



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:24 AM UTC

PDB ID : 2XER / pdb_00002xer
Title : Human PatL1 C-terminal domain (loop variant with sulfates)
Authors : Tritschler, F.; Weichenrieder, O.
Deposited on : 2010-05-17
Resolution : 2.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

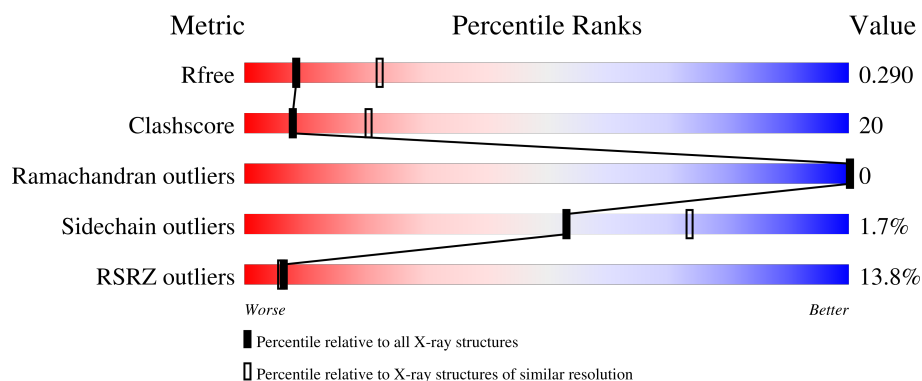
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	248	12% 56% 34% • 6%
1	B	248	12% 59% 29% • 11%
1	C	248	14% 61% 31% • 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5587 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 PAT1 HOMOLOG 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1876	1198	328	339	11			
1	B	221	Total	C	N	O	S	0	0	0
			1790	1149	312	318	11			
1	C	229	Total	C	N	O	S	0	0	0
			1857	1188	325	333	11			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	512	GLY	-	expression tag	UNP Q86TB9
A	513	PRO	-	expression tag	UNP Q86TB9
A	514	GLN	-	expression tag	UNP Q86TB9
A	515	ASP	-	expression tag	UNP Q86TB9
A	516	PRO	-	expression tag	UNP Q86TB9
A	664	GLY	GLN	engineered mutation	UNP Q86TB9
A	?	-	ALA	deletion	UNP Q86TB9
A	?	-	ALA	deletion	UNP Q86TB9
A	?	-	THR	deletion	UNP Q86TB9
A	?	-	PRO	deletion	UNP Q86TB9
A	?	-	ALA	deletion	UNP Q86TB9
A	?	-	LEU	deletion	UNP Q86TB9
A	?	-	SER	deletion	UNP Q86TB9
A	?	-	ASN	deletion	UNP Q86TB9
B	512	GLY	-	expression tag	UNP Q86TB9
B	513	PRO	-	expression tag	UNP Q86TB9
B	514	GLN	-	expression tag	UNP Q86TB9
B	515	ASP	-	expression tag	UNP Q86TB9
B	516	PRO	-	expression tag	UNP Q86TB9
B	664	GLY	GLN	engineered mutation	UNP Q86TB9
B	?	-	ALA	deletion	UNP Q86TB9
B	?	-	ALA	deletion	UNP Q86TB9
B	?	-	THR	deletion	UNP Q86TB9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PRO	deletion	UNP Q86TB9
B	?	-	ALA	deletion	UNP Q86TB9
B	?	-	LEU	deletion	UNP Q86TB9
B	?	-	SER	deletion	UNP Q86TB9
B	?	-	ASN	deletion	UNP Q86TB9
C	512	GLY	-	expression tag	UNP Q86TB9
C	513	PRO	-	expression tag	UNP Q86TB9
C	514	GLN	-	expression tag	UNP Q86TB9
C	515	ASP	-	expression tag	UNP Q86TB9
C	516	PRO	-	expression tag	UNP Q86TB9
C	664	GLY	GLN	engineered mutation	UNP Q86TB9
C	?	-	ALA	deletion	UNP Q86TB9
C	?	-	ALA	deletion	UNP Q86TB9
C	?	-	THR	deletion	UNP Q86TB9
C	?	-	PRO	deletion	UNP Q86TB9
C	?	-	ALA	deletion	UNP Q86TB9
C	?	-	LEU	deletion	UNP Q86TB9
C	?	-	SER	deletion	UNP Q86TB9
C	?	-	ASN	deletion	UNP Q86TB9

