



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:33 AM UTC

PDB ID : 1E8Y / pdb_00001e8y
Title : Structure determinants of phosphoinositide 3-kinase inhibition by wortmannin, LY294002, quercetin, myricetin and staurosporine
Authors : Walker, E.H.; Pacold, M.E.; Perisic, O.; Stephens, L.; Hawkins, P.T.; Wymann, M.P.; Williams, R.L.
Deposited on : 2000-10-03
Resolution : 2.00 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

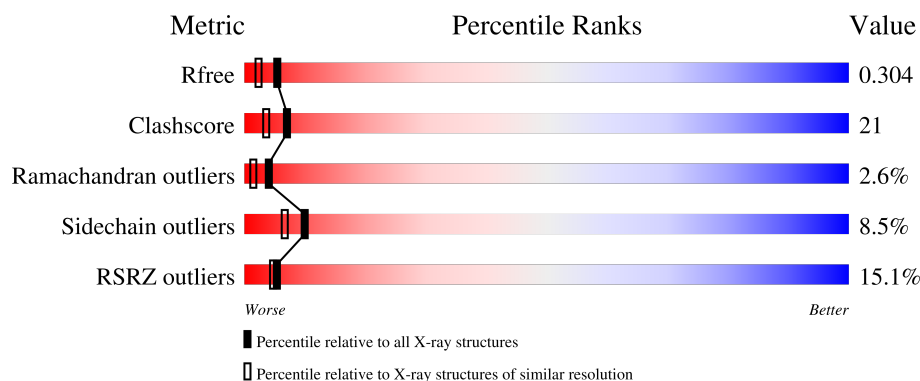
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	966	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6963 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 PHOSPHATIDYLINOSITOL 3-KINASE CATALYTIC SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	841	Total	C	N	O	S	0	0	0
			6815	4374	1164	1242	35			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	PRO	cloning artifact	UNP P48736
A	505	ALA	ARG	conflict	UNP P48736

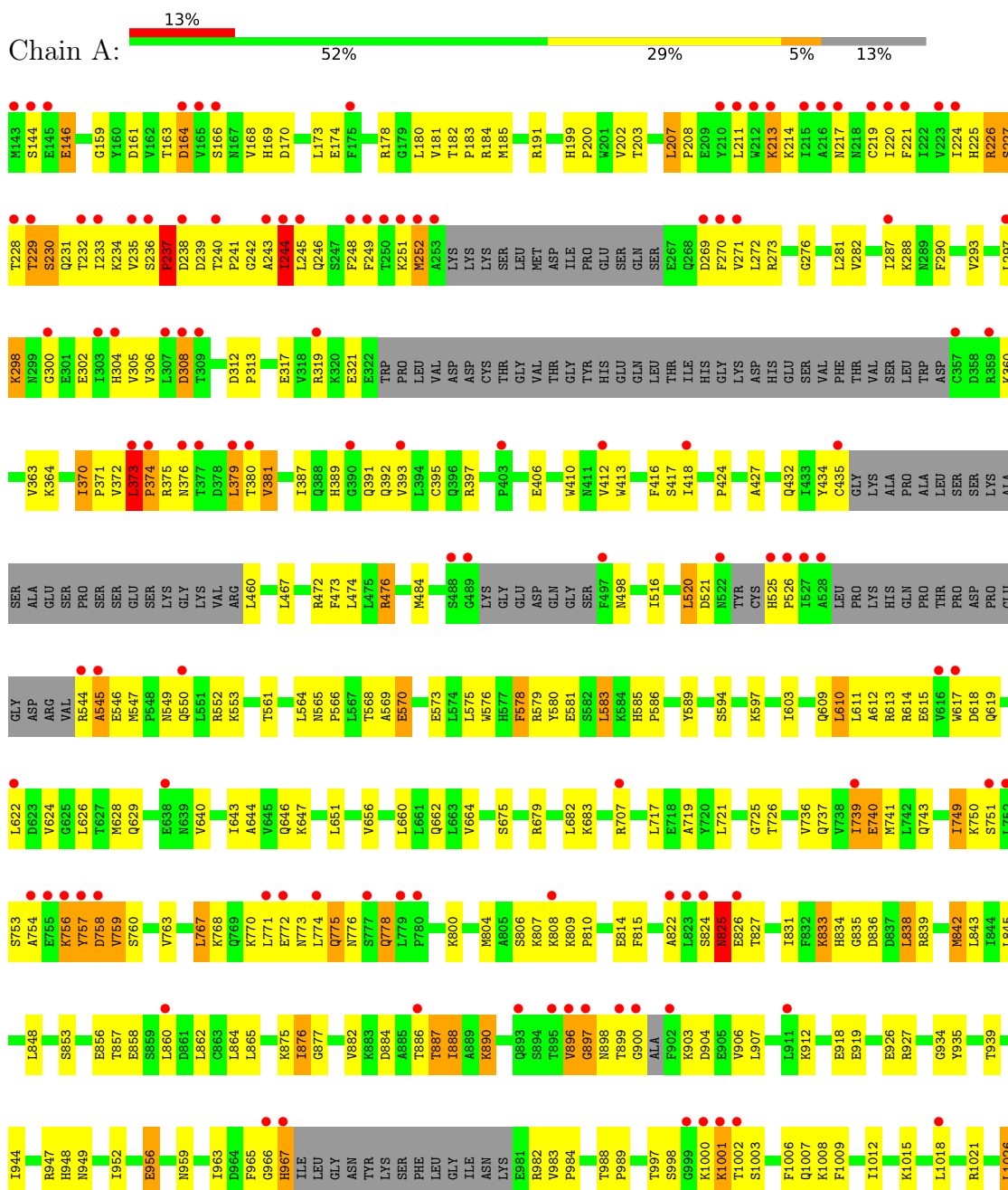
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	148	Total	O	0	0
			148	148		

