



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 06:34 PM UTC

PDB ID : 3HIZ / pdb_00003hiz
Title : Crystal structure of p110alpha H1047R mutant in complex with niSH2 of p85alpha
Authors : Amzel, L.M.; Vogelstein, B.; Gabelli, S.B.; Mandelker, D.
Deposited on : 2009-05-20
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 types of validation reports are described at

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

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

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

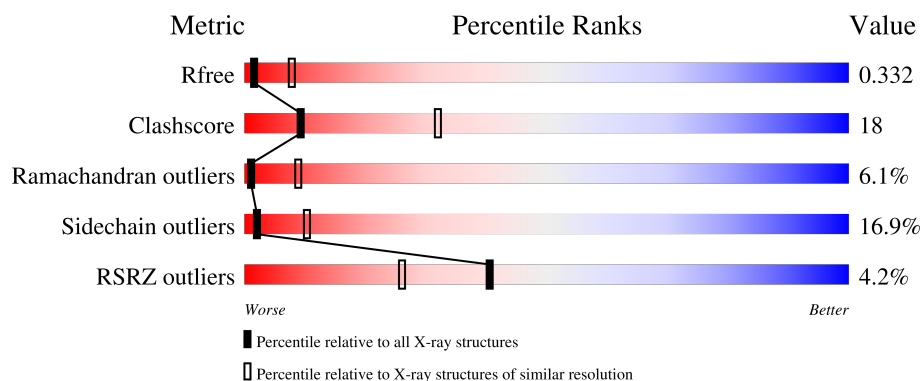
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	1096	
2	B	373	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10384 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-4,5-bisphosphate 3-kinase catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1024	Total	C	N	O	S	0	0	0
			8391	5365	1435	1525	66			

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	MET	-	expression tag	UNP P42336
A	-27	SER	-	expression tag	UNP P42336
A	-26	TYR	-	expression tag	UNP P42336
A	-25	TYR	-	expression tag	UNP P42336
A	-24	HIS	-	expression tag	UNP P42336
A	-23	HIS	-	expression tag	UNP P42336
A	-22	HIS	-	expression tag	UNP P42336
A	-21	HIS	-	expression tag	UNP P42336
A	-20	HIS	-	expression tag	UNP P42336
A	-19	HIS	-	expression tag	UNP P42336
A	-18	ASP	-	expression tag	UNP P42336
A	-17	TYR	-	expression tag	UNP P42336
A	-16	ASP	-	expression tag	UNP P42336
A	-15	ILE	-	expression tag	UNP P42336
A	-14	PRO	-	expression tag	UNP P42336
A	-13	THR	-	expression tag	UNP P42336
A	-12	THR	-	expression tag	UNP P42336
A	-11	GLU	-	expression tag	UNP P42336
A	-9	ASN	-	expression tag	UNP P42336
A	-8	LEU	-	expression tag	UNP P42336
A	-7	TYR	-	expression tag	UNP P42336
A	-6	PHE	-	expression tag	UNP P42336
A	-5	GLN	-	expression tag	UNP P42336
A	-4	GLY	-	expression tag	UNP P42336
A	-3	ALA	-	expression tag	UNP P42336
A	-2	MET	-	expression tag	UNP P42336

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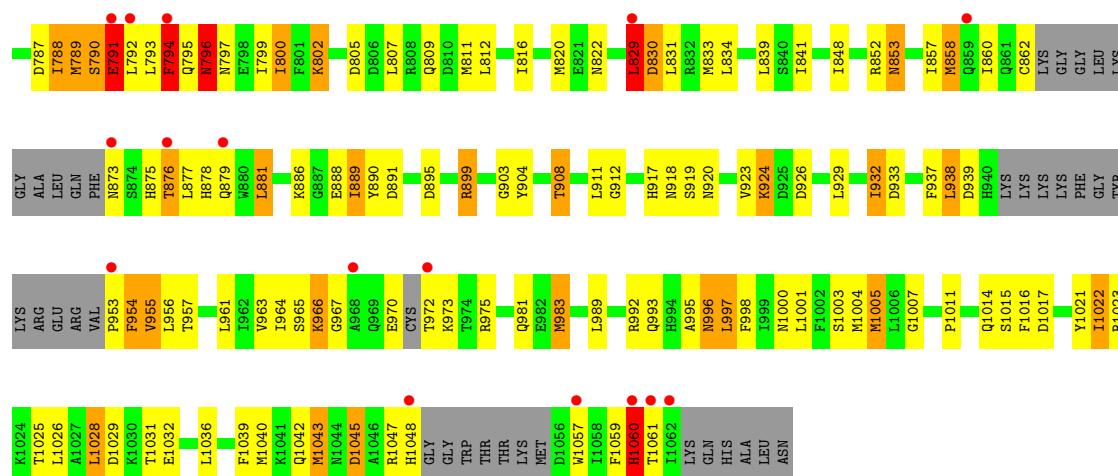
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P42336
A	0	SER	-	expression tag	UNP P42336
A	1047	ARG	HIS	engineered mutation	UNP P42336

- Molecule 2 is a protein called Phosphatidylinositol 3-kinase regulatory subunit alpha.

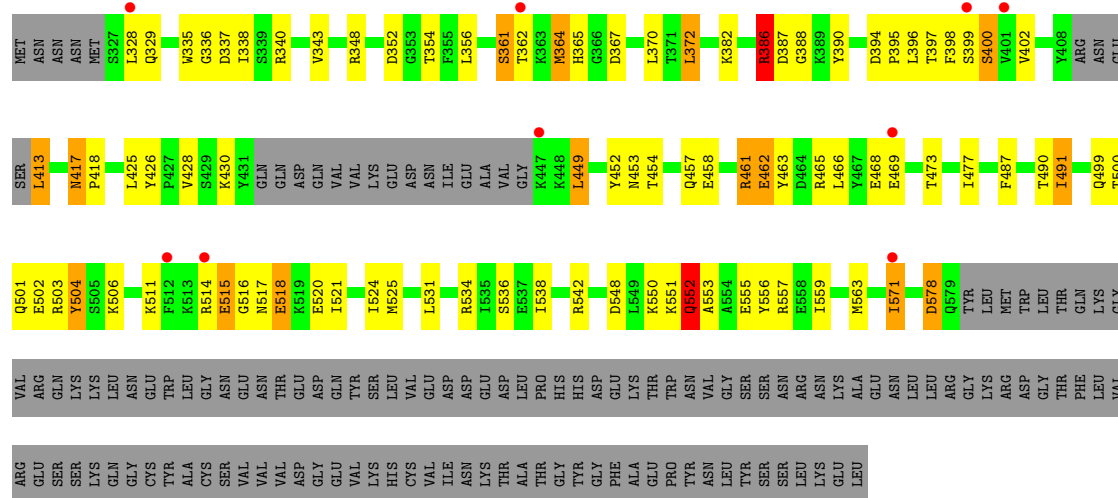
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	234	Total	C	N	O	S	0	0	0
			1993	1251	355	382	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	330	ASN	ASP	engineered mutation	UNP P27986



• Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	115.32Å 120.70Å 153.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.51 – 3.30 47.51 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.51-3.30) 99.4 (47.51-3.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.260 , 0.333 0.261 , 0.332	Depositor DCC
R_{free} test set	1658 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	85.8	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	10384	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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	0.72	7/8582 (0.1%)	1.03	22/11597 (0.2%)
2	B	0.56	0/2026	0.91	2/2709 (0.1%)
All	All	0.70	7/10608 (0.1%)	1.01	24/14306 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1060	HIS	CE1-NE2	13.07	1.45	1.32
1	A	1060	HIS	CG-CD2	9.24	1.46	1.35
1	A	1060	HIS	CG-ND1	7.02	1.46	1.38
1	A	228	LYS	CD-CE	6.94	1.73	1.52
1	A	796	ASN	CA-C	5.13	1.58	1.52
1	A	105	VAL	CA-CB	5.10	1.60	1.53
1	A	876	THR	CA-CB	5.03	1.61	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	797	ASN	N-CA-C	7.61	121.14	108.73
1	A	106	GLY	N-CA-C	-6.93	106.16	113.58
1	A	605	ASN	N-CA-C	-6.80	105.53	114.31
1	A	365	GLU	N-CA-C	6.79	119.28	109.84
1	A	532	LYS	N-CA-C	-6.49	105.22	113.01
1	A	795	GLN	N-CA-C	6.28	118.05	108.07
1	A	127	GLU	N-CA-C	-6.15	105.03	112.54
1	A	407	CYS	N-CA-C	6.14	123.88	110.80
1	A	792	LEU	N-CA-C	-6.13	102.28	110.55
1	A	198	VAL	N-CA-C	6.05	116.80	111.90
1	A	964	ILE	N-CA-C	-5.85	102.03	109.58
1	A	791	GLU	N-CA-C	5.59	117.38	111.28
1	A	184	LYS	N-CA-C	-5.51	106.69	113.41
1	A	1026	LEU	N-CA-C	-5.50	101.02	109.76
1	A	189	GLN	N-CA-C	5.40	117.18	109.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	794	PHE	N-CA-C	5.31	122.11	110.80
1	A	678	LYS	N-CA-C	5.28	117.03	111.28
1	A	370	ASN	N-CA-C	5.21	117.92	108.69
2	B	552	GLN	N-CA-C	-5.21	105.20	112.45
1	A	333	ALA	N-CA-C	5.11	117.12	110.43
1	A	649	LEU	N-CA-C	5.07	117.20	111.11
1	A	-15	ILE	N-CA-C	5.07	119.83	108.88
2	B	490	THR	N-CA-C	-5.04	105.70	111.14
1	A	228	LYS	CG-CD-CE	-5.03	99.73	111.30

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	8391	0	8357	332	0
2	B	1993	0	1974	47	0
All	All	10384	0	10331	375	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 18.