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

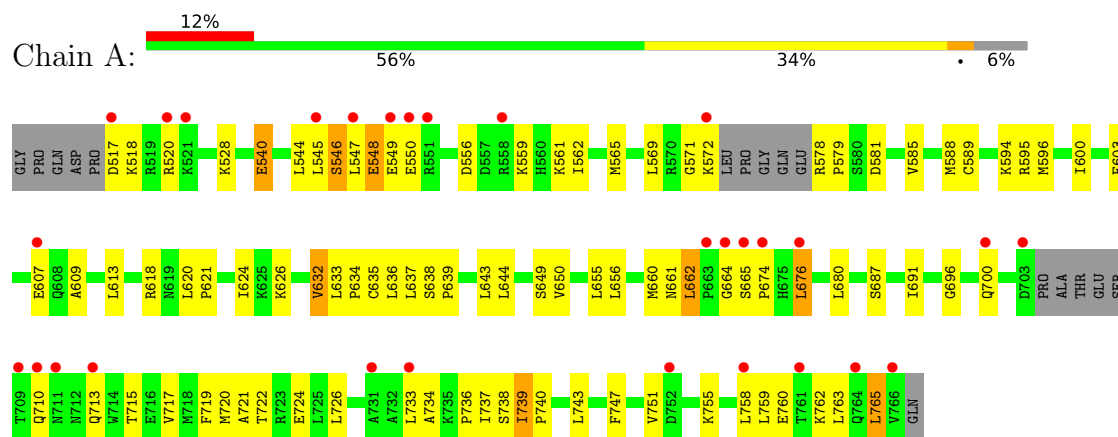
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total	O	0	0
			14	14		
3	B	13	Total	O	0	0
			13	13		
3	C	17	Total	O	0	0
			17	17		

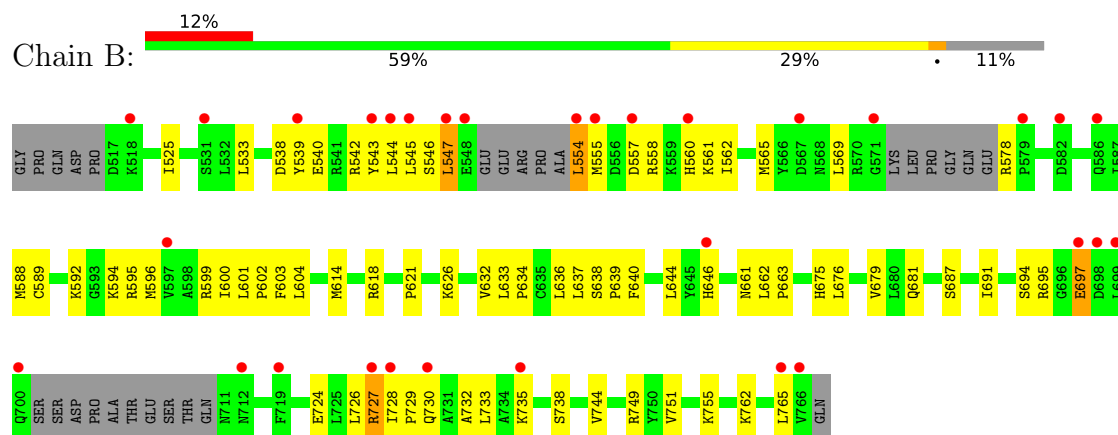
3 Residue-property plots

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.

