



Preliminary Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2021 – 06:32 PM JST

Deposition ID : D_1300024352

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System during initial deposition but before annotation of the structure.

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
Xtrriage (Phenix)	:	1.13
EDS	:	2.23.1
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)	:	2.23.1

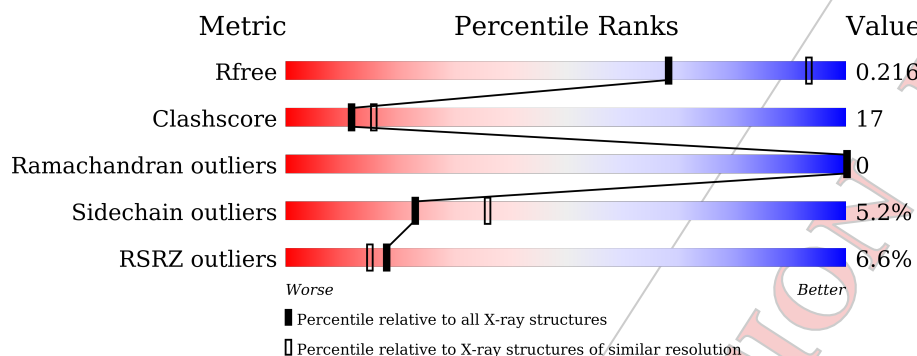
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	884	6% 65% 28% • •

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6852 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 Alanine aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	859	6720	4235	1171	1297	17	0	0	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	initiating methionine	UNP A4F9D7
A	-22	GLY	-	expression tag	UNP A4F9D7
A	-21	SER	-	expression tag	UNP A4F9D7
A	-20	SER	-	expression tag	UNP A4F9D7
A	-19	HIS	-	expression tag	UNP A4F9D7
A	-18	HIS	-	expression tag	UNP A4F9D7
A	-17	HIS	-	expression tag	UNP A4F9D7
A	-16	HIS	-	expression tag	UNP A4F9D7
A	-15	HIS	-	expression tag	UNP A4F9D7
A	-14	HIS	-	expression tag	UNP A4F9D7
A	-13	HIS	-	expression tag	UNP A4F9D7
A	-12	HIS	-	expression tag	UNP A4F9D7
A	-11	HIS	-	expression tag	UNP A4F9D7
A	-10	HIS	-	expression tag	UNP A4F9D7
A	-9	SER	-	expression tag	UNP A4F9D7
A	-8	SER	-	expression tag	UNP A4F9D7
A	-7	GLY	-	expression tag	UNP A4F9D7
A	-6	LEU	-	expression tag	UNP A4F9D7
A	-5	VAL	-	expression tag	UNP A4F9D7
A	-4	PRO	-	expression tag	UNP A4F9D7
A	-3	ARG	-	expression tag	UNP A4F9D7
A	-2	GLY	-	expression tag	UNP A4F9D7
A	-1	SER	-	expression tag	UNP A4F9D7
A	0	HIS	-	expression tag	UNP A4F9D7
A	1	VAL	-	expression tag	UNP A4F9D7

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total 1	Zn 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	131	Total 131	O 131	0	0

4 Data and refinement statistics [i](#)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.82Å 111.58Å 156.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.18 – 2.66 36.18 – 2.66	Depositor EDS
% Data completeness (in resolution range)	99.4 (36.18-2.66) 99.4 (36.18-2.66)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.18.2 3874	Depositor
R, R_{free}	0.202 , 0.216 0.202 , 0.216	Depositor DCC
R_{free} test set	1995 reflections (6.65%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6852	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.98	8/6880 (0.1%)	0.84	14/9378 (0.1%)