All (375) 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:873:ASN:HB3	1:A:876:THR:HB	1.21	1.18
1:A:599:MET:HB3	1:A:1004:MET:HE1	1.34	1.06
1:A:904:TYR:O	1:A:908:THR:HB	1.58	1.03
1:A:278:MET:HE2	1:A:278:MET:HA	1.40	1.03
1:A:829:LEU:HA	1:A:830:ASP:CB	1.90	1.00
1:A:995:ALA:O	1:A:996:ASN:HB2	1.64	0.97
1:A:829:LEU:HA	1:A:830:ASP:HB2	1.48	0.95
1:A:739:MET:HG2	1:A:744:PHE:CE1	2.06	0.91
1:A:599:MET:HB3	1:A:1004:MET:CE	2.01	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:LEU:HG	1:A:583:MET:HE1	1.52	0.89
1:A:873:ASN:HB3	1:A:876:THR:CB	2.03	0.89
1:A:788:ILE:H	1:A:788:ILE:HD12	1.40	0.87
1:A:745:MET:HE2	1:A:745:MET:HA	1.58	0.85
1:A:561:ILE:HD12	1:A:564:ILE:HD11	1.58	0.85
1:A:305:PRO:HG3	1:A:693:ARG:HD3	1.59	0.84
1:A:873:ASN:CB	1:A:876:THR:HB	2.05	0.84
1:A:413:LYS:HE3	1:A:414:GLY:H	1.43	0.82
1:A:108:ARG:HH11	1:A:108:ARG:HA	1.45	0.81
1:A:308:SER:HB2	1:A:309:ARG:HH21	1.45	0.81
1:A:367:LEU:HD11	1:A:389:TYR:HB3	1.62	0.81
1:A:890:TYR:OH	1:A:966:LYS:HB3	1.82	0.80
1:A:158:SER:HB3	1:A:159:PRO:HD3	1.65	0.79
1:A:529:GLU:O	1:A:531:LEU:N	2.16	0.79
1:A:772:MET:HE2	1:A:772:MET:HA	1.65	0.77
1:A:705:GLN:O	1:A:709:MET:HG2	1.84	0.77
1:A:328:TRP:CE3	1:A:577:ARG:HD2	2.20	0.77
1:A:858:MET:SD	1:A:1057:TRP:CE3	2.78	0.76
1:A:299:MET:HG2	1:A:697:MET:H	1.50	0.75
1:A:408:SER:H	1:A:421:PRO:HB2	1.50	0.75
2:B:461:ARG:O	2:B:465:ARG:HG2	1.88	0.74
1:A:439:GLY:O	1:A:476:GLU:HA	1.87	0.73
1:A:392:TYR:HB3	1:A:394:PRO:HD2	1.71	0.73
1:A:572:VAL:HG21	1:A:583:MET:HG2	1.70	0.73
1:A:189:GLN:HE21	1:A:210:LYS:HE2	1.53	0.72
1:A:283:PRO:C	1:A:284:ASN:HD22	1.97	0.72
1:A:858:MET:SD	1:A:1057:TRP:HE3	2.11	0.72
1:A:235:SER:OG	1:A:238:GLN:HB2	1.88	0.72
1:A:750:GLY:HA2	1:A:761:LEU:O	1.89	0.72
1:A:955:VAL:HG23	1:A:956:LEU:H	1.54	0.72
1:A:529:GLU:C	1:A:531:LEU:H	1.97	0.72
1:A:727:THR:OG1	1:A:730:VAL:HG23	1.90	0.70
1:A:995:ALA:O	1:A:996:ASN:CB	2.38	0.70
1:A:642:GLU:HG2	1:A:647:ASN:CG	2.17	0.70
1:A:372:ASN:HB3	1:A:387:LEU:HD21	1.74	0.70
1:A:776:LYS:O	1:A:778:PRO:HD3	1.91	0.70
1:A:612:ARG:NH1	1:A:642:GLU:OE1	2.26	0.69
1:A:407:CYS:HA	1:A:421:PRO:HB2	1.73	0.68
1:A:20:ILE:HD11	1:A:89:LEU:CD2	2.23	0.68
1:A:278:MET:HA	1:A:278:MET:CE	2.20	0.68
1:A:125:VAL:O	1:A:126:CYS:HB3	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:503:ARG:O	2:B:504:TYR:HB2	1.94	0.67
1:A:431:ASP:HB3	1:A:433:THR:H	1.60	0.67
1:A:401:ARG:NH2	1:A:458:PRO:O	2.20	0.67
1:A:181:ILE:HD13	1:A:278:MET:HE3	1.75	0.67
1:A:709:MET:O	1:A:713:ILE:HG13	1.95	0.66
1:A:216:VAL:HG22	1:A:219:GLN:HG3	1.78	0.66
1:A:351:ILE:C	1:A:353:LYS:H	2.03	0.66
1:A:-22:HIS:HA	1:A:924:LYS:HE2	1.78	0.66
2:B:487:PHE:HB3	2:B:542:ARG:HD3	1.77	0.66
1:A:507:SER:O	1:A:509:SER:N	2.28	0.66
1:A:791:GLU:OE2	1:A:796:ASN:HB3	1.96	0.66
1:A:805:ASP:O	1:A:807:LEU:HD12	1.97	0.65
1:A:561:ILE:HD12	1:A:564:ILE:CD1	2.25	0.65
1:A:956:LEU:HD22	1:A:961:LEU:HG	1.78	0.65
1:A:376:VAL:HG21	1:A:382:ARG:H	1.62	0.65
1:A:852:ARG:O	1:A:853:ASN:HB2	1.95	0.65
1:A:858:MET:SD	1:A:918:ASN:HB2	2.36	0.65
1:A:765:ARG:NH1	1:A:782:ASN:OD1	2.30	0.64
1:A:812:LEU:HD23	1:A:937:PHE:HZ	1.62	0.64
1:A:9:GLU:O	1:A:10:LEU:HB2	1.98	0.64
1:A:365:GLU:CD	1:A:365:GLU:N	2.55	0.64
1:A:788:ILE:H	1:A:788:ILE:CD1	2.10	0.64
1:A:561:ILE:O	1:A:564:ILE:HG13	1.97	0.64
1:A:721:GLN:O	1:A:723:LYS:N	2.31	0.64
1:A:829:LEU:HA	1:A:830:ASP:HB3	1.77	0.64
1:A:992:ARG:HG3	1:A:992:ARG:HH11	1.62	0.63
2:B:502:GLU:O	2:B:506:LYS:HB2	1.98	0.63
1:A:268:SER:HA	1:A:273:ILE:CG2	2.28	0.63
2:B:473:THR:HG23	2:B:552:GLN:HE22	1.63	0.62
1:A:-25:TYR:O	1:A:-23:HIS:N	2.29	0.62
1:A:361:TYR:HA	1:A:366:PRO:HD3	1.81	0.62
1:A:373:THR:HG22	1:A:375:ARG:H	1.63	0.62
1:A:30:MET:HE1	1:A:57:PRO:HD2	1.80	0.62
1:A:540:LEU:HD21	1:A:1016:PHE:HB3	1.81	0.62
1:A:357:ARG:HH11	1:A:371:VAL:HG13	1.64	0.61
1:A:1039:PHE:O	1:A:1042:GLN:HB2	1.99	0.61
1:A:857:ILE:HD12	1:A:877:LEU:HD11	1.82	0.61
1:A:345:ASN:OD1	2:B:557:ARG:HG2	2.01	0.61
1:A:60:GLN:H	1:A:60:GLN:NE2	1.99	0.61
1:A:599:MET:HE1	1:A:631:TYR:HB2	1.82	0.61
2:B:503:ARG:HH11	2:B:504:TYR:H	1.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:SER:HA	1:A:477:PHE:HB2	1.82	0.61
1:A:135:GLU:OE2	1:A:644:TYR:HB3	2.01	0.60
1:A:739:MET:HB3	1:A:766:LEU:HD11	1.82	0.60
1:A:981:GLN:HG2	1:A:1043:MET:HE1	1.83	0.60
1:A:340:CYS:HB3	1:A:382:ARG:HG3	1.84	0.60
1:A:527:ASP:O	1:A:530:GLN:HG2	2.02	0.59
1:A:633:ILE:HG22	1:A:1005:MET:HE1	1.84	0.59
2:B:390:TYR:HB2	2:B:398:PHE:O	2.01	0.59
1:A:924:LYS:HG2	1:A:926:ASP:OD1	2.01	0.59
1:A:299:MET:HA	1:A:697:MET:HG2	1.83	0.59
1:A:367:LEU:CD1	1:A:389:TYR:HB3	2.32	0.59
1:A:640:LYS:HG2	1:A:680:VAL:HG21	1.84	0.59
1:A:178:PRO:HG2	1:A:181:ILE:HG13	1.85	0.59
1:A:268:SER:HA	1:A:273:ILE:HG21	1.84	0.59
1:A:271:LYS:O	1:A:275:SER:HB3	2.03	0.58
1:A:408:SER:H	1:A:421:PRO:CB	2.16	0.58
1:A:407:CYS:H	1:A:422:LEU:HB2	1.67	0.58
1:A:682:GLN:HG2	1:A:686:LEU:HD22	1.84	0.58
1:A:351:ILE:C	1:A:353:LYS:N	2.61	0.58
1:A:397:PRO:HG2	1:A:400:ALA:HB2	1.84	0.58
1:A:756:ASN:C	1:A:756:ASN:HD22	2.11	0.58
1:A:1011:PRO:HA	1:A:1014:GLN:HE21	1.69	0.58
1:A:745:MET:HA	1:A:745:MET:CE	2.30	0.58
1:A:20:ILE:HD11	1:A:89:LEU:HD23	1.85	0.57
1:A:877:LEU:HD22	1:A:963:VAL:HG21	1.85	0.57
1:A:812:LEU:HD23	1:A:937:PHE:CZ	2.38	0.57
1:A:355:TYR:HB3	1:A:374:GLN:HA	1.86	0.57
2:B:338:ILE:CD1	2:B:343:VAL:HG22	2.35	0.57
1:A:211:ILE:HD12	1:A:212:ASN:H	1.70	0.56
1:A:365:GLU:CD	1:A:365:GLU:H	2.12	0.56
1:A:1029:ASP:HB3	2:B:361:SER:HB3	1.88	0.56
1:A:480:PHE:O	1:A:481:SER:C	2.46	0.56
1:A:57:PRO:HB2	1:A:58:LEU:HD12	1.86	0.56
2:B:354:THR:HA	2:B:426:TYR:HB2	1.88	0.56