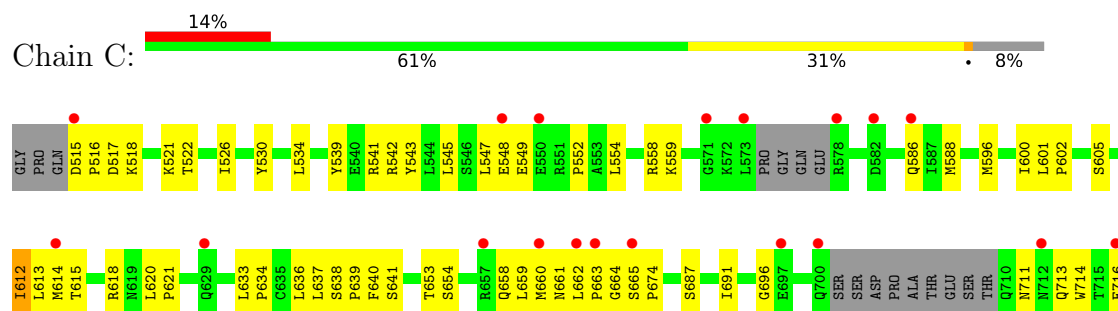
• Molecule 1: PAT1 HOMOLOG 1

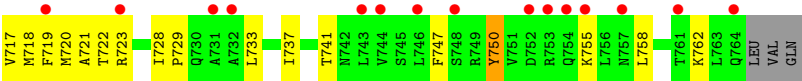


• Molecule 1: PAT1 HOMOLOG 1



• Molecule 1: PAT1 HOMOLOG 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	61.00Å 100.10Å 141.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.19 – 2.95 47.19 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.7 (47.19-2.95) 98.7 (47.19-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.96Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.247 , 0.289 0.247 , 0.290	Depositor DCC
R_{free} test set	952 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.8	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	0.89	EDS
Total number of atoms	5587	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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: SO4

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	0.57	2/1904 (0.1%)	0.77	2/2569 (0.1%)
1	B	0.42	0/1816	0.76	2/2449 (0.1%)
1	C	0.41	0/1886	0.74	1/2545 (0.0%)
All	All	0.47	2/5606 (0.0%)	0.76	5/7563 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	546	SER	C-O	-5.69	1.19	1.24
1	A	540	GLU	C-O	-5.22	1.18	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	547	LEU	N-CA-C	-9.10	102.18	113.28
1	B	727	ARG	N-CA-C	7.41	119.14	111.14
1	A	662	LEU	N-CA-C	-6.68	100.86	110.08
1	C	750	TYR	N-CA-C	6.10	120.80	112.68
1	A	548	GLU	N-CA-C	-5.02	102.58	110.36

There are no chirality outliers.

There are no planarity outliers.

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	1876	0	1973	92	2
1	B	1790	0	1893	68	0
1	C	1857	0	1954	76	0
2	B	5	0	0	0	0
2	C	15	0	0	0	0
3	A	14	0	0	0	0
3	B	13	0	0	0	0
3	C	17	0	0	2	0
All	All	5587	0	5820	223	2

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 20.