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	485	GLY	C-O	-6.82	1.12	1.23
1	A	226	ALA	C-O	5.73	1.34	1.23
1	A	275	GLU	CD-OE1	-5.40	1.19	1.25
1	A	59	TRP	CB-CG	-5.33	1.40	1.50
1	A	286	TYR	CE1-CZ	-5.25	1.31	1.38
1	A	568	GLU	C-O	-5.15	1.13	1.23
1	A	230	GLU	N-CA	5.08	1.56	1.46
1	A	482	ALA	C-O	-5.03	1.13	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	536	LEU	CA-CB-CG	7.95	133.59	115.30
1	A	542	ASP	CB-CA-C	6.57	123.53	110.40
1	A	292	VAL	CB-CA-C	5.91	122.64	111.40
1	A	225	ARG	O-C-N	-5.80	113.42	122.70
1	A	756	HIS	C-N-CA	-5.68	107.50	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	837	LEU	CB-CG-CD1	-5.62	101.45	111.00
1	A	837	LEU	CA-CB-CG	-5.62	102.38	115.30
1	A	292	VAL	CA-CB-CG1	5.54	119.21	110.90
1	A	230	GLU	C-N-CA	5.53	135.51	121.70
1	A	829	LEU	CB-CG-CD2	5.46	120.28	111.00
1	A	229	ALA	C-N-CA	-5.18	108.75	121.70
1	A	390	ILE	CB-CA-C	-5.06	101.47	111.60
1	A	228	LEU	CB-CG-CD1	-5.02	102.47	111.00
1	A	66	ARG	CG-CD-NE	-5.01	101.28	111.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	347	THR	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6720	0	6449	229	0
2	C	1	0	0	0	0
3	B	131	0	0	9	0
All	All	6852	0	6449	229	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 17.