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: PHOSPHATIDYLINOSITOL 3-KINASE CATALYTIC SUBUNIT





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.23Å 66.25Å 102.64Å 90.00° 97.85° 90.00°	Depositor
Resolution (Å)	68.96 – 2.00 68.96 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.6 (68.96-2.00) 92.7 (68.96-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.245 , 0.305 0.244 , 0.304	Depositor DCC
R_{free} test set	2287 reflections (3.93%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6963	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% 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	0.89	4/6960 (0.1%)	1.07	22/9413 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	484	MET	SD-CE	7.36	1.98	1.79
1	A	842	MET	SD-CE	-6.70	1.62	1.79
1	A	882	VAL	CA-CB	5.55	1.60	1.54
1	A	656	VAL	C-O	-5.18	1.18	1.24

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	LEU	N-CA-C	-10.47	100.50	113.28
1	A	644	ALA	N-CA-C	-7.66	102.53	111.03
1	A	308	ASP	N-CA-C	7.04	117.56	108.34
1	A	244	ILE	N-CA-C	-6.88	95.03	109.34
1	A	585	HIS	CA-C-N	6.61	126.86	119.32
1	A	585	HIS	C-N-CA	6.61	126.86	119.32
1	A	159	GLY	N-CA-C	-5.83	107.12	115.64
1	A	919	GLU	N-CA-C	-5.65	104.81	110.97
1	A	825	ASN	N-CA-C	-5.65	105.73	113.30
1	A	904	ASP	N-CA-C	5.62	118.17	111.71
1	A	833	LYS	N-CA-C	5.55	118.27	109.50
1	A	484	MET	N-CA-C	5.52	118.59	110.59
1	A	387	ILE	N-CA-C	-5.42	100.07	107.99
1	A	956	GLU	N-CA-C	-5.35	106.02	112.54
1	A	683	LYS	N-CA-C	5.32	116.76	111.07
1	A	191	ARG	N-CA-C	5.27	117.93	110.50
1	A	594	SER	N-CA-C	-5.27	106.63	113.16
1	A	578	PHE	CA-C-N	5.23	128.66	120.82
1	A	578	PHE	C-N-CA	5.23	128.66	120.82
1	A	163	THR	N-CA-C	-5.21	106.51	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	864	LEU	N-CA-C	-5.11	104.13	110.41
1	A	948	HIS	N-CA-C	-5.10	102.14	110.20