All (223) 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:662:LEU:HD23	1:A:674:PRO:HB3	1.54	0.90
1:B:751:VAL:CG1	1:B:755:LYS:HB2	2.13	0.78
1:A:758:LEU:O	1:A:762:LYS:HB2	1.84	0.77
1:B:542:ARG:HB3	1:B:554:LEU:HD21	1.68	0.76
1:A:676:LEU:HD12	1:A:680:LEU:HG	1.66	0.76
1:A:662:LEU:HD23	1:A:674:PRO:CB	2.15	0.75
1:A:594:LYS:HD2	1:A:632:VAL:HG23	1.68	0.75
1:A:661:ASN:HB3	1:A:674:PRO:HA	1.66	0.75
1:A:751:VAL:CG1	1:A:755:LYS:HB2	2.17	0.73
1:A:739:ILE:HD11	1:A:765:LEU:HD12	1.70	0.73
1:B:544:LEU:O	1:B:547:LEU:CD1	2.37	0.72
1:C:718:MET:HG2	1:C:750:TYR:CZ	2.24	0.72
1:C:588:MET:HE1	1:C:636:LEU:HD11	1.72	0.72
1:C:660:MET:HE1	1:C:717:VAL:O	1.89	0.71
1:A:520:ARG:CZ	1:A:520:ARG:HB2	2.20	0.71
1:A:644:LEU:HD12	1:A:691:ILE:HG22	1.73	0.70
1:B:730:GLN:OE1	1:B:762:LYS:HA	1.91	0.69
1:C:662:LEU:O	1:C:663:PRO:C	2.33	0.68
1:A:520:ARG:HB2	1:A:520:ARG:NH1	2.09	0.68
1:A:676:LEU:HD11	1:A:680:LEU:HD11	1.76	0.68
1:A:676:LEU:CD1	1:A:680:LEU:HG	2.24	0.67
1:B:555:MET:HE3	1:C:741:THR:HG22	1.75	0.66
1:A:607:GLU:OE1	1:A:607:GLU:N	2.29	0.65
1:B:697:GLU:O	1:B:697:GLU:HG2	1.95	0.65
1:B:544:LEU:O	1:B:547:LEU:HD11	1.96	0.65
1:C:661:ASN:O	1:C:661:ASN:CG	2.40	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:696:GLY:HA3	1:C:714:TRP:CH2	2.31	0.65
1:B:638:SER:HB3	1:B:639:PRO:HD3	1.78	0.64
1:A:548:GLU:O	1:A:549:GLU:HB2	1.96	0.64
1:A:687:SER:O	1:A:691:ILE:HG12	1.97	0.64
1:A:540:GLU:OE1	1:A:603:PHE:CZ	2.51	0.64
1:C:714:TRP:CZ2	1:C:718:MET:HE3	2.33	0.64
1:C:718:MET:HG2	1:C:750:TYR:CE2	2.33	0.63
1:B:744:VAL:HG22	1:B:765:LEU:HD13	1.80	0.62
1:B:596:MET:O	1:B:600:ILE:HG13	1.99	0.62
1:B:695:ARG:HA	1:C:559:LYS:HZ1	1.64	0.62
1:A:649:SER:OG	1:A:700:GLN:NE2	2.33	0.62
1:A:520:ARG:NH1	1:A:520:ARG:CB	2.62	0.61
1:B:637:LEU:HB3	1:C:543:TYR:OH	1.99	0.61
1:C:662:LEU:O	1:C:664:GLY:O	2.19	0.61
1:B:544:LEU:O	1:B:547:LEU:HD12	1.99	0.61
1:A:650:VAL:HA	1:A:710:GLN:NE2	2.14	0.61
1:C:601:LEU:HD21	1:C:612:ILE:HG21	1.82	0.60
1:C:716:GLU:HG3	1:C:720:MET:HE3	1.81	0.60
1:A:588:MET:O	1:A:594:LYS:HE2	2.01	0.60
1:A:676:LEU:HG	1:A:724:GLU:HG2	1.82	0.60
1:C:660:MET:O	1:C:674:PRO:HA	2.01	0.60
1:B:546:SER:HB3	1:C:737:ILE:HG23	1.84	0.60
1:C:660:MET:CE	1:C:721:ALA:HB2	2.32	0.59
1:A:662:LEU:CD2	1:A:674:PRO:HB3	2.29	0.59
1:B:561:LYS:O	1:B:565:MET:HG3	2.03	0.59
1:C:596:MET:O	1:C:600:ILE:HG13	2.03	0.59
1:A:662:LEU:HD23	1:A:674:PRO:HG3	1.84	0.58
1:A:662:LEU:HD23	1:A:674:PRO:CG	2.33	0.58
1:C:542:ARG:NH1	1:C:554:LEU:HD11	2.19	0.58
1:A:638:SER:HB3	1:A:639:PRO:HD3	1.84	0.58
1:B:646:HIS:ND1	1:C:605:SER:HB3	2.19	0.58
1:A:562:ILE:HD12	1:A:603:PHE:HB3	1.85	0.58
1:C:517:ASP:O	1:C:521:LYS:HG3	2.04	0.58
1:A:595:ARG:HD2	1:A:635:CYS:SG	2.44	0.57
1:C:714:TRP:CZ2	1:C:718:MET:CE	2.87	0.57
1:A:661:ASN:ND2	1:A:665:SER:O	2.38	0.57
1:B:544:LEU:O	1:B:544:LEU:HD23	2.05	0.56
1:C:637:LEU:HD13	1:C:737:ILE:HD12	1.85	0.56
1:A:548:GLU:C	1:A:550:GLU:H	2.11	0.56
1:C:658:GLN:O	1:C:661:ASN:N	2.38	0.56
1:C:714:TRP:O	1:C:717:VAL:HG22	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:LEU:CD2	1:A:674:PRO:HG3	2.37	0.55
1:A:548:GLU:O	1:A:549:GLU:CB	2.54	0.55
1:A:696:GLY:O	1:A:700:GLN:HG2	2.08	0.54
1:B:733:LEU:HD12	1:B:762:LYS:HG2	1.90	0.54
1:A:656:LEU:HB3	1:A:717:VAL:HG11	1.89	0.54
1:A:636:LEU:C	1:A:639:PRO:HD2	2.33	0.54
1:B:601:LEU:N	1:B:602:PRO:HD2	2.22	0.54