All (229) 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:A:835:PRO:O	1:A:839:ARG:HG3	1.55	1.05
1:A:784:TYR:HA	1:A:787:ARG:HG2	1.44	0.97
1:A:672:LEU:HD22	1:A:676:GLN:HB3	1.42	0.96
1:A:637:GLU:OE2	1:A:641:ARG:HD2	1.74	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:ARG:NH2	1:A:712:ALA:HB1	1.93	0.84
1:A:825:ALA:O	1:A:829:LEU:HG	1.78	0.83
1:A:818:ASP:HB3	1:A:821:THR:HG22	1.60	0.82
1:A:757:ASP:HB3	1:A:760:LEU:HB2	1.60	0.81
1:A:288:PHE:CG	1:A:292:VAL:HG11	2.16	0.81
1:A:732:ARG:HH21	1:A:763:ALA:HB1	1.45	0.81
1:A:288:PHE:HB3	1:A:292:VAL:HG11	1.60	0.80
1:A:753:ARG:O	1:A:757:ASP:HB2	1.81	0.79
1:A:188:LYS:HD3	1:A:424:TRP:CH2	2.19	0.77
1:A:836:ALA:HA	1:A:839:ARG:HD2	1.66	0.77
1:A:288:PHE:CB	1:A:292:VAL:HG11	2.16	0.76
1:A:752:GLN:O	1:A:756:HIS:HB2	1.86	0.76
1:A:61:ASP:HB3	1:A:137:LYS:HE3	1.69	0.75
1:A:235:GLU:O	1:A:239:ILE:HG13	1.86	0.75
1:A:816:ALA:O	1:A:821:THR:HG21	1.88	0.74
1:A:754:ALA:HB2	1:A:768:ILE:CG2	2.19	0.73
1:A:512:HIS:HE1	3:B:12:HOH:O	1.72	0.72
1:A:732:ARG:HD3	1:A:763:ALA:HB1	1.71	0.70
1:A:791:GLU:O	1:A:794:GLU:HG2	1.91	0.70
1:A:796:TRP:CD2	1:A:837:LEU:HD13	2.26	0.70
1:A:19:GLU:OE1	1:A:50:ARG:NH1	2.25	0.69
1:A:62:LEU:HB2	1:A:141:THR:HG23	1.74	0.69
1:A:609:GLU:HG2	1:A:614:VAL:HG22	1.73	0.69
1:A:285:ASP:OD1	1:A:285:ASP:N	2.25	0.69
1:A:72:LEU:HB3	1:A:77:LEU:HD21	1.75	0.68
1:A:27:LEU:HA	1:A:42:GLY:O	1.92	0.68
1:A:749:LYS:O	1:A:753:ARG:HG3	1.93	0.68
1:A:828:TRP:CE3	1:A:829:LEU:HD23	2.29	0.68
1:A:690:LEU:HD23	1:A:693:LEU:HB2	1.76	0.68
1:A:828:TRP:HE3	1:A:829:LEU:HD23	1.57	0.68
1:A:172:VAL:HG22	1:A:182:HIS:CD2	2.29	0.68
1:A:792:ILE:HD11	1:A:808:VAL:HB	1.76	0.67
1:A:384:GLU:O	1:A:384:GLU:HG2	1.92	0.67
1:A:286:TYR:CD1	1:A:300:ARG:HG3	2.31	0.66
1:A:646:LEU:HB3	1:A:667:LEU:HG	1.79	0.65
1:A:236:ARG:HA	1:A:239:ILE:HD12	1.78	0.65
1:A:458:ASN:OD1	1:A:490:ARG:HG3	1.97	0.64
1:A:612:ILE:O	1:A:616:GLN:HG3	1.97	0.64
1:A:754:ALA:HB2	1:A:768:ILE:HG21	1.79	0.64
1:A:727:THR:HG22	3:B:178:HOH:O	1.97	0.64
1:A:119:ASP:HB3	1:A:122:ASP:OD1	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:796:TRP:CE3	1:A:837:LEU:CD1	2.81	0.63
1:A:826:ASP:HA	1:A:829:LEU:HD12	1.80	0.62
1:A:459:MET:HE1	1:A:461:ARG:HB2	1.81	0.62
1:A:784:TYR:HA	1:A:787:ARG:CG	2.27	0.62
1:A:540:ASN:HD21	1:A:545:THR:H	1.46	0.62
1:A:151:THR:HB	1:A:187:THR:O	2.00	0.61
1:A:857:PHE:O	1:A:860:SER:HB3	2.00	0.61
1:A:421:ARG:HG2	1:A:422:HIS:CE1	2.35	0.61
1:A:828:TRP:HZ2	1:A:837:LEU:HD23	1.66	0.61
1:A:727:THR:CG2	3:B:178:HOH:O	2.48	0.61
1:A:419:PHE:O	1:A:423:ALA:HB2	2.01	0.61
1:A:654:GLU:HB2	1:A:657:SER:HB3	1.83	0.61
