD12	2.49	0.41
1:D:908:VAL:O	1:D:912:ILE:HG13	2.21	0.41
1:C:690:ARG:NE	1:C:692:MET:HE1	2.36	0.41
1:D:567:LEU:HD22	1:D:602:VAL:HG22	1.98	0.41
1:A:532:LEU:HD22	1:A:649:ILE:HD12	2.03	0.41
1:A:705:ARG:NH1	1:A:936:GLU:OE1	2.47	0.41
1:A:831:GLU:O	1:A:835:ILE:HD12	2.20	0.41
1:B:571:THR:HG21	1:B:595:VAL:HG21	2.02	0.41
1:B:604:MET:SD	1:B:608:TYR:CD1	3.14	0.41
1:B:746:ARG:HG2	1:B:750:TYR:CD2	2.55	0.41
1:B:814:LEU:HA	1:B:814:LEU:HD23	1.75	0.41
1:C:598:ILE:O	1:C:598:ILE:HG23	2.21	0.41
1:C:640:ILE:CD1	1:C:664:LEU:HD21	2.51	0.41
1:D:732:LEU:HD23	1:D:732:LEU:HA	1.88	0.41
1:B:663:TYR:C	1:B:665:LYS:N	2.79	0.41
1:B:908:VAL:O	1:B:912:ILE:HG13	2.21	0.41
1:D:537:VAL:HG22	1:D:542:VAL:HG13	2.02	0.41
1:A:546:GLN:O	1:A:547:GLU:HG3	2.21	0.40
1:A:871:ILE:HD13	1:A:874:MET:CE	2.51	0.40
1:B:692:MET:CE	1:B:922:MET:CE	2.79	0.40
1:D:601:ASN:O	1:D:602:VAL:C	2.64	0.40
1:D:801:ILE:O	1:D:805:LEU:HG	2.20	0.40
1:A:722:VAL:HG21	1:D:931:VAL:HG13	2.03	0.40
1:A:813:LYS:CA	2:A:1001:HOH:O	2.65	0.40
1:A:930:ARG:O	1:A:934:GLN:HG3	2.20	0.40
1:C:744:VAL:HG13	1:C:774:VAL:HG21	2.03	0.40
1:D:561:TYR:CB	2:D:1031:HOH:O	2.69	0.40
1:D:667:GLU:HG2	1:D:672:PRO:HB2	2.02	0.40
1:B:647:VAL:HG11	1:B:654:ILE:HD13	2.03	0.40
1:D:602:VAL:HB	1:D:608:TYR:CB	2.52	0.40
1:A:662:LEU:HD21	1:A:932:TRP:CH2	2.57	0.40
1:B:695:VAL:O	1:B:696:GLU:C	2.63	0.40
1:B:716:TRP:CD2	1:B:746:ARG:HD2	2.57	0.40
1:D:633:SER:O	1:D:636:ARG:HB2	2.21	0.40
1:A:754:TRP:CH2	1:A:788:LYS:HG3	2.57	0.40
1:C:584:THR:O	1:C:585:LYS:C	2.65	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:846:TYR:CG	1:C:847:PRO:HD3	2.57	0.40
1:C:868:SER:O	1:C:869:SER:C	2.65	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	384/423 (91%)	338 (88%)	45 (12%)	1 (0%)	36	70
1	B	388/423 (92%)	332 (86%)	53 (14%)	3 (1%)	16	50
1	C	389/423 (92%)	336 (86%)	52 (13%)	1 (0%)	36	70
1	D	380/423 (90%)	316 (83%)	60 (16%)	4 (1%)	11	43
All	All	1541/1692 (91%)	1322 (86%)	210 (14%)	9 (1%)	21	56

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	719	GLU
1	B	758	ASN
1	D	745	GLN
1	B	569	PHE
1	D	602	VAL
1	B	754	TRP
1	C	899	LYS
1	D	590	ILE
1	D	592	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	340/379 (90%)	334 (98%)	6 (2%)	51	77
1	B	355/379 (94%)	343 (97%)	12 (3%)	32	66
1	C	353/379 (93%)	341 (97%)	12 (3%)	32	66
1	D	350/379 (92%)	340 (97%)	10 (3%)	37	70
All	All	1398/1516 (92%)	1358 (97%)	40 (3%)	37	70

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	544	MET
1	A	583	LYS
1	A	588	VAL
1	A	627	THR
1	A	674	PHE
1	A	762	SER
1	B	535	ILE
1	B	569	PHE
1	B	579	ARG
1	B	707	LEU
1	B	715	THR
1	B	737	VAL
1	B	762	SER
1	B	785	LEU
1	B	829	THR
1	B	911	THR
1	B	912	ILE
1	B	938	LEU
1	C	538	ARG
1	C	562	LEU
1	C	595	VAL
1	C	610	VAL
1	C	646	LEU
1	C	662	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	702	PHE
1	C	780	GLU
1	C	814	LEU
1	C	837	THR
1	C	863	LYS
1	C	912	ILE
1	D	571	THR
1	D	656	LYS
1	D	724	GLU
1	D	798	LYS
1	D	808	THR
1	D	837	THR
1	D	888	LEU
1	D	912	ILE
1	D	936	GLU
1	D	950	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	578	HIS
1	A	675	GLN
1	A	738	HIS
1	A	739	ASN
1	A	790	GLN
1	A	830	GLN
1	A	834	GLN
1	A	856	ASN
1	A	918	ASN
1	A	934	GLN
1	B	611	HIS
1	B	645	GLN
1	B	675	GLN
1	B	745	GLN
1	B	760	ASN
1	B	809	GLN
1	B	810	ASN
1	B	851	GLN
1	B	904	GLN
1	C	611	HIS
1	C	628	HIS
1	C	675	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	678	ASN
1	C	738	HIS
1	C	777	GLN
1	C	809	GLN
1	C	830	GLN
1	C	934	GLN
1	D	543	HIS
1	D	641	ASN
1	D	741	GLN
1	D	909	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	396/423 (93%)	-1.37	0 100 100	33, 56, 80, 97	2 (0%)
1	B	399/423 (94%)	-1.33	0 100 100	24, 55, 80, 101	6 (1%)
1	C	398/423 (94%)	-1.34	0 100 100	25, 56, 84, 104	5 (1%)
1	D	398/423 (94%)	-1.35	0 100 100	28, 54, 84, 127	9 (2%)
All	All	1591/1692 (94%)	-1.35	0 100 100	24, 55, 82, 127	22 (1%)

There are no RSRZ outliers to report.

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.