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	6815	0	6848	287	0
2	A	148	0	0	6	0
All	All	6963	0	6848	287	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 (287) 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:181:VAL:HG12	1:A:185:MET:HE2	1.30	1.13
1:A:1035:LEU:HD12	1:A:1048:ILE:HD13	1.33	1.11
1:A:804:MET:HE3	1:A:810:PRO:HG2	1.35	1.08
1:A:525:HIS:HB3	1:A:526:PRO:HD3	1.46	0.94
1:A:373:LEU:HD22	1:A:406:GLU:HG2	1.50	0.93
1:A:544:ARG:HH21	1:A:546:GLU:HB3	1.32	0.92
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.21	0.88
1:A:1044:SER:O	1:A:1045:LYS:HG3	1.74	0.86
1:A:576:TRP:CZ3	1:A:579:ARG:HD2	2.12	0.85
1:A:804:MET:HE3	1:A:810:PRO:CG	2.07	0.84
1:A:181:VAL:CG1	1:A:185:MET:HE2	2.07	0.82
1:A:240:THR:O	1:A:244:ILE:HG23	1.78	0.82
1:A:224:ILE:HD13	1:A:233:ILE:HD13	1.64	0.80
1:A:360:LYS:HE2	1:A:417:SER:HA	1.65	0.78
1:A:237:PRO:HA	1:A:287:ILE:HD11	1.65	0.78
1:A:576:TRP:CH2	1:A:579:ARG:HD2	2.18	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ALA:HA	1:A:246:GLN:HG3	1.65	0.77
1:A:379:LEU:HD13	1:A:380:THR:H	1.50	0.75
1:A:225:HIS:HE1	1:A:304:HIS:HD2	1.34	0.75
1:A:217:ASN:HD22	1:A:219:CYS:HB2	1.51	0.74
1:A:1039:MET:HB3	1:A:1040:PRO:HD2	1.70	0.74
1:A:614:ARG:HG2	1:A:617:TRP:HB3	1.71	0.73
1:A:568:THR:HG22	1:A:570:GLU:H	1.52	0.73
1:A:370:ILE:HD13	1:A:371:PRO:HD2	1.69	0.73
1:A:217:ASN:ND2	1:A:219:CYS:HB2	2.05	0.72
1:A:1043:THR:C	1:A:1045:LYS:H	1.98	0.71
1:A:580:TYR:HE2	1:A:613:ARG:HD3	1.56	0.70
1:A:220:ILE:HD11	1:A:237:PRO:HG3	1.74	0.69
1:A:395:CYS:HB3	1:A:416:PHE:HD2	1.55	0.69
1:A:807:LYS:H	1:A:807:LYS:HD2	1.57	0.69
1:A:202:VAL:HG12	1:A:203:THR:N	2.07	0.69
1:A:293:VAL:O	1:A:297:LEU:HG	1.93	0.69
1:A:939:THR:HG21	2:A:2128:HOH:O	1.93	0.68
1:A:1021:ARG:HE	1:A:1056:THR:CG2	2.07	0.68
1:A:888:ILE:HG22	1:A:949:ASN:OD1	1.92	0.68
1:A:1000:LYS:HA	1:A:1076:ARG:NH1	2.08	0.68
1:A:174:GLU:HB3	1:A:178:ARG:HH12	1.59	0.68
1:A:887:THR:HG22	1:A:890:LYS:H	1.58	0.68
1:A:997:THR:HG22	1:A:998:SER:N	2.09	0.68
1:A:1026:LEU:O	1:A:1029:ILE:HG22	1.93	0.67
1:A:1021:ARG:HE	1:A:1056:THR:HG22	1.58	0.67
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.77	0.66
1:A:622:LEU:HD21	1:A:651:LEU:CD2	2.26	0.65
1:A:373:LEU:N	1:A:374:PRO:HD2	2.12	0.65
1:A:1060:ASN:HD21	1:A:1062:GLU:HB2	1.60	0.65
1:A:896:VAL:HG12	1:A:897:GLY:H	1.60	0.64
1:A:1002:THR:HG22	1:A:1003:SER:H	1.62	0.64
1:A:860:LEU:HD11	1:A:1015:LYS:HG2	1.77	0.64
1:A:565:ASN:OD1	1:A:566:PRO:HD2	1.98	0.64
1:A:758:ASP:OD1	1:A:759:VAL:N	2.31	0.64
1:A:170:ASP:OD2	1:A:476:ARG:NH2	2.30	0.63
1:A:886:THR:HG22	1:A:887:THR:H	1.61	0.63
1:A:395:CYS:SG	1:A:418:ILE:HG13	2.39	0.63
1:A:251:LYS:O	1:A:251:LYS:HD3	1.99	0.62
1:A:1006:PHE:O	1:A:1009:PHE:HB3	1.99	0.62
1:A:1042:LEU:HD22	1:A:1042:LEU:O	1.99	0.62
1:A:233:ILE:H	1:A:233:ILE:HD12	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1008:LYS:O	1:A:1012:ILE:HG13	1.99	0.62
1:A:231:GLN:HG3	1:A:232:THR:H	1.64	0.62
1:A:379:LEU:HB3	1:A:435:CYS:SG	2.41	0.61
1:A:220:ILE:HD12	1:A:287:ILE:CD1	2.30	0.61
1:A:370:ILE:HD13	1:A:371:PRO:CD	2.30	0.61
1:A:815:PHE:O	1:A:827:THR:HB	2.01	0.61
1:A:888:ILE:HD13	1:A:952:ILE:HG22	1.82	0.61
1:A:982:ARG:HD2	1:A:1090:LEU:HD13	1.83	0.61
1:A:768:LYS:O	1:A:772:GLU:HG2	2.01	0.60
