



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 03:54 pm BST

PDB ID : 6P5L
Title : Crystal Structure of Ubl123 with an EZH2 peptide
Authors : Saridakis, V.
Deposited on : 2019-05-30
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

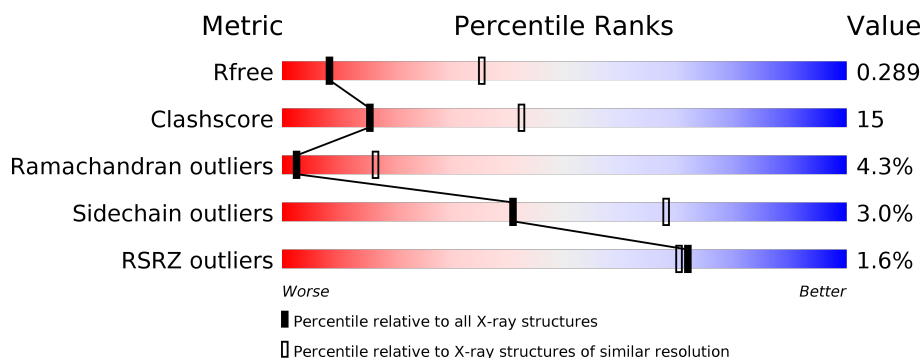
1 Overall quality at a glance

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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 on 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	356	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 63%, yellow 28%, orange 5%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 63% 28% 5% • </div> </div>
1	B	356	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, green 61%, yellow 30%, orange 5%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 61% 30% • • </div> </div>
2	D	8	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 25%, green 38%, yellow 38%, grey 25%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 25% 38% 38% 25% </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5622 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 carboxyl-terminal hydrolase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2784	1760	474	532	18			
1	B	340	Total	C	N	O	S	0	0	0
			2780	1757	477	530	16			

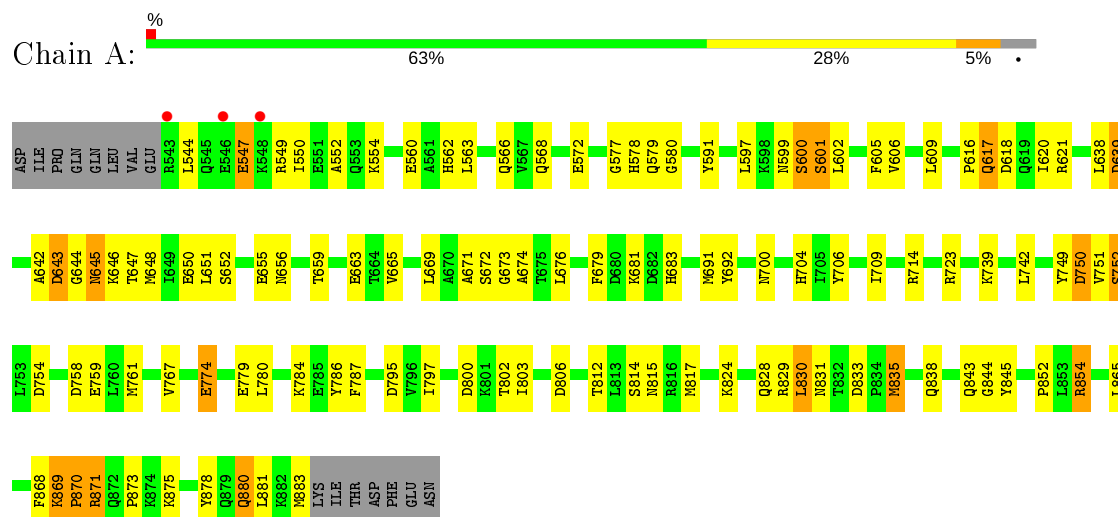
- Molecule 2 is a protein called PRO-ARG-LYS-LYS-LYS-ARG-LYS-HIS.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	6	Total	C	N	O	0	0	0
			58	36	16	6			