1:A:789:MET:HB3	1:A:793:LEU:HD12	1.87	0.56
1:A:508:TYR:CG	1:A:509:SER:N	2.74	0.55
1:A:670:HIS:CE1	1:A:811:MET:HE1	2.41	0.55
1:A:720:LYS:O	1:A:721:GLN:HB3	2.05	0.55
1:A:175:PRO:HB3	1:A:269:GLN:HE22	1.71	0.55
1:A:744:PHE:CE2	1:A:748:LEU:HD13	2.42	0.55
1:A:216:VAL:HG23	1:A:218:GLU:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:449:LEU:HG	2:B:452:TYR:HD2	1.70	0.55
2:B:463:TYR:HE1	2:B:563:MET:HE3	1.72	0.55
1:A:195:TRP:H	1:A:195:TRP:CD1	2.25	0.55
1:A:568:LEU:HG	1:A:583:MET:CE	2.30	0.55
1:A:992:ARG:HG3	1:A:992:ARG:NH1	2.21	0.55
1:A:912:GLY:HA3	1:A:1021:TYR:CE2	2.43	0.55
1:A:793:LEU:O	1:A:794:PHE:HD1	1.89	0.54
1:A:140:ARG:HB3	1:A:307:TYR:CE2	2.43	0.54
1:A:529:GLU:C	1:A:531:LEU:N	2.64	0.54
1:A:-15:ILE:HG13	1:A:187:LYS:HD3	1.90	0.54
1:A:308:SER:HB2	1:A:309:ARG:NH2	2.17	0.54
1:A:-23:HIS:O	1:A:924:LYS:HE2	2.08	0.54
1:A:788:ILE:HD12	1:A:788:ILE:N	2.17	0.54
1:A:614:PHE:HA	1:A:617:ARG:NH1	2.22	0.54
1:A:408:SER:N	1:A:421:PRO:HB2	2.21	0.54
1:A:831:LEU:HD23	1:A:899:ARG:HG3	1.89	0.54
1:A:997:LEU:O	1:A:1001:LEU:HG	2.08	0.53
1:A:634:GLN:HB3	1:A:1004:MET:SD	2.47	0.53
1:A:344:VAL:HG21	1:A:422:LEU:HD13	1.91	0.53
1:A:9:GLU:O	1:A:10:LEU:CB	2.56	0.53
2:B:364:MET:O	2:B:365:HIS:HB2	2.08	0.53
1:A:441:MET:O	1:A:475:LEU:N	2.41	0.53
1:A:438:SER:HB2	1:A:478:ASP:O	2.08	0.53
1:A:122:GLY:O	1:A:123:MET:CB	2.57	0.53
1:A:427:ILE:HD11	1:A:443:LEU:HD22	1.90	0.53
1:A:284:ASN:HD22	1:A:284:ASN:N	2.03	0.53
1:A:790:SER:OG	1:A:791:GLU:N	2.41	0.53
1:A:108:ARG:HB3	1:A:112:ILE:HG13	1.90	0.53
2:B:473:THR:HG23	2:B:552:GLN:NE2	2.23	0.53
1:A:243:VAL:O	1:A:244:LEU:C	2.52	0.53
1:A:413:LYS:HE3	1:A:414:GLY:N	2.19	0.53
1:A:858:MET:HG2	1:A:918:ASN:HB2	1.91	0.53
1:A:106:GLY:O	1:A:108:ARG:N	2.41	0.52
2:B:338:ILE:HD12	2:B:343:VAL:HG22	1.91	0.52
1:A:131:VAL:O	1:A:132:LYS:HB2	2.09	0.52
1:A:642:GLU:HG2	1:A:647:ASN:OD1	2.09	0.52
1:A:1059:PHE:O	1:A:1060:HIS:CB	2.57	0.52
1:A:215:CYS:O	1:A:267:LEU:HB2	2.09	0.52
2:B:548:ASP:O	2:B:552:GLN:HB2	2.09	0.52
1:A:136:VAL:HG13	1:A:686:LEU:HD21	1.91	0.52
1:A:503:GLU:C	1:A:505:GLY:H	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:955:VAL:HG23	1:A:956:LEU:N	2.23	0.52
1:A:932:ILE:HG12	1:A:933:ASP:N	2.25	0.51
1:A:1015:SER:OG	1:A:1017:ASP:HB2	2.10	0.51
1:A:756:ASN:O	1:A:759:HIS:HB2	2.10	0.51
2:B:449:LEU:HG	2:B:452:TYR:CD2	2.46	0.51
1:A:63:GLN:HB2	1:A:68:TYR:CZ	2.45	0.51
2:B:356:LEU:HD23	2:B:428:VAL:HG21	1.92	0.51
1:A:858:MET:HG2	1:A:918:ASN:CB	2.41	0.51
1:A:965:SER:O	1:A:967:GLY:N	2.44	0.51
1:A:1000:ASN:O	1:A:1004:MET:HG3	2.11	0.51
1:A:20:ILE:HD11	1:A:89:LEU:HD21	1.93	0.50
1:A:71:VAL:HG22	1:A:81:GLU:HA	1.92	0.50
1:A:175:PRO:HB3	1:A:269:GLN:NE2	2.26	0.50
2:B:524:ILE:HG22	2:B:525:MET:HE2	1.93	0.50
1:A:718:ILE:O	1:A:724:LYS:HB2	2.11	0.50
1:A:876:THR:HA	1:A:879:GLN:HB3	1.93	0.50
1:A:682:GLN:O	1:A:686:LEU:HB2	2.11	0.50
1:A:857:ILE:HB	1:A:918:ASN:HB3	1.94	0.50
1:A:38:ARG:NH2	1:A:743:ASP:OD2	2.45	0.50
1:A:730:VAL:O	1:A:733:LYS:HB2	2.12	0.50
1:A:743:ASP:OD1	1:A:744:PHE:N	2.45	0.50
2:B:458:GLU:HA	2:B:461:ARG:HB2	1.94	0.50
1:A:404:LEU:HD13	1:A:473:LEU:HD23	1.93	0.50
1:A:799:ILE:HG22	1:A:800:ILE:N	2.27	0.50
2:B:518:GLU:O	2:B:520:GLU:N	2.35	0.50
2:B:534:ARG:O	2:B:538:ILE:HG13	2.12	0.50
1:A:189:GLN:HB3	1:A:212:ASN:HA	1.93	0.49
1:A:378:CYS:O	1:A:380:ASN:N	2.45	0.49
1:A:895:ASP:O	1:A:899:ARG:HB2	2.11	0.49
2:B:514:ARG:C	2:B:516:GLY:H	2.20	0.49
1:A:45:ILE:HD11	1:A:89:LEU:HD22	1.94	0.49
1:A:401:ARG:HB2	1:A:427:ILE:O	2.13	0.49
1:A:809:GLN:NE2	1:A:1011:PRO:HD2	2.27	0.49
1:A:876:THR:HA	1:A:879:GLN:CB	2.42	0.49
1:A:336:ILE:HD13	1:A:402:LEU:HD22	1.94	0.49
1:A:633:ILE:HB	1:A:634:GLN:NE2	2.28	0.49
1:A:108:ARG:HG3	1:A:111:LYS:HB3	1.94	0.49
1:A:454:ASP:HA	2:B:348:ARG:NH2	2.27	0.49
1:A:852:ARG:O	1:A:853:ASN:CB	2.61	0.49
1:A:243:VAL:HG12	1:A:244:LEU:N	2.28	0.49
1:A:576:SER:HB3	1:A:579:GLU:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:MET:HE1	1:A:631:TYR:CB	2.44	0.48
1:A:726:GLU:HB2	1:A:730:VAL:HB	1.95	0.48
1:A:745:MET:O	1:A:749:GLN:HB2	2.13	0.48
1:A:337:LYS:HB3	1:A:476:GLU:HB3	1.95	0.48
1:A:123:MET:HE1	1:A:685:GLY:HA3	1.96	0.48
1:A:421:PRO:HD2	1:A:455:LEU:HA	1.94	0.48
1:A:529:GLU:C	1:A:529:GLU:CD	2.81	0.48
1:A:1040:MET:C	1:A:1042:GLN:H	2.20	0.48
1:A:410:LYS:HB3	1:A:411:GLY:H	1.49	0.48
1:A:718:ILE:HG23	1:A:722:GLU:HB3	1.95	0.48
2:B:335:TRP:O	2:B:337:ASP:N	2.46	0.48
1:A:23:GLU:O	1:A:98:PHE:HA	2.14	0.48
1:A:660:ASN:OD1	1:A:660:ASN:C	2.57	0.48
1:A:807:LEU:HD21	1:A:848:ILE:HD11	1.96	0.47
1:A:225:ILE:O	1:A:227:LYS:N	2.45	0.47
1:A:337:LYS:HA	1:A:386:TRP:HA	1.96	0.47
1:A:401:ARG:HH11	1:A:462:THR:HG22	1.80	0.47
2:B:328:LEU:HA	2:B:402:VAL:HG21	1.96	0.47
1:A:744:PHE:CZ	1:A:748:LEU:HD13	2.50	0.47
1:A:500:VAL:O	1:A:503:GLU:HB2	2.15	0.47
1:A:1023:ARG:HA	1:A:1028:LEU:HD22	1.96	0.47
1:A:63:GLN:O	1:A:65:GLU:N	2.47	0.47
1:A:92:LEU:HB2	1:A:94:LEU:HG	1.96	0.47
1:A:558:CYS:SG	1:A:564:ILE:HD12	2.55	0.47
1:A:953:PRO:O	1:A:954:PHE:HB2	2.15	0.47
1:A:407:CYS:CA	1:A:421:PRO:HB2	2.41	0.47
1:A:881:LEU:HD23	1:A:881:LEU:HA	1.80	0.47
2:B:578:ASP:OD1	2:B:578:ASP:N	2.48	0.47
1:A:876:THR:HG23	1:A:879:GLN:HB3	1.97	0.47
1:A:64:ASP:O	1:A:65:GLU:HB2	2.15	0.46
1:A:1040:MET:C	1:A:1042:GLN:N	2.73	0.46
1:A:540:LEU:HD13	1:A:1023:ARG:HD2	1.98	0.46
1:A:858:MET:HG2	1:A:918:ASN:C	2.41	0.46
1:A:393:ILE:N	1:A:394:PRO:CD	2.78	0.46
1:A:912:GLY:HA3	1:A:1021:TYR:HE2	1.80	0.46
1:A:367:LEU:HD23	1:A:367:LEU:O	2.16	0.46
1:A:456:LEU:O	1:A:457:ASN:C	2.59	0.46
1:A:572:VAL:CG2	1:A:583:MET:HE2	2.46	0.46