1:A:888:ILE:CG2	1:A:949:ASN:OD1	2.49	0.60
1:A:622:LEU:HD21	1:A:651:LEU:HD23	1.82	0.60
1:A:544:ARG:HH21	1:A:546:GLU:CB	2.12	0.60
1:A:568:THR:CG2	1:A:569:ALA:N	2.64	0.60
1:A:886:THR:HG22	1:A:887:THR:N	2.17	0.60
1:A:1043:THR:O	1:A:1045:LYS:N	2.28	0.59
1:A:287:ILE:HD12	1:A:288:LYS:N	2.18	0.59
1:A:614:ARG:HH11	1:A:646:GLN:HE22	1.50	0.59
1:A:221:PHE:HE2	1:A:234:LYS:HD2	1.67	0.59
1:A:568:THR:HG22	1:A:569:ALA:N	2.18	0.59
1:A:1060:ASN:ND2	1:A:1062:GLU:H	2.01	0.58
1:A:202:VAL:CG1	1:A:203:THR:N	2.66	0.58
1:A:629:GLN:OE1	2:A:2062:HOH:O	2.17	0.58
1:A:410:TRP:O	1:A:412:VAL:HG23	2.02	0.58
1:A:547:MET:HE3	1:A:578:PHE:CD1	2.38	0.58
1:A:749:ILE:CD1	1:A:770:LYS:HD2	2.33	0.58
1:A:927:ARG:HE	1:A:959:ASN:HD22	1.50	0.58
1:A:173:LEU:HB2	2:A:2011:HOH:O	2.02	0.58
1:A:363:VAL:HG23	1:A:520:LEU:CD1	2.33	0.58
1:A:568:THR:HG22	1:A:570:GLU:N	2.19	0.58
1:A:947:ARG:NH2	1:A:963:ILE:O	2.35	0.58
1:A:207:LEU:HD23	1:A:208:PRO:HD2	1.85	0.58
1:A:757:TYR:HA	1:A:809:LYS:NZ	2.19	0.58
1:A:372:VAL:HG12	1:A:374:PRO:HD2	1.85	0.57
1:A:756:LYS:O	1:A:758:ASP:OD2	2.22	0.57
1:A:180:LEU:C	1:A:183:PRO:HD2	2.29	0.57
1:A:379:LEU:HD13	1:A:380:THR:HG22	1.85	0.57
1:A:169:HIS:HE1	2:A:2043:HOH:O	1.87	0.57
1:A:363:VAL:HG23	1:A:520:LEU:HD13	1.86	0.57
1:A:888:ILE:CD1	1:A:952:ILE:HG22	2.34	0.57
1:A:903:LYS:O	1:A:906:VAL:HG23	2.04	0.57
1:A:213:LYS:HD3	1:A:214:LYS:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ILE:HD12	1:A:287:ILE:HD11	1.87	0.56
1:A:379:LEU:CD1	1:A:380:THR:H	2.15	0.56
1:A:757:TYR:HA	1:A:809:LYS:HZ1	1.70	0.56
1:A:1043:THR:C	1:A:1045:LYS:N	2.62	0.56
1:A:614:ARG:HD2	1:A:618:ASP:OD1	2.06	0.56
1:A:1042:LEU:HD22	1:A:1042:LEU:C	2.31	0.56
1:A:774:LEU:O	1:A:776:ASN:N	2.39	0.56
1:A:903:LYS:HB2	1:A:906:VAL:CG2	2.36	0.56
1:A:824:SER:OG	1:A:826:GLU:HG3	2.05	0.55
1:A:161:ASP:O	1:A:164:ASP:HB3	2.07	0.55
1:A:615:GLU:O	1:A:619:GLN:HG3	2.07	0.55
1:A:271:VAL:HG23	1:A:282:VAL:HG12	1.89	0.55
1:A:856:GLU:C	1:A:858:GLU:H	2.15	0.55
1:A:381:VAL:HG22	1:A:434:TYR:O	2.07	0.54
1:A:252:MET:HE3	1:A:252:MET:HA	1.89	0.54
1:A:238:ASP:OD1	1:A:238:ASP:O	2.26	0.54
1:A:997:THR:HG22	1:A:998:SER:H	1.73	0.54
1:A:1035:LEU:HA	1:A:1039:MET:HG2	1.89	0.54
1:A:1085:ASN:O	1:A:1087:PHE:N	2.41	0.54
1:A:373:LEU:CD2	1:A:406:GLU:HG2	2.32	0.53
1:A:373:LEU:N	1:A:374:PRO:CD	2.72	0.53
1:A:624:VAL:O	1:A:628:MET:HG2	2.08	0.53
1:A:989:PRO:HG2	1:A:1080:TRP:CD1	2.44	0.53
1:A:825:ASN:N	1:A:825:ASN:ND2	2.57	0.53
1:A:233:ILE:HD12	1:A:233:ILE:N	2.23	0.52
1:A:549:ASN:HD21	1:A:553:LYS:NZ	2.08	0.52
1:A:888:ILE:HD13	1:A:952:ILE:CG2	2.39	0.52
1:A:1042:LEU:O	1:A:1042:LEU:HD13	2.10	0.52
1:A:174:GLU:HB3	1:A:178:ARG:NH1	2.24	0.52
1:A:800:LYS:HD3	1:A:814:GLU:OE1	2.09	0.52
1:A:1002:THR:O	1:A:1003:SER:HB3	2.09	0.52
1:A:736:VAL:O	1:A:740:GLU:HB2	2.10	0.52
1:A:1000:LYS:HA	1:A:1076:ARG:CZ	2.40	0.52
1:A:182:THR:HB	1:A:183:PRO:HD3	1.92	0.51
1:A:1002:THR:HG22	1:A:1003:SER:N	2.25	0.51
1:A:611:LEU:O	1:A:614:ARG:HB2	2.10	0.51
1:A:424:PRO:HG2	1:A:427:ALA:HB2	1.92	0.51
1:A:525:HIS:HB3	1:A:526:PRO:CD	2.31	0.51
1:A:569:ALA:O	1:A:573:GLU:HG3	2.11	0.51
1:A:660:LEU:O	1:A:664:VAL:HG23	2.11	0.51
1:A:214:LYS:NZ	1:A:300:GLY:HA2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ARG:NH2	1:A:321:GLU:OE1	2.43	0.51