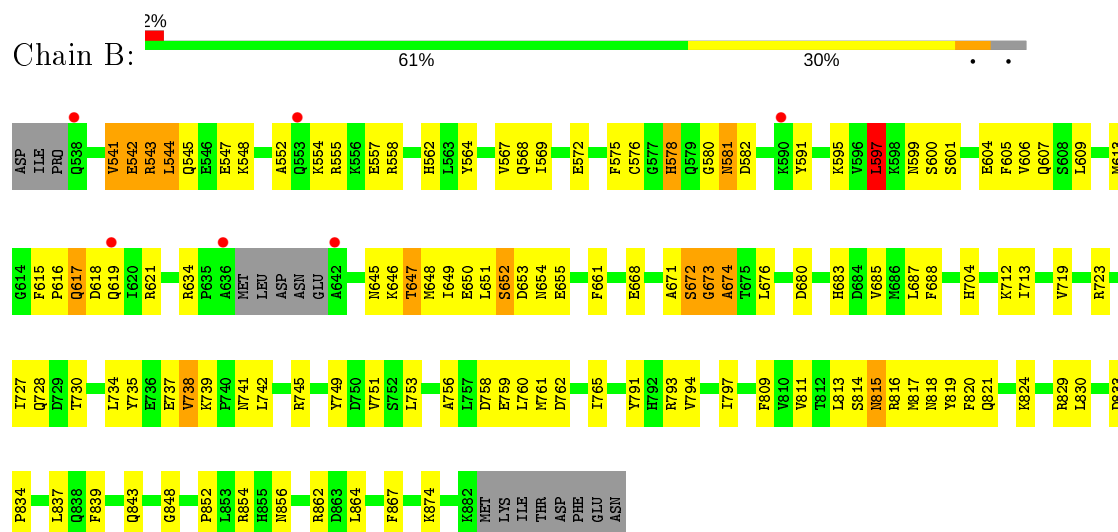
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 carboxyl-terminal hydrolase 7



• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7



• Molecule 2: PRO-ARG-LYS-LYS-LYS-ARG-LYS-HIS



PRO						
R490						
R491						
K492						
R493						
R494						
K495						
HIS						

4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	165.45Å 165.45Å 110.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.61 – 3.30 29.61 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.61-3.30) 99.5 (29.61-3.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 3.31Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.231 , 0.289 0.231 , 0.289	Depositor DCC
R_{free} test set	1993 reflections (8.43%)	wwPDB-VP
Wilson B-factor (Å ²)	117.6	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 66.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5622	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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	0.44	0/2843	1.09	17/3840 (0.4%)
1	B	0.39	0/2838	0.86	3/3832 (0.1%)
2	D	0.37	0/57	0.71	0/69
All	All	0.42	0/5738	0.98	20/7741 (0.3%)