1:A:712:LEU:HD12	1:A:712:LEU:HA	1.61	0.46
1:A:71:VAL:HG21	1:A:102:ILE:HD11	1.97	0.46
1:A:446:TRP:CH2	1:A:466:PRO:HD3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:PRO:HB2	1:A:593:ILE:HG22	1.98	0.45
2:B:514:ARG:O	2:B:516:GLY:N	2.48	0.45
1:A:992:ARG:HH12	1:A:1028:LEU:H	1.64	0.45
2:B:338:ILE:HD12	2:B:343:VAL:CG2	2.45	0.45
2:B:462:GLU:O	2:B:466:LEU:N	2.47	0.45
1:A:102:ILE:HB	1:A:103:GLU:H	1.60	0.45
1:A:192:VAL:HG12	1:A:283:PRO:HG2	1.99	0.45
1:A:231:SER:HB3	1:A:234:LEU:HB2	1.97	0.45
1:A:875:HIS:O	1:A:878:HIS:HB3	2.16	0.45
1:A:917:HIS:CE1	1:A:920:ASN:HD22	2.35	0.45
1:A:194:ILE:O	1:A:194:ILE:HG22	2.16	0.45
1:A:395:ASP:OD1	1:A:577:ARG:HB3	2.16	0.45
1:A:234:LEU:O	1:A:235:SER:C	2.58	0.45
1:A:195:TRP:CD1	1:A:195:TRP:N	2.85	0.45
1:A:251:ILE:HD12	1:A:290:LYS:HG2	1.99	0.45
1:A:796:ASN:HD22	1:A:796:ASN:H	1.65	0.45
1:A:158:SER:HB3	1:A:159:PRO:CD	2.41	0.44
1:A:122:GLY:O	1:A:123:MET:HB2	2.17	0.44
1:A:229:THR:O	1:A:230:ARG:C	2.60	0.44
1:A:599:MET:HE2	1:A:635:LEU:HD21	1.99	0.44
1:A:1043:MET:C	1:A:1045:ASP:H	2.24	0.44
1:A:433:THR:O	1:A:434:ASP:HB2	2.17	0.44
1:A:241:LEU:O	1:A:242:CYS:HB3	2.16	0.44
2:B:394:ASP:HB2	2:B:395:PRO:HD3	1.99	0.44
1:A:774:SER:HB2	1:A:776:LYS:O	2.16	0.44
1:A:1045:ASP:OD1	1:A:1045:ASP:N	2.51	0.44
2:B:491:ILE:HD13	2:B:542:ARG:HE	1.83	0.44
1:A:-16:ASP:O	1:A:-14:PRO:HD2	2.17	0.44
2:B:390:TYR:HD1	2:B:399:SER:HA	1.83	0.44
1:A:121:ILE:HD11	1:A:689:GLU:HA	1.99	0.44
1:A:401:ARG:HA	1:A:429:LEU:HG	1.99	0.44
1:A:380:ASN:O	1:A:380:ASN:ND2	2.39	0.43
1:A:27:PRO:HD3	1:A:101:VAL:HB	2.00	0.43
2:B:518:GLU:C	2:B:520:GLU:H	2.22	0.43
1:A:84:ASP:OD1	1:A:84:ASP:C	2.61	0.43
1:A:816:ILE:O	1:A:820:MET:HG3	2.19	0.43
2:B:338:ILE:HD11	2:B:343:VAL:HG22	2.01	0.43
2:B:477:ILE:HG13	2:B:552:GLN:NE2	2.33	0.43
1:A:108:ARG:CG	1:A:111:LYS:HB3	2.48	0.43
2:B:553:ALA:O	2:B:556:TYR:HB3	2.18	0.43
1:A:24:CYS:SG	1:A:49:LEU:HD13	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:ARG:NH2	1:A:582:GLN:OE1	2.51	0.43
1:A:791:GLU:HA	1:A:791:GLU:OE1	2.17	0.43
1:A:378:CYS:HB2	1:A:379:SER:H	1.58	0.43
1:A:539:PRO:HB3	1:A:600:GLU:OE2	2.19	0.43
1:A:612:ARG:O	1:A:616:VAL:HG23	2.19	0.43
1:A:147:CYS:HB3	1:A:694:ALA:HB2	2.00	0.43
1:A:217:PRO:HB3	1:A:252:LEU:HD12	2.00	0.43
1:A:756:ASN:C	1:A:756:ASN:ND2	2.76	0.43
1:A:739:MET:HA	1:A:744:PHE:CD1	2.53	0.43
1:A:241:LEU:O	1:A:242:CYS:CB	2.67	0.43
1:A:365:GLU:N	1:A:365:GLU:OE2	2.50	0.43
1:A:446:TRP:HA	1:A:465:ASN:HD22	1.83	0.43
1:A:833:MET:SD	1:A:903:GLY:HA3	2.59	0.42
1:A:937:PHE:HB3	1:A:938:LEU:H	1.45	0.42
1:A:857:ILE:HD11	1:A:923:VAL:HG23	2.00	0.42
1:A:939:ASP:HB2	1:A:1021:TYR:CD1	2.54	0.42
1:A:39:GLU:HG2	1:A:742:PRO:HG2	2.01	0.42
1:A:858:MET:CG	1:A:918:ASN:HB2	2.49	0.42
1:A:538:ASP:O	1:A:541:SER:HB2	2.19	0.42
1:A:875:HIS:O	1:A:878:HIS:N	2.50	0.42
1:A:59:HIS:O	1:A:62:LEU:HB3	2.19	0.42
1:A:125:VAL:O	1:A:126:CYS:CB	2.62	0.42
1:A:410:LYS:HB2	2:B:571:ILE:HD11	2.02	0.42
1:A:1047:ARG:O	1:A:1048:HIS:C	2.63	0.42
2:B:417:ASN:HA	2:B:418:PRO:HD3	1.93	0.42
1:A:27:PRO:HG3	1:A:68:TYR:CE1	2.55	0.42
1:A:253:LYS:HD2	1:A:260:TYR:CZ	2.55	0.42
1:A:275:SER:O	1:A:279:LEU:HD12	2.20	0.42
1:A:787:ASP:O	1:A:790:SER:HB3	2.20	0.42
2:B:399:SER:O	2:B:400:SER:HB3	2.19	0.42
1:A:62:LEU:O	1:A:63:GLN:HG2	2.20	0.42
1:A:255:CYS:SG	1:A:284:ASN:O	2.77	0.42
1:A:485:LYS:HB3	1:A:485:LYS:HE2	1.82	0.42
1:A:598:ALA:O	1:A:601:LEU:HB2	2.20	0.42
1:A:467:ASN:HD21	1:A:469:GLU:HG2	1.85	0.42
1:A:504:ALA:HA	1:A:506:PHE:CE2	2.54	0.42
1:A:777:ARG:HD2	1:A:777:ARG:HA	1.83	0.42
1:A:138:ASP:O	1:A:139:PHE:C	2.63	0.41
1:A:222:ALA:HA	1:A:225:ILE:HD12	2.01	0.41
1:A:772:MET:HA	1:A:772:MET:CE	2.42	0.41
1:A:917:HIS:CE1	1:A:920:ASN:ND2	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1059:PHE:O	1:A:1060:HIS:HB3	2.19	0.41
1:A:68:TYR:O	1:A:69:ILE:HB	2.19	0.41
1:A:352:ASP:O	1:A:353:LYS:O	2.37	0.41
1:A:647:ASN:ND2	1:A:650:VAL:H	2.18	0.41
1:A:691:TYR:O	1:A:695:CYS:HB3	2.20	0.41
1:A:802:LYS:HE2	1:A:805:ASP:OD2	2.20	0.41
1:A:938:LEU:HD22	1:A:1022:ILE:HG23	2.02	0.41
1:A:108:ARG:HG3	1:A:111:LYS:CB	2.49	0.41
1:A:406:ILE:HG22	1:A:422:LEU:HD12	2.01	0.41
1:A:424:TRP:CH2	1:A:460:GLY:HA3	2.55	0.41
1:A:671:LEU:HD11	1:A:687:LEU:HD13	2.03	0.41
1:A:187:LYS:HE3	1:A:187:LYS:HB3	1.86	0.41
1:A:561:ILE:CD1	1:A:564:ILE:HD11	2.40	0.41
1:A:765:ARG:HH12	1:A:796:ASN:HB2	1.85	0.41
1:A:799:ILE:CG2	1:A:800:ILE:N	2.82	0.41
1:A:1000:ASN:HA	1:A:1003:SER:HB2	2.02	0.41
2:B:515:GLU:C	2:B:517:ASN:H	2.29	0.41
1:A:816:ILE:HG21	1:A:911:LEU:HD21	2.02	0.41
1:A:899:ARG:NE	1:A:983:MET:HE1	2.36	0.41
1:A:187:LYS:H	1:A:187:LYS:HD2	1.85	0.41
1:A:507:SER:O	1:A:508:TYR:CD1	2.74	0.41
1:A:652:PHE:O	1:A:653:LEU:C	2.63	0.41
2:B:328:LEU:HB3	2:B:329:GLN:H	1.73	0.41
2:B:503:ARG:O	2:B:504:TYR:CB	2.66	0.41
2:B:563:MET:HE2	2:B:563:MET:HB3	1.94	0.41
1:A:767:GLU:H	1:A:767:GLU:CD	2.28	0.41
1:A:50:PHE:CG	1:A:65:GLU:HG3	2.57	0.40
1:A:888:GLU:HG3	1:A:889:ILE:H	1.85	0.40
1:A:647:ASN:HD22	1:A:649:LEU:N	2.19	0.40
2:B:372:LEU:HD22	2:B:413:LEU:HD13	2.03	0.40
1:A:43:ILE:HG13	1:A:44:THR:N	2.36	0.40
1:A:820:MET:HG2	1:A:998:PHE:CZ	2.56	0.40
1:A:989:LEU:HD11	1:A:1036:LEU:HD22	2.04	0.40
1:A:253:LYS:HB2	1:A:260:TYR:CD2	2.55	0.40
1:A:255:CYS:HG	1:A:284:ASN:C	2.29	0.40
1:A:568:LEU:CG	1:A:583:MET:HE1	2.36	0.40
1:A:724:LYS:O	1:A:731:GLN:NE2	2.54	0.40
2:B:364:MET:HG3	2:B:386:ARG:NH2	2.37	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	1006/1096 (92%)	787 (78%)	156 (16%)	63 (6%)	1	8
2	B	228/373 (61%)	186 (82%)	30 (13%)	12 (5%)	1	10
All	All	1234/1469 (84%)	973 (79%)	186 (15%)	75 (6%)	1	9