1:A:672:LEU:CD2	1:A:680:MET:HE1	2.31	0.60
1:A:56:ALA:O	1:A:93:LEU:HD12	2.02	0.60
1:A:796:TRP:CG	1:A:837:LEU:HD13	2.36	0.60
1:A:757:ASP:OD2	1:A:760:LEU:HD22	2.01	0.60
1:A:836:ALA:HA	1:A:839:ARG:CD	2.32	0.60
1:A:218:ILE:HG22	1:A:220:LEU:HD23	1.83	0.60
1:A:708:VAL:HG11	1:A:718:ILE:HD11	1.84	0.60
1:A:611:GLU:HB2	1:A:614:VAL:HG13	1.82	0.59
1:A:144:ASP:HB3	3:B:44:HOH:O	2.02	0.59
1:A:215:GLN:HG3	1:A:255:PRO:HB3	1.84	0.59
1:A:691:GLU:O	1:A:691:GLU:HG2	2.02	0.59
1:A:754:ALA:HB2	1:A:768:ILE:HG22	1.84	0.59
1:A:837:LEU:O	1:A:841:VAL:HG23	2.03	0.59
1:A:828:TRP:CZ2	1:A:837:LEU:HD23	2.37	0.59
1:A:672:LEU:HD22	1:A:680:MET:CE	2.32	0.59
1:A:757:ASP:CB	1:A:760:LEU:HB2	2.29	0.59
1:A:751:TRP:HH2	1:A:788:TYR:HB2	1.68	0.58
1:A:559:LEU:HD11	1:A:575:CYS:HB3	1.84	0.58
1:A:8:ARG:HD2	3:B:237:HOH:O	2.04	0.57
1:A:172:VAL:CG2	1:A:182:HIS:CD2	2.86	0.57
1:A:672:LEU:HD22	1:A:676:GLN:CB	2.25	0.57
1:A:585:GLU:OE2	1:A:850:ARG:NH1	2.36	0.57
1:A:327:LEU:HD22	1:A:429:LEU:HD13	1.86	0.57
1:A:260:LYS:HD2	1:A:260:LYS:C	2.26	0.55
1:A:111:GLY:HA3	1:A:270:ASN:OD1	2.06	0.55
1:A:15:ALA:HA	1:A:148:LEU:HD21	1.88	0.55
1:A:30:SER:HA	1:A:159:PRO:HD3	1.87	0.55
1:A:61:ASP:CB	1:A:137:LYS:HE3	2.35	0.55
1:A:133:THR:HG23	1:A:322:TRP:CE2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:LYS:CD	1:A:424:TRP:CH2	2.88	0.54
1:A:672:LEU:HD21	1:A:680:MET:HE1	1.88	0.54
1:A:288:PHE:HB3	1:A:292:VAL:CG1	2.33	0.54
1:A:275:GLU:O	1:A:275:GLU:HG2	2.07	0.54
1:A:236:ARG:NH1	1:A:297:TYR:CG	2.76	0.53
1:A:672:LEU:CD2	1:A:676:GLN:HB3	2.27	0.53
1:A:524:GLU:HG3	3:B:65:HOH:O	2.09	0.53
1:A:165:ILE:HD12	1:A:165:ILE:N	2.23	0.53
1:A:276:ASN:HB2	1:A:279:CYS:O	2.08	0.53
1:A:494:LEU:C	1:A:494:LEU:HD12	2.30	0.52
1:A:743:THR:HG23	1:A:746:ALA:H	1.73	0.52
1:A:664:VAL:HG21	1:A:693:LEU:HD22	1.92	0.52
1:A:722:LEU:HD12	1:A:738:ARG:HH22	1.74	0.52
1:A:788:TYR:OH	1:A:808:VAL:HG23	2.10	0.52
1:A:645:ARG:HG3	1:A:649:LEU:HD12	1.90	0.52
1:A:156:VAL:HG21	1:A:197:LEU:HD21	1.92	0.52
1:A:646:LEU:CB	1:A:667:LEU:HG	2.39	0.52
1:A:64:ALA:HB1	1:A:104:ASP:O	2.09	0.51
1:A:722:LEU:HD12	1:A:738:ARG:NH2	2.25	0.51
1:A:708:VAL:HG21	1:A:718:ILE:HG12	1.92	0.51
1:A:760:LEU:HG	1:A:761:PRO:HD2	1.92	0.51
1:A:21:GLN:NE2	1:A:50:ARG:HG3	2.26	0.51
1:A:607:GLY:CA	1:A:649:LEU:HD21	2.40	0.51
1:A:341:VAL:HG23	1:A:349:ALA:HB3	1.94	0.50
1:A:228:LEU:N	1:A:228:LEU:HD23	2.25	0.50
1:A:341:VAL:CG2	1:A:349:ALA:HB3	2.41	0.50
1:A:331:PHE:CD1	1:A:331:PHE:C	2.85	0.50
1:A:466:ILE:HD12	1:A:470:GLY:HA2	1.93	0.50
1:A:236:ARG:NH1	1:A:297:TYR:CD1	2.80	0.50