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
All	All	0	2

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	645	ASN	CB-CG-OD1	28.58	178.76	121.60
1	A	645	ASN	CB-CG-ND2	-16.71	76.59	116.70
1	A	880	GLN	CG-CD-NE2	-13.98	83.14	116.70
1	B	597	LEU	CB-CG-CD1	13.17	133.38	111.00
1	B	544	LEU	CB-CG-CD2	-11.79	90.95	111.00
1	A	830	LEU	CA-CB-CG	10.01	138.32	115.30
1	A	880	GLN	CA-CB-CG	-9.17	93.23	113.40
1	B	544	LEU	CB-CG-CD1	8.61	125.64	111.00
1	A	645	ASN	OD1-CG-ND2	-8.38	102.62	121.90
1	A	784	LYS	CD-CE-NZ	7.99	130.07	111.70
1	A	865	LEU	CB-CG-CD2	-7.22	98.72	111.00
1	A	875	LYS	CD-CE-NZ	-7.18	95.19	111.70
1	A	830	LEU	CB-CG-CD1	6.33	121.77	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	880	GLN	N-CA-CB	-6.33	99.21	110.60
1	A	871	ARG	CB-CA-C	-5.67	99.06	110.40
1	A	880	GLN	CG-CD-OE1	5.59	132.79	121.60
1	A	871	ARG	N-CA-CB	5.37	120.26	110.60
1	A	880	GLN	CB-CG-CD	5.19	125.09	111.60
1	A	774	GLU	CA-CB-CG	-5.17	102.03	113.40
1	A	547	GLU	CA-CB-CG	-5.11	102.16	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	880	GLN	Sidechain
1	B	607	GLN	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	2784	0	2727	86	0
1	B	2780	0	2725	87	0
2	D	58	0	77	4	0
All	All	5622	0	5529	165	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (165) 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:719:VAL:HG12	1:B:723:ARG:HD2	1.50	0.91
1:B:578:HIS:NE2	1:B:580:GLY:O	2.10	0.85
1:A:869:LYS:HB3	1:A:870:PRO:HD2	1.63	0.80
1:A:704:HIS:O	1:A:723:ARG:NH2	2.16	0.79
1:B:647:THR:N	1:B:650:GLU:OE2	2.22	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:541:VAL:HG13	1:B:544:LEU:HD12	1.72	0.71
1:B:672:SER:O	1:B:674:ALA:N	2.24	0.70
1:A:779:GLU:OE1	1:A:779:GLU:N	2.25	0.69
1:B:621:ARG:HD2	1:B:676:LEU:HD21	1.74	0.68
1:B:815:ASN:HB3	1:B:862:ARG:HB2	1.76	0.68
1:A:671:ALA:O	1:A:673:GLY:N	2.25	0.67
1:B:616:PRO:O	1:B:618:ASP:N	2.28	0.67
1:B:542:GLU:O	1:B:545:GLN:N	2.28	0.66
1:B:548:LYS:O	1:B:552:ALA:N	2.29	0.65
1:A:616:PRO:O	1:A:618:ASP:N	2.30	0.65
1:A:691:MET:HE2	1:A:700:ASN:HB2	1.78	0.65
1:A:761:MET:SD	2:D:495:LYS:HE2	2.38	0.63
1:A:652:SER:OG	1:A:655:GLU:O	2.16	0.63
1:A:646:LYS:HB2	1:A:651:LEU:HD21	1.81	0.62
1:A:691:MET:HG2	1:A:692:TYR:N	2.14	0.62
1:B:713:ILE:HG12	1:B:753:LEU:HD23	1.81	0.61
1:B:818:ASN:ND2	1:B:821:GLN:HG3	2.14	0.61
1:B:555:ARG:HA	1:B:558:ARG:NE	2.16	0.60
1:B:760:LEU:HD12	1:B:761:MET:H	1.66	0.60
1:B:758:ASP:N	1:B:758:ASP:OD1	2.33	0.60
1:A:642:ALA:C	1:A:644:GLY:H	2.04	0.59
1:A:671:ALA:C	1:A:673:GLY:H	2.05	0.59
1:A:843:GLN:O	1:A:845:TYR:N	2.34	0.59
1:A:679:PHE:HD1	1:A:706:TYR:HD2	1.50	0.59
1:A:759:GLU:HG2	2:D:492:LYS:HD2	1.85	0.58
1:A:852:PRO:HB2	1:B:854:ARG:HH22	1.67	0.58
1:A:639:ASP:OD2	1:A:642:ALA:HB3	2.04	0.58
1:B:652:SER:OG	1:B:655:GLU:N	2.37	0.58
1:A:566:GLN:N	1:A:656:ASN:OD1	2.31	0.57
1:A:639:ASP:HB3	1:A:643:ASP:H	1.70	0.57
1:A:620:ILE:HA	1:A:676:LEU:HD13	1.86	0.57