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-15	ILE
1	A	-14	PRO
1	A	64	ASP
1	A	65	GLU
1	A	110	GLU
1	A	123	MET
1	A	126	CYS
1	A	158	SER
1	A	202	ASN
1	A	353	LYS
1	A	375	ARG
1	A	384	ASN
1	A	508	TYR
1	A	525	GLU
1	A	530	GLN
1	A	830	ASP
1	A	966	LYS
1	A	996	ASN
2	B	336	GLY
2	B	400	SER
2	B	515	GLU
1	A	-24	HIS
1	A	107	ASN
1	A	157	ASN
1	A	226	ARG

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Mol	Chain	Res	Type
1	A	235	SER
1	A	348	ILE
1	A	352	ASP
1	A	379	SER
1	A	407	CYS
1	A	422	LEU
1	A	452	LEU
1	A	504	ALA
1	A	722	GLU
1	A	853	ASN
1	A	860	ILE
1	A	886	LYS
1	A	954	PHE
1	A	955	VAL
2	B	352	ASP
2	B	386	ARG
2	B	518	GLU
1	A	7	SER
1	A	10	LEU
1	A	109	GLU
1	A	209	LEU
1	A	350	ASP
1	A	721	GLN
1	A	829	LEU
1	A	1007	GLY
1	A	1060	HIS
2	B	425	LEU
2	B	504	TYR
1	A	-17	TYR
1	A	69	ILE
1	A	104	PRO
1	A	213	HIS
1	A	227	LYS
1	A	553	SER
1	A	790	SER
2	B	340	ARG
2	B	361	SER
2	B	417	ASN
1	A	207	TYR
1	A	242	CYS
1	A	332	SER
1	A	431	ASP