1:A:215:GLN:OE1	1:A:249:HIS:HB3	2.13	0.49
1:A:732:ARG:HH21	1:A:763:ALA:CB	2.21	0.49
1:A:659:HIS:O	1:A:663:PHE:CD2	2.65	0.49
1:A:681:ARG:NH2	1:A:712:ALA:CB	2.71	0.49
1:A:823:ALA:O	1:A:827:ARG:HG3	2.13	0.49
1:A:672:LEU:CD2	1:A:680:MET:CE	2.91	0.49
1:A:71:VAL:HG22	1:A:76:GLU:HG3	1.95	0.48
1:A:21:GLN:HE22	1:A:50:ARG:HG3	1.79	0.48
1:A:205:TRP:O	1:A:206:ARG:HD2	2.13	0.48
1:A:812:PHE:CD1	1:A:813:PRO:HD2	2.49	0.48
1:A:112:GLU:HB3	1:A:135:ASP:OD2	2.13	0.48
1:A:499:TYR:HB2	1:A:536:LEU:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:VAL:HG23	1:A:695:VAL:O	2.12	0.48
1:A:796:TRP:CE3	1:A:837:LEU:HD12	2.49	0.48
1:A:318:THR:O	1:A:426:ASN:HA	2.13	0.47
1:A:607:GLY:HA3	1:A:649:LEU:HD21	1.96	0.47
1:A:796:TRP:CD2	1:A:837:LEU:CD1	2.97	0.47
1:A:738:ARG:O	1:A:741:ILE:HG13	2.15	0.47
1:A:556:LEU:HD21	1:A:588:LEU:HD13	1.97	0.47
1:A:769:ILE:O	1:A:770:SER:C	2.51	0.47
1:A:815:TRP:HB3	3:B:102:HOH:O	2.14	0.47
1:A:275:GLU:HG3	1:A:310:HIS:HB3	1.96	0.47
1:A:93:LEU:HD23	1:A:97:ASN:ND2	2.30	0.47
1:A:133:THR:CG2	1:A:380:LEU:HD22	2.45	0.46
1:A:607:GLY:HA2	1:A:649:LEU:CD2	2.46	0.46
1:A:749:LYS:C	1:A:753:ARG:HG3	2.35	0.46
1:A:53:THR:HG22	1:A:53:THR:O	2.15	0.46
1:A:788:TYR:O	1:A:792:ILE:HB	2.16	0.46
1:A:119:ASP:OD1	1:A:120:PRO:HD2	2.16	0.46
1:A:502:ASP:OD2	1:A:505:THR:OG1	2.26	0.46
1:A:808:VAL:HG22	1:A:840:LEU:HD13	1.98	0.45
1:A:421:ARG:HG2	1:A:422:HIS:ND1	2.31	0.45
1:A:540:ASN:ND2	1:A:545:THR:H	2.14	0.45
1:A:792:ILE:CG2	1:A:793:ASP:N	2.78	0.45
1:A:825:ALA:CB	1:A:845:ARG:HD2	2.47	0.45
1:A:110:THR:O	1:A:115:HIS:ND1	2.40	0.45
1:A:150:ALA:O	1:A:189:PRO:HA	2.16	0.45
1:A:158:ALA:HB3	1:A:182:HIS:CE1	2.51	0.45
1:A:568:GLU:HB2	1:A:571:PRO:HG2	1.98	0.45
1:A:664:VAL:HG11	1:A:699:LEU:HD11	1.98	0.45
1:A:796:TRP:CE3	1:A:837:LEU:HD13	2.49	0.45
1:A:760:LEU:HD12	1:A:760:LEU:HA	1.76	0.45
1:A:632:PRO:O	1:A:636:PRO:HD3	2.17	0.44
1:A:796:TRP:HZ2	1:A:836:ALA:HB3	1.82	0.44
1:A:232:LEU:HD23	1:A:234:ALA:HB2	2.00	0.44
1:A:464:LEU:HD12	1:A:464:LEU:C	2.38	0.44
1:A:598:LEU:HD21	1:A:642:PHE:HD1	1.83	0.44
1:A:671:VAL:O	1:A:671:VAL:HG12	2.16	0.44
1:A:66:ARG:O	1:A:66:ARG:HG3	2.12	0.44
1:A:128:TYR:HE2	1:A:267:PRO:O	2.01	0.44
1:A:3:PRO:CB	1:A:4:PRO:HD2	2.47	0.44
1:A:8:ARG:HD3	1:A:321:TRP:CD1	2.53	0.44
1:A:757:ASP:CG	1:A:760:LEU:HB2	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:792:ILE:HG23	1:A:793:ASP:N	2.33	0.44
1:A:464:LEU:HD12	1:A:464:LEU:O	2.17	0.44
1:A:6:LEU:HD12	1:A:10:GLN:OE1	2.17	0.43
1:A:164:VAL:CG1	1:A:197:LEU:HD11	2.47	0.43
1:A:219:PRO:O	1:A:260:LYS:HB2	2.18	0.43
1:A:672:LEU:HD22	1:A:680:MET:HE3	2.00	0.43