1:C:614:MET:HE1	1:C:658:GLN:HG3	1.90	0.54
1:C:719:PHE:HB3	1:C:723:ARG:NH1	2.22	0.54
1:A:607:GLU:CD	1:A:607:GLU:H	2.15	0.54
1:B:533:LEU:HB2	1:B:565:MET:HE1	1.89	0.54
1:A:662:LEU:CD2	1:A:674:PRO:CB	2.84	0.54
1:C:518:LYS:HE2	1:C:586:GLN:NE2	2.23	0.54
1:B:614:MET:HE3	1:B:618:ARG:HH21	1.73	0.53
1:A:540:GLU:OE1	1:A:603:PHE:CE1	2.60	0.53
1:A:596:MET:HG2	1:A:600:ILE:HD11	1.90	0.53
1:A:676:LEU:CD1	1:A:680:LEU:CD1	2.87	0.53
1:A:565:MET:O	1:A:569:LEU:HG	2.09	0.52
1:B:557:ASP:CG	1:B:560:HIS:HB3	2.34	0.52
1:A:620:LEU:O	1:A:624:ILE:HG13	2.09	0.52
1:A:660:MET:HE1	1:A:721:ALA:HB2	1.91	0.52
1:B:588:MET:O	1:B:594:LYS:HD2	2.10	0.52
1:A:760:GLU:HA	1:A:765:LEU:HB2	1.92	0.52
1:B:562:ILE:HD12	1:B:603:PHE:HB3	1.92	0.52
1:C:687:SER:O	1:C:691:ILE:HG12	2.10	0.52
1:A:720:MET:HE3	1:A:720:MET:HA	1.93	0.51
1:B:592:LYS:HG3	1:B:595:ARG:HH21	1.76	0.51
1:B:557:ASP:OD2	1:B:560:HIS:HB3	2.11	0.50
1:C:601:LEU:N	1:C:602:PRO:HD2	2.27	0.50
1:B:594:LYS:HE2	1:B:632:VAL:CG2	2.41	0.50
1:A:738:SER:O	1:A:740:PRO:HD3	2.11	0.50
1:B:691:ILE:O	1:B:694:SER:HB3	2.11	0.50
1:B:697:GLU:HG3	1:B:749:ARG:CZ	2.42	0.50
1:C:515:ASP:HB3	1:C:516:PRO:HD3	1.92	0.50
1:B:634:PRO:HB2	1:C:547:LEU:HD22	1.92	0.50
1:A:763:LEU:HB2	1:A:765:LEU:HD13	1.93	0.50
1:A:581:ASP:O	1:A:585:VAL:HG23	2.12	0.50
1:B:545:LEU:HD12	1:B:545:LEU:O	2.11	0.50
1:B:730:GLN:OE1	1:B:762:LYS:HG3	2.12	0.50
1:C:755:LYS:HA	1:C:758:LEU:HG	1.94	0.49
1:A:751:VAL:HG11	1:A:755:LYS:HB2	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:654:SER:O	1:C:658:GLN:HG2	2.13	0.49
1:A:596:MET:O	1:A:600:ILE:HG13	2.12	0.48
1:A:676:LEU:CD1	1:A:680:LEU:HD11	2.42	0.48
1:C:661:ASN:O	1:C:661:ASN:OD1	2.30	0.48
1:A:676:LEU:CD1	1:A:680:LEU:CG	2.91	0.48
1:C:545:LEU:HD22	3:C:2017:HOH:O	2.11	0.48
1:C:620:LEU:HB3	1:C:621:PRO:HD3	1.95	0.48
1:C:733:LEU:HD12	1:C:762:LYS:HG2	1.96	0.48
1:B:558:ARG:HH22	1:C:641:SER:HB2	1.77	0.48
1:B:558:ARG:O	1:B:562:ILE:HG12	2.13	0.48
1:B:687:SER:O	1:B:691:ILE:HD13	2.14	0.48
1:A:594:LYS:HD2	1:A:632:VAL:CG2	2.43	0.47
1:C:662:LEU:C	1:C:664:GLY:N	2.68	0.47
1:B:744:VAL:CG2	1:B:765:LEU:HD13	2.45	0.47
1:C:548:GLU:O	1:C:549:GLU:HG2	2.13	0.47
1:A:713:GLN:O	1:A:717:VAL:HG23	2.13	0.47
1:C:541:ARG:HD2	3:C:2004:HOH:O	2.13	0.47
1:C:713:GLN:O	1:C:717:VAL:HG13	2.14	0.47
1:A:578:ARG:HB2	1:A:579:PRO:HD2	1.95	0.47
1:C:633:LEU:N	1:C:634:PRO:CD	2.77	0.47
1:C:636:LEU:O	1:C:639:PRO:HG2	2.14	0.47
1:C:722:THR:HG22	1:C:747:PHE:CD1	2.50	0.47
1:A:540:GLU:OE1	1:A:603:PHE:HZ	1.97	0.47
1:A:739:ILE:HD11	1:A:765:LEU:CD1	2.41	0.47
1:B:661:ASN:CG	1:B:662:LEU:H	2.22	0.47
1:A:520:ARG:CB	1:A:520:ARG:HH11	2.26	0.46
1:A:726:LEU:HD12	1:A:759:LEU:HD21	1.97	0.46
1:C:662:LEU:N	1:C:663:PRO:CD	2.78	0.46
1:B:724:GLU:OE2	1:B:727:ARG:NH2	2.39	0.46
1:C:714:TRP:CE2	1:C:718:MET:HE3	2.50	0.46
1:A:676:LEU:HD12	1:A:680:LEU:CG	2.42	0.46
1:B:592:LYS:HG3	1:B:595:ARG:NH2	2.30	0.46
1:C:653:THR:HG21	1:C:713:GLN:HG2	1.97	0.46
1:A:595:ARG:HD2	1:A:595:ARG:HA	1.73	0.46
1:B:681:GLN:HG2	1:B:732:ALA:O	2.16	0.46
1:A:633:LEU:N	1:A:634:PRO:CD	2.78	0.46
1:B:539:TYR:HB3	1:B:543:TYR:CE2	2.51	0.46
1:B:728:ILE:HD12	1:B:729:PRO:HD2	1.98	0.46
1:B:735:LYS:CE	1:C:552:PRO:HA	2.47	0.45
1:C:596:MET:HG2	1:C:600:ILE:HD11	1.97	0.45
1:A:637:LEU:HD23	1:A:737:ILE:HG21	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:665:SER:HA	1:C:674:PRO:HD3	1.87	0.45