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Mol	Chain	Res	Type
1	A	1061	THR
1	A	298	PRO
1	A	542	GLU
1	A	409	VAL
1	A	381	PRO
1	A	122	GLY
1	A	366	PRO
2	B	388	GLY

5.3.2 Protein sidechains [i](#)

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	941/999 (94%)	780 (83%)	161 (17%)	2	10
2	B	218/342 (64%)	183 (84%)	35 (16%)	2	12
All	All	1159/1341 (86%)	963 (83%)	196 (17%)	2	10

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-18	ASP
1	A	-16	ASP
1	A	-11	GLU
1	A	6	SER
1	A	14	HIS
1	A	16	MET
1	A	22	VAL
1	A	23	GLU
1	A	31	ILE
1	A	32	VAL
1	A	37	LEU
1	A	60	GLN
1	A	62	LEU
1	A	67	SER
1	A	75	GLN

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Mol	Chain	Res	Type
1	A	92	LEU
1	A	93	ARG
1	A	100	LYS
1	A	102	ILE
1	A	108	ARG
1	A	115	ARG
1	A	125	VAL
1	A	130	MET
1	A	137	GLN
1	A	151	VAL
1	A	153	LEU
1	A	171	VAL
1	A	173	SER
1	A	179	LYS
1	A	185	LEU
1	A	186	ASP
1	A	187	LYS
1	A	193	VAL
1	A	196	VAL
1	A	202	ASN
1	A	203	ASP
1	A	211	ILE
1	A	216	VAL
1	A	223	GLU
1	A	227	LYS
1	A	233	LEU
1	A	236	SER
1	A	238	GLN
1	A	241	LEU
1	A	242	CYS
1	A	243	VAL
1	A	244	LEU
1	A	245	GLU
1	A	247	GLN
1	A	249	LYS
1	A	251	ILE
1	A	264	LYS
1	A	267	LEU
1	A	273	ILE
1	A	282	MET
1	A	284	ASN
1	A	287	LEU