1:A:797:ILE:CD1	1:A:873:PRO:HB2	2.35	0.56
1:B:567:VAL:HG11	1:B:605:PHE:CE2	2.40	0.56
1:A:835:MET:HG3	1:B:834:PRO:HB2	1.87	0.55
1:A:852:PRO:HB2	1:B:854:ARG:NH2	2.21	0.55
1:B:727:ILE:O	1:B:730:THR:OG1	2.21	0.55
1:A:800:ASP:N	1:A:806:ASP:OD2	2.32	0.55
1:A:714:ARG:HD2	1:A:750:ASP:OD1	2.07	0.55
1:B:543:ARG:O	1:B:547:GLU:HG3	2.07	0.55
1:A:767:VAL:HG21	1:A:787:PHE:HE2	1.72	0.54
1:A:577:GLY:O	1:A:579:GLN:NE2	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:597:LEU:O	1:B:600:SER:OG	2.26	0.53
1:B:811:VAL:HG22	1:B:829:ARG:NH2	2.25	0.52
1:A:647:THR:O	1:A:650:GLU:HG2	2.09	0.52
1:B:554:LYS:O	1:B:558:ARG:NE	2.41	0.52
1:A:679:PHE:HD1	1:A:706:TYR:CD2	2.28	0.52
1:A:800:ASP:HB2	1:A:878:TYR:CZ	2.44	0.52
1:B:621:ARG:HD2	1:B:676:LEU:CD2	2.38	0.52
1:B:817:MET:HA	1:B:821:GLN:OE1	2.09	0.52
1:B:572:GLU:HB2	1:B:661:PHE:HE1	1.75	0.52
1:A:758:ASP:N	1:A:758:ASP:OD1	2.43	0.51
1:B:809:PHE:CZ	1:B:830:LEU:HD11	2.45	0.51
1:B:680:ASP:OD1	1:B:683:HIS:N	2.43	0.51
2:D:494:ARG:HG3	2:D:495:LYS:H	1.76	0.51
1:B:634:ARG:NH2	1:B:738:VAL:O	2.43	0.51
1:A:602:LEU:HA	1:A:648:MET:CE	2.41	0.51
1:A:572:GLU:OE2	1:A:704:HIS:ND1	2.44	0.51
1:A:797:ILE:HD12	1:A:873:PRO:HB2	1.93	0.51
1:B:741:ASN:HB2	1:B:791:TYR:CD2	2.46	0.50
1:A:665:VAL:HG23	1:A:676:LEU:HD12	1.93	0.50
1:A:838:GLN:OE1	1:B:856:ASN:HB3	2.11	0.50
1:A:560:GLU:O	1:A:563:LEU:HB2	2.12	0.49
1:A:616:PRO:C	1:A:618:ASP:H	2.15	0.49
1:B:734:LEU:HD13	1:B:749:TYR:CZ	2.47	0.49
1:B:578:HIS:CD2	1:B:580:GLY:H	2.30	0.49
1:B:564:TYR:CD2	1:B:595:LYS:HE2	2.47	0.49
1:B:645:ASN:O	1:B:646:LYS:HG2	2.12	0.49
1:A:547:GLU:HG2	1:A:550:ILE:HD11	1.94	0.49
1:A:759:GLU:HA	2:D:492:LYS:HE3	1.94	0.49
1:B:704:HIS:O	1:B:723:ARG:NH2	2.46	0.49
1:B:735:TYR:HD2	1:B:745:ARG:HA	1.78	0.48
1:B:837:LEU:HD13	1:B:839:PHE:CZ	2.48	0.48
1:A:602:LEU:O	1:A:606:VAL:HG23	2.14	0.48
1:A:835:MET:HE3	1:B:819:TYR:HE2	1.79	0.48
1:A:835:MET:HE3	1:B:819:TYR:CE2	2.49	0.48
1:B:797:ILE:N	1:B:874:LYS:O	2.34	0.48
1:B:600:SER:HB2	1:B:604:GLU:OE1	2.14	0.47
1:B:824:LYS:CD	1:B:834:PRO:HG3	2.44	0.47
1:A:597:LEU:O	1:A:600:SER:HB3	2.15	0.47
1:A:854:ARG:NH1	1:B:854:ARG:HD2	2.29	0.47
1:A:602:LEU:HA	1:A:648:MET:HE1	1.95	0.47
1:A:709:ILE:HG22	1:A:754:ASP:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:843:GLN:HG3	1:B:848:GLY:O	2.14	0.47
1:A:639:ASP:CB	1:A:643:ASP:H	2.27	0.46
1:B:688:PHE:CE2	1:B:704:HIS:HB3	2.50	0.46
1:A:824:LYS:O	1:A:828:GLN:HG3	2.16	0.46
1:A:800:ASP:OD1	1:A:802:THR:OG1	2.22	0.46
1:B:651:LEU:C	1:B:653:ASP:H	2.19	0.46
1:B:811:VAL:HG22	1:B:829:ARG:CZ	2.45	0.46
1:A:709:ILE:CG2	1:A:754:ASP:HB2	2.45	0.46
1:A:568:GLN:O	1:A:659:THR:HA	2.15	0.46
1:A:868:PHE:O	1:A:869:LYS:HD3	2.16	0.45
1:A:568:GLN:HB3	1:A:591:TYR:CD2	2.51	0.45
1:B:554:LYS:O	1:B:558:ARG:NH2	2.50	0.45
1:B:568:GLN:HB3	1:B:591:TYR:CD2	2.52	0.45
1:B:739:LYS:HG2	1:B:742:LEU:HB3	1.98	0.45
1:A:620:ILE:CA	1:A:676:LEU:HD13	2.46	0.45
1:B:634:ARG:CZ	1:B:765:ILE:HD12	2.47	0.45