1:A:722:THR:HG22	1:A:747:PHE:CD1	2.52	0.45
1:B:633:LEU:N	1:B:634:PRO:CD	2.79	0.45
1:B:694:SER:O	1:C:559:LYS:NZ	2.49	0.45
1:B:695:ARG:HA	1:C:559:LYS:NZ	2.30	0.45
1:C:522:THR:O	1:C:526:ILE:HG13	2.17	0.45
1:C:615:THR:HA	1:C:618:ARG:NH1	2.31	0.45
1:B:558:ARG:NH2	1:C:641:SER:CB	2.79	0.45
1:C:539:TYR:CE2	1:C:554:LEU:HD23	2.52	0.45
1:A:520:ARG:HH11	1:A:520:ARG:HB3	1.82	0.44
1:A:571:GLY:O	1:A:572:LYS:O	2.34	0.44
1:B:663:PRO:HB3	1:B:724:GLU:OE2	2.17	0.44
1:B:595:ARG:HG2	1:B:595:ARG:O	2.16	0.44
1:B:614:MET:CE	1:B:618:ARG:HH21	2.29	0.44
1:B:751:VAL:HG12	1:B:755:LYS:HB2	1.95	0.44
1:A:517:ASP:CG	1:A:518:LYS:H	2.26	0.44
1:A:520:ARG:CZ	1:A:520:ARG:CB	2.93	0.44
1:B:738:SER:HA	1:C:554:LEU:O	2.18	0.43
1:A:676:LEU:HD11	1:A:680:LEU:CD1	2.44	0.43
1:A:637:LEU:CD2	1:A:737:ILE:HB	2.49	0.43
1:A:571:GLY:O	1:A:572:LYS:C	2.62	0.43
1:A:660:MET:O	1:A:661:ASN:CB	2.64	0.43
1:B:565:MET:O	1:B:569:LEU:HG	2.18	0.43
1:A:528:LYS:HB2	1:A:528:LYS:HE2	1.79	0.42
1:A:547:LEU:HD23	1:A:547:LEU:HA	1.83	0.42
1:B:621:PRO:HG2	1:B:675:HIS:ND1	2.35	0.42
1:A:589:CYS:SG	1:A:626:LYS:HG3	2.60	0.42
1:C:637:LEU:HD23	1:C:641:SER:OG	2.19	0.42
1:A:613:LEU:HG	1:A:655:LEU:HD22	2.01	0.42
1:C:638:SER:N	1:C:639:PRO:HD2	2.34	0.42
1:B:588:MET:HE1	1:B:636:LEU:HD11	2.00	0.42
1:B:751:VAL:CG1	1:B:755:LYS:CB	2.92	0.42
1:A:722:THR:O	1:A:726:LEU:HD13	2.19	0.42
1:A:561:LYS:O	1:A:565:MET:HG3	2.20	0.42
1:A:660:MET:O	1:A:661:ASN:HB3	2.20	0.42
1:C:637:LEU:HD11	1:C:687:SER:CB	2.49	0.42
1:C:728:ILE:HA	1:C:729:PRO:HD3	1.91	0.42
1:A:581:ASP:OD2	1:A:618:ARG:HD2	2.19	0.42
1:B:589:CYS:SG	1:B:626:LYS:HG3	2.60	0.42
1:B:694:SER:C	1:C:559:LYS:HZ2	2.27	0.42
1:B:726:LEU:CD1	1:B:755:LYS:HD3	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:526:ILE:O	1:C:530:TYR:HB2	2.19	0.42
1:A:733:LEU:HD23	1:A:733:LEU:HA	1.92	0.42
1:C:660:MET:HE1	1:C:721:ALA:N	2.35	0.42
1:B:601:LEU:HD23	1:B:604:LEU:HD12	2.01	0.41
1:A:620:LEU:N	1:A:621:PRO:CD	2.83	0.41
1:A:715:THR:O	1:A:719:PHE:HD2	2.04	0.41
1:B:538:ASP:OD2	1:B:542:ARG:HD3	2.20	0.41
1:C:661:ASN:C	1:C:663:PRO:HD2	2.45	0.41
1:B:533:LEU:HD21	1:B:599:ARG:HB2	2.02	0.41
1:B:578:ARG:HG3	1:B:578:ARG:O	2.20	0.41
1:C:696:GLY:HA3	1:C:714:TRP:CZ2	2.55	0.41
1:A:739:ILE:HD12	1:A:743:LEU:HD12	2.02	0.41
1:C:613:LEU:HD13	1:C:640:PHE:CD1	2.55	0.41
1:C:633:LEU:O	1:C:636:LEU:HB2	2.20	0.41
1:C:662:LEU:O	1:C:664:GLY:N	2.52	0.41
1:A:739:ILE:CD1	1:A:765:LEU:HD12	2.44	0.41
1:B:543:TYR:C	1:B:545:LEU:N	2.78	0.41
1:B:676:LEU:O	1:B:679:VAL:HG22	2.20	0.41
1:B:640:PHE:O	1:B:644:LEU:HG	2.21	0.41
1:C:614:MET:CE	1:C:658:GLN:HG3	2.50	0.41
1:A:548:GLU:C	1:A:550:GLU:N	2.78	0.41
1:A:664:GLY:O	1:A:665:SER:C	2.63	0.41
1:C:722:THR:HG22	1:C:747:PHE:CE1	2.56	0.41
1:A:609:ALA:HB1	1:A:643:LEU:HD22	2.03	0.41
1:A:734:ALA:O	1:A:736:PRO:HD3	2.21	0.41
1:A:739:ILE:CD1	1:A:743:LEU:HD12	2.51	0.41
1:B:557:ASP:OD1	1:B:560:HIS:HB3	2.21	0.41
1:A:546:SER:O	1:A:546:SER:OG	2.30	0.41
1:B:525:ILE:HD13	1:B:525:ILE:HA	1.99	0.40
1:A:556:ASP:O	1:A:559:LYS:HE2	2.20	0.40
1:C:539:TYR:CD1	1:C:558:ARG:HD2	2.56	0.40
1:C:659:LEU:HA	1:C:659:LEU:HD23	1.90	0.40
1:C:658:GLN:C	1:C:661:ASN:H	2.28	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:LEU:CD2	1:A:650:VAL:CG2[2_555]	1.86	0.34
1:A:549:GLU:O	1:A:578:ARG:NH1[2_555]	1.88	0.32