1:A:725:GLY:HA3	2:A:2096:HOH:O	2.11	0.50
1:A:804:MET:CE	1:A:831:ILE:HG12	2.41	0.50
1:A:774:LEU:C	1:A:776:ASN:N	2.67	0.50
1:A:317:GLU:O	1:A:726:THR:HG23	2.11	0.50
1:A:226:ARG:O	1:A:227:SER:HB2	2.12	0.50
1:A:983:VAL:HG22	1:A:984:PRO:HD2	1.93	0.50
1:A:839:ARG:HA	1:A:842:MET:CE	2.42	0.50
1:A:856:GLU:C	1:A:858:GLU:N	2.69	0.50
1:A:235:VAL:HG12	1:A:236:SER:N	2.27	0.50
1:A:373:LEU:H	1:A:374:PRO:CD	2.25	0.49
1:A:583:LEU:O	1:A:583:LEU:HD23	2.13	0.49
1:A:525:HIS:CB	1:A:526:PRO:HD3	2.32	0.49
1:A:544:ARG:O	1:A:545:ALA:HB3	2.12	0.49
1:A:838:LEU:HD23	1:A:877:GLY:HA3	1.95	0.49
1:A:750:LYS:NZ	1:A:834:HIS:HD2	2.11	0.49
1:A:860:LEU:HD21	1:A:1015:LYS:CE	2.42	0.49
1:A:308:ASP:N	1:A:308:ASP:OD1	2.45	0.49
1:A:164:ASP:OD1	1:A:166:SER:HB2	2.13	0.49
1:A:988:THR:HB	1:A:989:PRO:HD2	1.95	0.48
1:A:997:THR:CG2	1:A:998:SER:N	2.76	0.48
1:A:373:LEU:H	1:A:374:PRO:HD2	1.79	0.48
1:A:242:GLY:O	1:A:246:GLN:HG3	2.13	0.48
1:A:860:LEU:HD21	1:A:1015:LYS:NZ	2.28	0.48
1:A:389:HIS:O	1:A:392:GLN:HB3	2.14	0.48
1:A:546:GLU:OE2	1:A:552:ARG:NH1	2.42	0.48
1:A:629:GLN:HG2	1:A:1029:ILE:HG13	1.95	0.48
1:A:808:LYS:HD2	1:A:835:GLY:HA3	1.96	0.48
1:A:220:ILE:CD1	1:A:237:PRO:HG3	2.41	0.48
1:A:561:THR:HG21	1:A:565:ASN:ND2	2.28	0.48
1:A:808:LYS:HE3	1:A:836:ASP:OD1	2.14	0.48
1:A:561:THR:HG21	1:A:565:ASN:HD22	1.78	0.47
1:A:1056:THR:HG23	1:A:1056:THR:O	2.14	0.47
1:A:240:THR:HG22	1:A:242:GLY:H	1.79	0.47
1:A:474:LEU:HD23	1:A:525:HIS:N	2.28	0.47
1:A:1086:TRP:C	1:A:1087:PHE:CD1	2.92	0.47
1:A:213:LYS:HD3	1:A:214:LYS:H	1.80	0.47
1:A:896:VAL:O	1:A:897:GLY:O	2.32	0.47
1:A:899:THR:HG22	1:A:899:THR:O	2.15	0.47
1:A:741:MET:HE1	1:A:778:GLN:O	2.15	0.47
1:A:807:LYS:H	1:A:807:LYS:CD	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:876:ILE:HG12	1:A:877:GLY:N	2.30	0.47
1:A:302:GLU:HB2	1:A:304:HIS:CE1	2.49	0.47
1:A:580:TYR:CE2	1:A:613:ARG:HD3	2.44	0.47
1:A:739:ILE:HG13	1:A:740:GLU:N	2.30	0.47
1:A:1042:LEU:CD1	1:A:1042:LEU:H	2.27	0.47
1:A:675:SER:O	1:A:679:ARG:HG3	2.15	0.47
1:A:579:ARG:HG2	1:A:610:LEU:HD11	1.97	0.46
1:A:1055:LEU:O	1:A:1056:THR:HG22	2.15	0.46
1:A:614:ARG:HH11	1:A:646:GLN:NE2	2.11	0.46
1:A:1003:SER:O	1:A:1007:GLN:HG3	2.15	0.46
1:A:213:LYS:NZ	1:A:214:LYS:HB2	2.31	0.46
1:A:544:ARG:NH2	1:A:546:GLU:HB3	2.14	0.46
1:A:760:SER:O	1:A:763:VAL:HG12	2.15	0.46
1:A:825:ASN:H	1:A:825:ASN:HD22	1.64	0.46
1:A:935:TYR:O	1:A:939:THR:HG22	2.16	0.46
1:A:199:HIS:O	1:A:200:PRO:C	2.57	0.46
1:A:628:MET:HE1	1:A:662:GLN:HB3	1.97	0.46
1:A:774:LEU:C	1:A:776:ASN:H	2.23	0.46
1:A:240:THR:HG23	1:A:241:PRO:HD2	1.97	0.46
1:A:1038:GLY:C	1:A:1039:MET:HE2	2.41	0.46
1:A:739:ILE:O	1:A:743:GLN:HG3	2.15	0.46
1:A:1000:LYS:HG2	1:A:1076:ARG:HB3	1.97	0.46
1:A:202:VAL:CG1	1:A:203:THR:H	2.28	0.46
1:A:862:LEU:HB3	1:A:934:GLY:HA3	1.98	0.46
1:A:1042:LEU:HD23	1:A:1048:ILE:HD11	1.98	0.46
1:A:211:LEU:HD21	1:A:298:LYS:HA	1.97	0.45
1:A:233:ILE:H	1:A:233:ILE:CD1	2.29	0.45
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.97	0.45
1:A:589:TYR:CD1	1:A:589:TYR:N	2.83	0.45
1:A:224:ILE:N	1:A:224:ILE:HD12	2.31	0.45
1:A:472:ARG:O	1:A:473:PHE:HB2	2.16	0.45
1:A:467:LEU:O	1:A:476:ARG:HD2	2.17	0.45
1:A:583:LEU:HD23	1:A:583:LEU:C	2.40	0.45
1:A:757:TYR:HD1	1:A:757:TYR:O	1.98	0.45
1:A:804:MET:HE2	1:A:831:ILE:HG12	1.98	0.45