1:B:609:LEU:HD11	1:B:613:MET:CE	2.47	0.45
1:A:833:ASP:OD2	1:B:824:LYS:NZ	2.37	0.45
1:A:843:GLN:C	1:A:845:TYR:H	2.19	0.45
1:B:651:LEU:O	1:B:653:ASP:N	2.50	0.45
1:A:621:ARG:HD2	1:A:706:TYR:OH	2.16	0.45
1:B:727:ILE:HG23	1:B:728:GLN:O	2.17	0.45
1:B:794:VAL:N	1:B:813:LEU:O	2.47	0.44
1:B:820:PHE:O	1:B:824:LYS:HG2	2.17	0.44
1:A:642:ALA:C	1:A:644:GLY:N	2.71	0.44
1:A:780:LEU:HD13	1:A:786:TYR:HA	2.00	0.44
1:B:572:GLU:HB2	1:B:661:PHE:CE1	2.53	0.44
1:B:581:ASN:O	1:B:582:ASP:HB2	2.17	0.44
1:B:751:VAL:CG2	1:B:756:ALA:HB2	2.48	0.44
1:A:605:PHE:O	1:A:609:LEU:N	2.49	0.44
1:B:671:ALA:O	1:B:673:GLY:N	2.49	0.44
1:B:837:LEU:HD23	1:B:837:LEU:HA	1.73	0.43
1:A:549:ARG:HA	1:A:552:ALA:HB3	2.00	0.43
1:A:749:TYR:O	1:A:751:VAL:N	2.49	0.43
1:A:669:LEU:HB3	1:A:674:ALA:CB	2.49	0.43
1:A:683:HIS:O	1:A:709:ILE:HG13	2.19	0.43
1:B:671:ALA:C	1:B:673:GLY:H	2.21	0.43
1:A:616:PRO:C	1:A:618:ASP:N	2.72	0.43
1:B:616:PRO:HB2	1:B:619:GLN:HG2	2.01	0.43
1:B:824:LYS:HD2	1:B:834:PRO:HG3	2.01	0.43
1:A:600:SER:OG	1:A:601:SER:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:774:GLU:HG2	1:A:774:GLU:O	2.19	0.42
1:B:581:ASN:HA	1:B:737:GLU:OE2	2.19	0.42
1:A:550:ILE:O	1:A:554:LYS:HB2	2.19	0.42
1:A:830:LEU:O	1:A:831:ASN:C	2.56	0.42
1:B:600:SER:O	1:B:648:MET:N	2.49	0.42
1:A:779:GLU:CD	1:A:779:GLU:H	2.14	0.42
1:A:854:ARG:NH1	1:B:852:PRO:HB2	2.34	0.42
1:B:685:VAL:HA	1:B:762:ASP:OD1	2.19	0.42
1:B:575:PHE:N	1:B:575:PHE:CD1	2.87	0.42
1:B:687:LEU:HD23	1:B:687:LEU:HA	1.85	0.42
1:A:663:GLU:OE1	1:A:706:TYR:OH	2.34	0.42
1:B:554:LYS:HD3	1:B:554:LYS:HA	1.78	0.42
1:B:759:GLU:O	1:B:761:MET:HG3	2.20	0.42
1:B:542:GLU:O	1:B:544:LEU:N	2.52	0.42
1:B:609:LEU:HD11	1:B:613:MET:SD	2.59	0.42
1:B:739:LYS:HG2	1:B:742:LEU:CB	2.50	0.42
1:B:735:TYR:CD2	1:B:745:ARG:HA	2.55	0.42
1:A:751:VAL:HG23	1:A:752:SER:O	2.20	0.42
1:A:803:ILE:HB	1:A:806:ASP:HB2	2.00	0.41
1:A:814:SER:HB3	1:A:817:MET:HG3	2.02	0.41
1:A:679:PHE:CD1	1:A:706:TYR:CD2	3.07	0.41
1:B:814:SER:C	1:B:816:ARG:H	2.23	0.41
1:B:864:LEU:HD23	1:B:864:LEU:HA	1.84	0.41
1:B:580:GLY:O	1:B:581:ASN:O	2.38	0.41
1:B:569:ILE:HG21	1:B:613:MET:HE3	2.02	0.41
1:A:550:ILE:HD13	1:A:550:ILE:HG21	1.81	0.41
1:A:562:HIS:CE1	1:A:563:LEU:HG	2.55	0.41
1:A:606:VAL:HG12	1:A:617:GLN:HG3	2.03	0.41
1:A:795:ASP:OD1	1:A:812:THR:OG1	2.29	0.41
1:A:838:GLN:HB2	1:A:881:LEU:HD11	2.03	0.41
1:A:679:PHE:CD1	1:A:706:TYR:HD2	2.35	0.40
1:A:578:HIS:CE1	1:A:580:GLY:H	2.40	0.40
1:A:638:LEU:HA	1:A:638:LEU:HD12	1.86	0.40
1:A:739:LYS:HG2	1:A:742:LEU:HB3	2.03	0.40
1:B:606:VAL:HG12	1:B:617:GLN:HG3	2.01	0.40
1:B:645:ASN:C	1:B:646:LYS:HG2	2.42	0.40
1:B:564:TYR:HD2	1:B:595:LYS:HG2	1.85	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	339/356 (95%)	293 (86%)	35 (10%)	11 (3%)	4	22
1	B	336/356 (94%)	272 (81%)	46 (14%)	18 (5%)	2	12
2	D	4/8 (50%)	2 (50%)	2 (50%)	0	100	100
All	All	679/720 (94%)	567 (84%)	83 (12%)	29 (4%)	2	16