1:A:538:LEU:HD23	1:A:538:LEU:HA	1.80	0.43
1:A:618:VAL:HA	1:A:621:GLN:HG2	2.01	0.43
1:A:750:ALA:O	1:A:751:TRP:C	2.55	0.43
1:A:459:MET:HE2	1:A:459:MET:HB3	1.63	0.43
1:A:796:TRP:CZ2	1:A:836:ALA:HB3	2.53	0.43
1:A:116:ARG:HG3	1:A:127:LEU:CD2	2.48	0.43
1:A:390:ILE:HG21	1:A:390:ILE:HD13	1.70	0.43
1:A:461:ARG:HG3	1:A:461:ARG:HH11	1.84	0.43
1:A:500:ASP:OD2	1:A:534:GLY:HA2	2.19	0.43
1:A:283:LEU:HD23	1:A:283:LEU:O	2.19	0.43
1:A:437:GLU:HG2	1:A:442:ARG:O	2.18	0.43
1:A:607:GLY:HA2	1:A:649:LEU:HD21	2.01	0.42
1:A:664:VAL:HG21	1:A:693:LEU:CD2	2.48	0.42
1:A:635:GLN:N	1:A:636:PRO:CD	2.82	0.42
1:A:47:VAL:HG13	1:A:99:LEU:HB3	2.00	0.42
1:A:170:GLY:HA2	1:A:184:PHE:HA	2.01	0.42
1:A:402:LEU:HB2	1:A:447:TRP:CZ2	2.54	0.42
1:A:7:THR:OG1	1:A:10:GLN:HG3	2.19	0.42
1:A:457:LEU:N	1:A:457:LEU:HD12	2.34	0.42
1:A:782:ALA:O	1:A:785:VAL:HG23	2.19	0.42
1:A:837:LEU:HD12	1:A:837:LEU:HA	1.73	0.42
1:A:197:LEU:HA	1:A:197:LEU:HD12	1.60	0.42
1:A:302:GLU:OE1	3:B:195:HOH:O	2.21	0.42
1:A:681:ARG:HH21	1:A:712:ALA:HB1	1.75	0.42
1:A:693:LEU:HD11	1:A:699:LEU:CD2	2.50	0.42
1:A:831:GLY:O	1:A:838:ARG:NH1	2.53	0.42
1:A:536:LEU:HD21	1:A:559:LEU:HD23	2.01	0.42
1:A:819:GLU:CD	1:A:819:GLU:H	2.23	0.42
1:A:160:GLN:HG2	1:A:178:GLY:O	2.19	0.42
1:A:175:THR:O	1:A:177:GLU:HG3	2.20	0.42
1:A:236:ARG:NH2	1:A:345:GLN:HE22	2.18	0.41
1:A:265:PHE:CD1	1:A:282:PHE:HB2	2.55	0.41
1:A:39:GLU:HG3	1:A:40:THR:HG23	2.02	0.41
1:A:708:VAL:CG1	1:A:741:ILE:HG12	2.50	0.41
1:A:760:LEU:HG	1:A:761:PRO:CD	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:TYR:HE2	1:A:263:GLN:OE1	2.02	0.41
1:A:512:HIS:CE1	3:B:12:HOH:O	2.58	0.41
1:A:721:GLU:O	1:A:721:GLU:HG3	2.20	0.41
1:A:460:LEU:HD12	1:A:547:CYS:SG	2.60	0.41
1:A:296:LEU:N	1:A:296:LEU:HD23	2.33	0.41
1:A:337:VAL:HG13	1:A:349:ALA:HB1	2.03	0.41
1:A:354:ALA:HA	1:A:358:LYS:HB2	2.03	0.41
1:A:446:TRP:CE3	1:A:447:TRP:HA	2.55	0.41
1:A:116:ARG:HG3	1:A:127:LEU:HD21	2.01	0.41
1:A:401:GLN:HA	1:A:401:GLN:HE21	1.86	0.40
1:A:761:PRO:HD2	1:A:764:ILE:HB	2.02	0.40
1:A:664:VAL:CG1	1:A:699:LEU:HD11	2.51	0.40
1:A:163:LYS:N	1:A:200:GLY:O	2.51	0.40
1:A:215:GLN:HG3	1:A:255:PRO:CB	2.50	0.40
1:A:256:TYR:HA	1:A:257:PRO:HD3	1.91	0.40
1:A:418:TYR:CE2	1:A:432:LEU:HB2	2.55	0.40
1:A:501:ASP:OD1	1:A:562:ARG:NH1	2.48	0.40
1:A:695:VAL:O	1:A:695:VAL:CG2	2.69	0.40
1:A:417:VAL:O	1:A:421:ARG:HB3	2.22	0.40
1:A:448:SER:CB	1:A:452:LEU:HD12	2.52	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	857/884 (97%)	840 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	693/717 (97%)	657 (95%)	36 (5%)	23 36