1:A:884:ASP:HB3	1:A:956:GLU:HG3	1.98	0.45
1:A:381:VAL:HA	1:A:434:TYR:O	2.16	0.45
1:A:884:ASP:O	1:A:956:GLU:HG3	2.16	0.45
1:A:287:ILE:HA	1:A:290:PHE:HD1	1.82	0.45
1:A:939:THR:OG1	1:A:944:ILE:HG13	2.17	0.45
1:A:965:PHE:O	1:A:967:HIS:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1018:LEU:HB2	2:A:2141:HOH:O	2.16	0.45
1:A:516:ILE:O	1:A:516:ILE:HG23	2.17	0.45
1:A:751:SER:C	1:A:753:SER:H	2.25	0.45
1:A:899:THR:O	1:A:900:GLY:C	2.59	0.44
1:A:622:LEU:CD2	1:A:651:LEU:HD23	2.46	0.44
1:A:737:GLN:O	1:A:741:MET:HG3	2.17	0.44
1:A:237:PRO:HA	1:A:287:ILE:CD1	2.41	0.44
1:A:628:MET:HB2	1:A:1029:ILE:HD12	2.00	0.44
1:A:547:MET:HG2	1:A:578:PHE:CD2	2.52	0.44
1:A:741:MET:HE1	1:A:778:GLN:C	2.43	0.44
1:A:169:HIS:C	1:A:169:HIS:CD2	2.95	0.44
1:A:579:ARG:HG2	1:A:610:LEU:CD1	2.47	0.43
1:A:552:ARG:HH21	1:A:581:GLU:CD	2.26	0.43
1:A:767:LEU:HD22	1:A:771:LEU:HG	2.00	0.43
1:A:246:GLN:C	1:A:248:PHE:H	2.26	0.43
1:A:544:ARG:CG	1:A:545:ALA:N	2.82	0.43
1:A:276:GLY:HA3	1:A:822:ALA:HA	1.99	0.43
1:A:498:ASN:OD1	1:A:498:ASN:C	2.61	0.43
1:A:912:LYS:HE2	1:A:918:GLU:OE2	2.19	0.43
1:A:273:ARG:O	1:A:306:VAL:HG12	2.18	0.43
1:A:287:ILE:HA	1:A:290:PHE:CD1	2.53	0.43
1:A:640:VAL:O	1:A:643:ILE:HG12	2.18	0.43
1:A:1021:ARG:NE	1:A:1056:THR:CG2	2.78	0.43
1:A:146:GLU:OE2	1:A:319:ARG:NH1	2.51	0.43
1:A:810:PRO:HB3	1:A:833:LYS:HB2	1.99	0.43
1:A:249:PHE:HZ	1:A:270:PHE:HD1	1.67	0.42
1:A:229:THR:O	1:A:230:SER:HB3	2.19	0.42
1:A:853:SER:O	1:A:857:THR:HG23	2.20	0.42
1:A:875:LYS:HE3	1:A:875:LYS:HB2	1.80	0.42
1:A:364:LYS:HB2	1:A:413:TRP:CE3	2.55	0.42
1:A:825:ASN:N	1:A:825:ASN:HD22	2.16	0.42
1:A:949:ASN:H	1:A:1083:GLN:NE2	2.01	0.42
1:A:184:ARG:HD3	1:A:719:ALA:O	2.20	0.42
1:A:544:ARG:CG	1:A:545:ALA:H	2.29	0.42
1:A:839:ARG:HA	1:A:842:MET:HE2	2.01	0.42
1:A:241:PRO:HG2	1:A:290:PHE:CZ	2.55	0.42
1:A:432:GLN:HB3	1:A:460:LEU:CD1	2.50	0.42
1:A:982:ARG:HD2	1:A:1090:LEU:CD1	2.49	0.42
1:A:239:ASP:HB3	1:A:244:ILE:HG22	2.02	0.42
1:A:1086:TRP:O	1:A:1087:PHE:CD1	2.72	0.42
1:A:860:LEU:HD21	1:A:1015:LYS:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1086:TRP:HH2	1:A:1090:LEU:HB3	1.85	0.41
1:A:757:TYR:O	1:A:758:ASP:HB3	2.20	0.41
1:A:207:LEU:CD2	1:A:208:PRO:HD2	2.49	0.41
1:A:1070:ASP:O	1:A:1074:VAL:HG23	2.20	0.41
1:A:174:GLU:OE1	1:A:178:ARG:NH1	2.53	0.41
1:A:397:ARG:HD3	1:A:397:ARG:HA	1.86	0.41
1:A:589:TYR:N	1:A:589:TYR:HD1	2.18	0.41
1:A:983:VAL:CG2	1:A:984:PRO:HD2	2.51	0.41
1:A:225:HIS:HE1	1:A:304:HIS:CD2	2.23	0.41
1:A:721:LEU:HD23	1:A:721:LEU:HA	1.97	0.41
1:A:609:GLN:O	1:A:612:ALA:HB3	2.20	0.41
1:A:146:GLU:CD	1:A:319:ARG:HH12	2.29	0.41
1:A:312:ASP:HA	1:A:313:PRO:HD2	1.87	0.41
1:A:372:VAL:CG1	1:A:374:PRO:HD2	2.51	0.41
1:A:380:THR:O	1:A:435:CYS:HA	2.21	0.41
1:A:597:LYS:HB2	1:A:603:ILE:HD13	2.03	0.41
1:A:773:ASN:O	1:A:776:ASN:HB2	2.21	0.40
1:A:774:LEU:O	1:A:775:GLN:C	2.64	0.40
1:A:927:ARG:NE	1:A:959:ASN:HD22	2.18	0.40
1:A:997:THR:CG2	1:A:998:SER:H	2.33	0.40
1:A:249:PHE:CZ	1:A:270:PHE:HD1	2.39	0.40
1:A:1001:LYS:HB3	1:A:1002:THR:H	1.68	0.40
1:A:552:ARG:NH2	1:A:581:GLU:CD	2.79	0.40
1:A:251:LYS:O	1:A:252:MET:HE3	2.21	0.40
1:A:806:SER:O	1:A:807:LYS:C	2.63	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	823/966 (85%)	745 (90%)	57 (7%)	21 (3%)	4 1