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	226/248 (91%)	214 (95%)	12 (5%)	0	100	100
1	B	213/248 (86%)	206 (97%)	7 (3%)	0	100	100
1	C	223/248 (90%)	216 (97%)	7 (3%)	0	100	100
All	All	662/744 (89%)	636 (96%)	26 (4%)	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	216/229 (94%)	211 (98%)	5 (2%)	44	67
1	B	206/229 (90%)	203 (98%)	3 (2%)	57	76
1	C	213/229 (93%)	210 (99%)	3 (1%)	59	77
All	All	635/687 (92%)	624 (98%)	11 (2%)	53	73

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	544	LEU
1	A	632	VAL
1	A	676	LEU
1	A	739	ILE
1	A	765	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	540	GLU
1	B	554	LEU
1	B	697	GLU
1	C	534	LEU
1	C	612	ILE
1	C	711	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	658	GLN
1	A	700	GLN
1	A	710	GLN
1	B	661	ASN
1	B	713	GLN
1	B	757	ASN
1	C	586	GLN
1	C	700	GLN
1	C	711	ASN
1	C	713	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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	C	1767	-	4,4,4	0.23	0	6,6,6	0.12	0
2	SO4	C	1765	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	C	1766	-	4,4,4	0.23	0	6,6,6	0.11	0
2	SO4	B	1767	-	4,4,4	0.23	0	6,6,6	0.08	0