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	47	VAL
1	A	66	ARG
1	A	84	GLU
1	A	97	ASN
1	A	98	GLU
1	A	141	THR
1	A	151	THR
1	A	220	LEU
1	A	227	SER
1	A	260	LYS
1	A	283	LEU
1	A	285	ASP
1	A	299	ARG
1	A	302	GLU
1	A	320	ARG
1	A	384	GLU
1	A	401	GLN
1	A	459	MET
1	A	521	GLU
1	A	536	LEU
1	A	538	LEU
1	A	549	MET
1	A	559	LEU
1	A	571	PRO
1	A	614	VAL
1	A	666	SER
1	A	671	VAL
1	A	674	GLU
1	A	722	LEU

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Mol	Chain	Res	Type
1	A	725	ASP
1	A	727	THR
1	A	758	ASP
1	A	780	LEU
1	A	792	ILE
1	A	808	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	ASN
1	A	182	HIS
1	A	270	ASN
1	A	512	HIS
1	A	540	ASN
1	A	554	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

PRELIMINARY VALIDATION REPORT

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	859/884 (97%)	0.20	57 (6%) 18 15	20, 45, 102, 124	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	723	GLU	5.2
1	A	178	GLY	5.2
1	A	213	ASP	4.9
1	A	291	ARG	4.7
1	A	759	GLN	4.6
1	A	214	GLY	4.5
1	A	726	GLN	4.4
1	A	728	ALA	4.2
1	A	827	ARG	4.0
1	A	860	SER	3.9
1	A	732	ARG	3.8
1	A	826	ASP	3.8
1	A	720	ALA	3.7
1	A	764	ILE	3.6
1	A	805	GLN	3.4
1	A	176	GLY	3.3
1	A	279	CYS	3.3
1	A	745	GLU	3.3
1	A	762	ASN	3.3
1	A	704	LEU	3.1
1	A	738	ARG	3.1
1	A	719	ASP	3.1
1	A	797	HIS	3.0
1	A	789	PHE	3.0
1	A	292	VAL	3.0
1	A	211	GLY	3.0
1	A	180	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	160	GLN	2.9
1	A	289	ARG	2.9
1	A	785	VAL	2.9
1	A	196	ALA	2.9
1	A	786	ARG	2.8
1	A	731	ARG	2.7
1	A	177	GLU	2.7
1	A	290	SER	2.6
1	A	655	PRO	2.6
1	A	80	SER	2.6
1	A	748	GLU	2.6
1	A	172	VAL	2.5
1	A	802	GLU	2.5
1	A	803	ARG	2.5
1	A	714	GLY	2.4
1	A	194	LEU	2.3
1	A	280	VAL	2.3
1	A	630	ALA	2.3
1	A	174	ASP	2.3
1	A	793	ASP	2.2
1	A	741	ILE	2.2
1	A	820	ASP	2.2
1	A	722	LEU	2.1
1	A	831	GLY	2.1
1	A	175	THR	2.1
1	A	161	ASP	2.1
1	A	718	ILE	2.1
1	A	715	GLU	2.1
1	A	212	ASP	2.1
1	A	801	SER	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 monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	C	1	1/?	0.85	0.17	32,32,32,32	1

6.5 Other polymers [i](#)

There are no such residues in this entry.