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	ASN
1	A	227	SER
1	A	230	SER
1	A	758	ASP
1	A	775	GLN
1	A	897	GLY
1	A	966	GLY
1	A	1040	PRO
1	A	1044	SER
1	A	1086	TRP
1	A	756	LYS
1	A	1045	LYS
1	A	373	LEU
1	A	545	ALA
1	A	754	ALA
1	A	1088	LEU
1	A	237	PRO
1	A	759	VAL
1	A	1091	VAL
1	A	374	PRO
1	A	244	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	755/864 (87%)	691 (92%)	64 (8%)	10 7

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	SER
1	A	146	GLU
1	A	164	ASP
1	A	168	VAL

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Mol	Chain	Res	Type
1	A	207	LEU
1	A	213	LYS
1	A	226	ARG
1	A	228	THR
1	A	229	THR
1	A	237	PRO
1	A	252	MET
1	A	269	ASP
1	A	281	LEU
1	A	298	LYS
1	A	370	ILE
1	A	373	LEU
1	A	375	ARG
1	A	379	LEU
1	A	381	VAL
1	A	391	GLN
1	A	393	VAL
1	A	476	ARG
1	A	520	LEU
1	A	521	ASP
1	A	550	GLN
1	A	570	GLU
1	A	575	LEU
1	A	583	LEU
1	A	586	PRO
1	A	610	LEU
1	A	626	LEU
1	A	647	LYS
1	A	682	LEU
1	A	707	ARG
1	A	717	LEU
1	A	739	ILE
1	A	740	GLU
1	A	749	ILE
1	A	757	TYR
1	A	767	LEU
1	A	778	GLN
1	A	825	ASN
1	A	838	LEU
1	A	843	LEU
1	A	845	LEU
1	A	848	LEU