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.

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	232/248 (93%)	0.74	29 (12%) 8 7	9, 41, 103, 162	0
1	B	221/248 (89%)	0.78	31 (14%) 6 6	15, 42, 102, 151	0
1	C	229/248 (92%)	0.76	34 (14%) 5 5	11, 42, 115, 153	0
All	All	682/744 (91%)	0.76	94 (13%) 6 6	9, 42, 107, 162	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	662	LEU	6.8
1	A	713	GLN	4.8
1	A	710	GLN	4.7
1	A	551	ARG	4.6
1	B	719	PHE	4.6
1	A	674	PRO	4.5
1	C	723	ARG	4.4
1	A	711	ASN	4.1
1	B	544	LEU	4.1
1	C	755	LYS	4.0
1	B	730	GLN	4.0
1	C	753	ARG	3.9
1	A	550	GLU	3.9
1	C	744	VAL	3.8
1	A	547	LEU	3.8
1	B	700	GLN	3.6
1	C	754	GLN	3.5
1	B	712	ASN	3.5
1	C	743	LEU	3.4
1	A	520	ARG	3.4
1	B	560	HIS	3.4
1	C	550	GLU	3.4
1	C	752	ASP	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	572	LYS	3.2
1	A	676	LEU	3.2
1	B	554	LEU	3.1
1	A	761	THR	3.1
1	C	761	THR	3.1
1	A	700	GLN	3.1
1	B	543	TYR	3.0
1	B	547	LEU	3.0
1	B	698	ASP	3.0
1	B	545	LEU	3.0
1	C	757	ASN	3.0
1	B	699	LEU	2.9
1	B	531	SER	2.9
1	B	586	GLN	2.9
1	C	719	PHE	2.9
1	A	558	ARG	2.9
1	C	660	MET	2.9
1	A	733	LEU	2.8
1	A	549	GLU	2.8
1	B	727	ARG	2.8
1	A	665	SER	2.8
1	A	709	THR	2.8
1	B	697	GLU	2.8
1	C	716	GLU	2.8
1	C	578	ARG	2.8
1	C	764	GLN	2.7
1	A	664	GLY	2.7
1	B	518	LYS	2.7
1	C	548	GLU	2.7
1	B	582	ASP	2.6
1	C	586	GLN	2.6
1	C	665	SER	2.6
1	B	539	TYR	2.6
1	A	521	LYS	2.6
1	B	728	ILE	2.6
1	A	517	ASP	2.6
1	B	548	GLU	2.5
1	C	515	ASP	2.5
1	C	731	ALA	2.5
1	B	571	GLY	2.5
1	A	607	GLU	2.5
1	B	735	LYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	731	ALA	2.4
1	C	573	LEU	2.4
1	B	597	VAL	2.3
1	B	555	MET	2.3
1	B	765	LEU	2.3
1	C	663	PRO	2.3
1	C	700	GLN	2.3
1	B	766	VAL	2.3
1	C	629	GLN	2.2
1	A	703	ASP	2.2
1	C	571	GLY	2.2
1	C	582	ASP	2.2
1	C	614	MET	2.2
1	A	764	GLN	2.2
1	A	752	ASP	2.1
1	B	567	ASP	2.1
1	C	732	ALA	2.1
1	B	646	HIS	2.1
1	A	663	PRO	2.1
1	C	748	SER	2.1
1	A	766	VAL	2.1
1	A	545	LEU	2.1
1	B	557	ASP	2.1
1	C	657	ARG	2.1
1	A	758	LEU	2.0
1	C	712	ASN	2.0
1	C	746	LEU	2.0
1	C	697	GLU	2.0
1	B	579	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	1767	5/5	0.76	0.14	86,88,88,88	0
2	SO4	C	1766	5/5	0.85	0.14	59,59,60,60	0
2	SO4	C	1767	5/5	0.90	0.13	85,85,85,86	0
2	SO4	C	1765	5/5	0.93	0.09	66,66,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.