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	617	GLN
1	A	645	ASN
1	A	672	SER
1	A	750	ASP
1	A	870	PRO
1	B	541	VAL
1	B	543	ARG
1	B	557	GLU
1	B	581	ASN
1	B	617	GLN
1	B	652	SER
1	B	673	GLY
1	B	674	ALA
1	B	599	ASN
1	B	672	SER
1	B	815	ASN
1	A	643	ASP
1	A	815	ASN
1	A	835	MET
1	A	869	LYS
1	B	542	GLU
1	B	654	ASN
1	B	578	HIS
1	A	829	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	668	GLU
1	A	844	GLY
1	B	647	THR
1	B	738	VAL
1	B	649	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	310/327 (95%)	300 (97%)	10 (3%)	39	67
1	B	309/327 (94%)	300 (97%)	9 (3%)	42	69
2	D	6/8 (75%)	6 (100%)	0	100	100
All	All	625/662 (94%)	606 (97%)	19 (3%)	41	68

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	544	LEU
1	A	599	ASN
1	A	600	SER
1	A	601	SER
1	A	639	ASP
1	A	681	LYS
1	A	752	SER
1	A	854	ARG
1	A	871	ARG
1	A	883	MET
1	B	562	HIS
1	B	576	CYS
1	B	597	LEU
1	B	601	SER
1	B	615	PHE
1	B	712	LYS
1	B	793	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	833	ASP
1	B	867	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	645	ASN
1	A	880	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 carbohydrates 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	341/356 (95%)	-0.00	3 (0%) 84 84	70, 106, 166, 199	0
1	B	340/356 (95%)	0.07	6 (1%) 68 67	83, 129, 180, 211	0
2	D	6/8 (75%)	1.42	2 (33%) 0 0	124, 127, 147, 156	0
All	All	687/720 (95%)	0.04	11 (1%) 72 70	70, 116, 176, 211	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	538	GLN	7.4
1	B	636	ALA	3.9
1	B	553	GLN	3.3
2	D	490	ARG	3.1
1	B	619	GLN	3.0
1	A	548	LYS	2.9
1	B	590	LYS	2.5
2	D	491	LYS	2.4
1	B	642	ALA	2.2
1	A	546	GLU	2.1
1	A	543	ARG	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.