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Mol	Chain	Res	Type
1	A	865	LEU
1	A	876	ILE
1	A	887	THR
1	A	888	ILE
1	A	890	LYS
1	A	896	VAL
1	A	898	ASN
1	A	907	LEU
1	A	926	GLU
1	A	967	HIS
1	A	1001	LYS
1	A	1026	LEU
1	A	1029	ILE
1	A	1042	LEU
1	A	1051	ILE
1	A	1089	HIS
1	A	1091	VAL
1	A	1092	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	169	HIS
1	A	217	ASN
1	A	225	HIS
1	A	304	HIS
1	A	389	HIS
1	A	391	GLN
1	A	483	HIS
1	A	549	ASN
1	A	554	GLN
1	A	629	GLN
1	A	646	GLN
1	A	743	GLN
1	A	766	GLN
1	A	773	ASN
1	A	825	ASN
1	A	834	HIS
1	A	951	ASN
1	A	959	ASN
1	A	967	HIS

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Mol	Chain	Res	Type
1	A	1041	GLN
1	A	1060	ASN
1	A	1083	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 ⓘ

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	841/966 (87%)	0.87	127 (15%) 5 5	17, 39, 75, 126	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	379	LEU	6.6
1	A	900	GLY	6.6
1	A	1087	PHE	6.2
1	A	1040	PRO	5.8
1	A	377	THR	5.6
1	A	1044	SER	5.3
1	A	253	ALA	5.3
1	A	526	PRO	5.2
1	A	1090	LEU	5.0
1	A	779	LEU	4.9
1	A	757	TYR	4.8
1	A	1088	LEU	4.7
1	A	1091	VAL	4.6
1	A	1089	HIS	4.5
1	A	1042	LEU	4.5
1	A	525	HIS	4.3
1	A	1092	LEU	4.3
1	A	373	LEU	4.2
1	A	899	THR	4.1
1	A	527	ILE	4.1
1	A	216	ALA	4.1
1	A	528	ALA	4.1
1	A	966	GLY	4.0
1	A	897	GLY	3.9
1	A	249	PHE	3.6
1	A	412	VAL	3.5
1	A	307	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	250	THR	3.4
1	A	774	LEU	3.4
1	A	251	LYS	3.4
1	A	211	LEU	3.4
1	A	221	PHE	3.4
1	A	374	PRO	3.3
1	A	164	ASP	3.3
1	A	1043	THR	3.3
1	A	233	ILE	3.2
1	A	823	LEU	3.2
1	A	967	HIS	3.2
1	A	489	GLY	3.2
1	A	212	TRP	3.1
1	A	238	ASP	3.1
1	A	244	ILE	3.1
1	A	497	PHE	3.1
1	A	144	SER	3.0
1	A	215	ILE	3.0
1	A	213	LYS	3.0
1	A	772	GLU	3.0
1	A	754	ALA	3.0
1	A	902	PHE	3.0
1	A	550	GLN	2.9
1	A	739	ILE	2.9
1	A	309	THR	2.9
1	A	252	MET	2.9
1	A	271	VAL	2.9
1	A	220	ILE	2.9
1	A	240	THR	2.9
1	A	755	GLU	2.8
1	A	219	CYS	2.8
1	A	418	ILE	2.8
1	A	777	SER	2.8
1	A	143	MET	2.8
1	A	488	SER	2.7
1	A	308	ASP	2.7
1	A	545	ALA	2.7
1	A	359	ARG	2.7
1	A	1041	GLN	2.7
1	A	303	ILE	2.7
1	A	544	ARG	2.7
1	A	376	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	357	CYS	2.6
1	A	166	SER	2.6
1	A	236	SER	2.6
1	A	771	LEU	2.6
1	A	1018	LEU	2.6
1	A	243	ALA	2.6
1	A	758	ASP	2.6
1	A	617	TRP	2.6
1	A	522	ASN	2.5
1	A	756	LYS	2.5
1	A	270	PHE	2.5
1	A	896	VAL	2.5
1	A	1002	THR	2.5
1	A	911	LEU	2.5
1	A	165	VAL	2.5
1	A	224	ILE	2.5
1	A	435	CYS	2.4
1	A	248	PHE	2.4
1	A	393	VAL	2.4
1	A	824	SER	2.4
1	A	1000	LYS	2.4
1	A	297	LEU	2.4
1	A	229	THR	2.4
1	A	380	THR	2.4
1	A	616	VAL	2.4
1	A	751	SER	2.3
1	A	893	GLN	2.3
1	A	826	GLU	2.3
1	A	287	ILE	2.3
1	A	235	VAL	2.3
1	A	886	THR	2.2
1	A	269	ASP	2.2
1	A	390	GLY	2.2
1	A	245	LEU	2.2
1	A	752	LEU	2.2
1	A	232	THR	2.2
1	A	780	PRO	2.2
1	A	145	GLU	2.2
1	A	300	GLY	2.2
1	A	860	LEU	2.2
1	A	403	PRO	2.1
1	A	895	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	175	PHE	2.1
1	A	223	VAL	2.1
1	A	1001	LYS	2.1
1	A	228	THR	2.1
1	A	1048	ILE	2.1
1	A	822	ALA	2.1
1	A	1045	LYS	2.1
1	A	304	HIS	2.1
1	A	707	ARG	2.1
1	A	808	LYS	2.1
1	A	217	ASN	2.0
1	A	638	GLU	2.0
1	A	622	LEU	2.0
1	A	319	ARG	2.0
1	A	999	GLY	2.0
1	A	210	TYR	2.0

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.