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Mol	Chain	Res	Type
1	A	296	GLN
1	A	300	ASP
1	A	306	SER
1	A	309	ARG
1	A	322	THR
1	A	328	TRP
1	A	335	ARG
1	A	351	ILE
1	A	354	ILE
1	A	365	GLU
1	A	367	LEU
1	A	368	CYS
1	A	378	CYS
1	A	380	ASN
1	A	384	ASN
1	A	402	LEU
1	A	409	VAL
1	A	413	LYS
1	A	431	ASP
1	A	435	THR
1	A	436	LEU
1	A	440	LYS
1	A	454	ASP
1	A	455	LEU
1	A	474	GLU
1	A	485	LYS
1	A	494	GLU
1	A	510	HIS
1	A	513	LEU
1	A	526	ASN
1	A	529	GLU
1	A	534	ILE
1	A	540	LEU
1	A	553	SER
1	A	561	ILE
1	A	564	ILE
1	A	585	CYS
1	A	588	LYS
1	A	589	ASP
1	A	628	LEU
1	A	637	GLN
1	A	638	VAL

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Mol	Chain	Res	Type
1	A	648	LEU
1	A	650	VAL
1	A	659	THR
1	A	672	LYS
1	A	680	VAL
1	A	686	LEU
1	A	687	LEU
1	A	712	LEU
1	A	715	LEU
1	A	722	GLU
1	A	723	LYS
1	A	726	GLU
1	A	736	VAL
1	A	745	MET
1	A	748	LEU
1	A	759	HIS
1	A	760	GLN
1	A	766	LEU
1	A	767	GLU
1	A	770	ARG
1	A	773	SER
1	A	776	LYS
1	A	788	ILE
1	A	789	MET
1	A	791	GLU
1	A	794	PHE
1	A	796	ASN
1	A	800	ILE
1	A	802	LYS
1	A	822	ASN
1	A	829	LEU
1	A	834	LEU
1	A	839	LEU
1	A	841	ILE
1	A	858	MET
1	A	862	CYS
1	A	881	LEU
1	A	889	ILE
1	A	891	ASP
1	A	899	ARG
1	A	908	THR
1	A	919	SER

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Mol	Chain	Res	Type
1	A	924	LYS
1	A	929	LEU
1	A	932	ILE
1	A	938	LEU
1	A	957	THR
1	A	970	GLU
1	A	972	THR
1	A	973	LYS
1	A	975	ARG
1	A	983	MET
1	A	993	GLN
1	A	997	LEU
1	A	1005	MET
1	A	1022	ILE
1	A	1025	THR
1	A	1028	LEU
1	A	1031	THR
1	A	1032	GLU
1	A	1043	MET
1	A	1045	ASP
2	B	362	THR
2	B	364	MET
2	B	367	ASP
2	B	370	LEU
2	B	372	LEU
2	B	382	LYS
2	B	386	ARG
2	B	387	ASP
2	B	396	LEU
2	B	397	THR
2	B	413	LEU
2	B	430	LYS
2	B	449	LEU
2	B	453	ASN
2	B	454	THR
2	B	457	GLN
2	B	461	ARG
2	B	462	GLU
2	B	468	GLU
2	B	469	GLU
2	B	491	ILE
2	B	499	GLN

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Mol	Chain	Res	Type
2	B	500	THR
2	B	501	GLN
2	B	511	LYS
2	B	521	ILE
2	B	531	LEU
2	B	536	SER
2	B	550	LYS
2	B	551	LYS
2	B	552	GLN
2	B	555	GLU
2	B	559	ILE
2	B	571	ILE
2	B	578	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-24	HIS
1	A	60	GLN
1	A	96	GLN
1	A	189	GLN
1	A	219	GLN
1	A	269	GLN
1	A	284	ASN
1	A	370	ASN
1	A	467	ASN
1	A	575	ASN
1	A	647	ASN
1	A	670	HIS
1	A	676	HIS
1	A	677	ASN
1	A	682	GLN
1	A	756	ASN
1	A	826	ASN
1	A	859	GLN
1	A	875	HIS
1	A	878	HIS
1	A	917	HIS
1	A	928	GLN
1	A	958	GLN
1	A	1014	GLN
1	A	1042	GLN

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Mol	Chain	Res	Type
2	B	344	ASN
2	B	385	HIS
2	B	415	GLN
2	B	475	GLN
2	B	501	GLN
2	B	564	ASN

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	1024/1096 (93%)	0.26	44 (4%) 40 25	33, 66, 92, 124	0
2	B	234/373 (62%)	0.62	9 (3%) 44 30	75, 111, 125, 128	0
All	All	1258/1469 (85%)	0.33	53 (4%) 40 26	33, 70, 120, 128	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	513	LEU	4.5
1	A	791	GLU	4.3
2	B	512	PHE	4.1
1	A	873	ASN	4.0
1	A	-15	ILE	3.8
1	A	794	PHE	3.7
1	A	235	SER	3.7
1	A	876	THR	3.4
2	B	514	ARG	3.1
1	A	-17	TYR	3.0
2	B	328	LEU	2.9
1	A	505	GLY	2.9
1	A	1062	ILE	2.9
2	B	447	LYS	2.7
1	A	91	ASP	2.6
1	A	299	MET	2.6
1	A	233	LEU	2.6
1	A	366	PRO	2.5
1	A	242	CYS	2.5
2	B	399	SER	2.5
1	A	1061	THR	2.5
1	A	1060	HIS	2.4
1	A	-16	ASP	2.4
1	A	307	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	829	LEU	2.4
1	A	408	SER	2.4
2	B	362	THR	2.3
1	A	879	GLN	2.3
2	B	401	VAL	2.3
1	A	455	LEU	2.3
1	A	351	ILE	2.3
1	A	792	LEU	2.3
1	A	347	ASN	2.3
1	A	1048	HIS	2.3
1	A	516	ARG	2.3
1	A	968	ALA	2.2
1	A	509	SER	2.2
1	A	30	MET	2.2
1	A	506	PHE	2.2
1	A	352	ASP	2.1
1	A	1057	TRP	2.1
1	A	375	ARG	2.1
1	A	256	GLY	2.1
1	A	415	ALA	2.1
1	A	859	GLN	2.1
1	A	953	PRO	2.1
2	B	469	GLU	2.1
1	A	90	CYS	2.1
1	A	236	SER	2.0
2	B	571	ILE	2.0
1	A	972	THR	2.0
1	A	365	GLU	2.0
1	A	-18	ASP	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 ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.