Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 11:03 pm BST

PDB ID	:	4OVU
Title	:	Crystal Structure of p110alpha in complex with niSH2 of p85alpha
Authors	:	Gabelli, S.B.; Vogelstein, B.; Miller, M.S.; Amzel, L.M.
Deposited on	:	2014-01-14
Resolution	:	2.96 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 (i) symbol.

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

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

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 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	Percentile Ranks	Value
Rfree		0.276
Clashscore		17
Ramachandran outliers		4.2%
Sidechain outliers		9.7%
RSRZ outliers		7.2%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
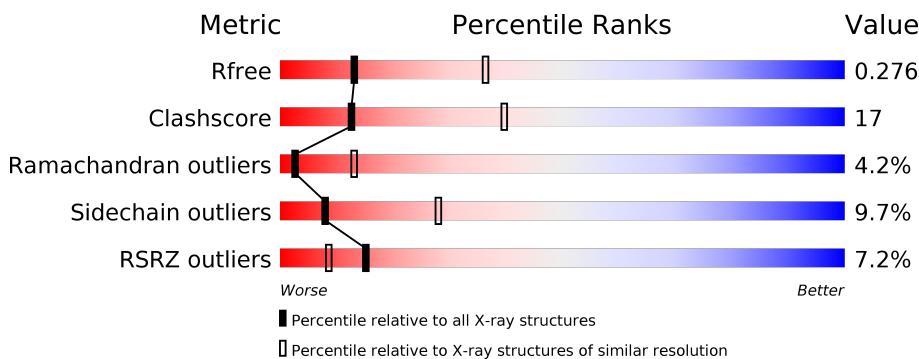
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	4% / 59% 30% 6% · 5%
2	B	279	18% / 59% 30% 6% · ·
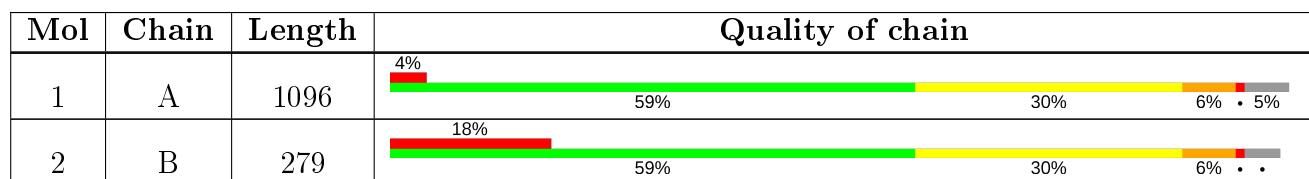
2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10848 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
			Total	C	N	O	S			
1	A	1044	8549	5463	1463	1554	69	0	1	0

There are 28 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	-10	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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	268	2281	1433	404	438	6	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	17	17	17	0	0
3	B	1	Total	O	0	0
			1	1		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform

• Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha
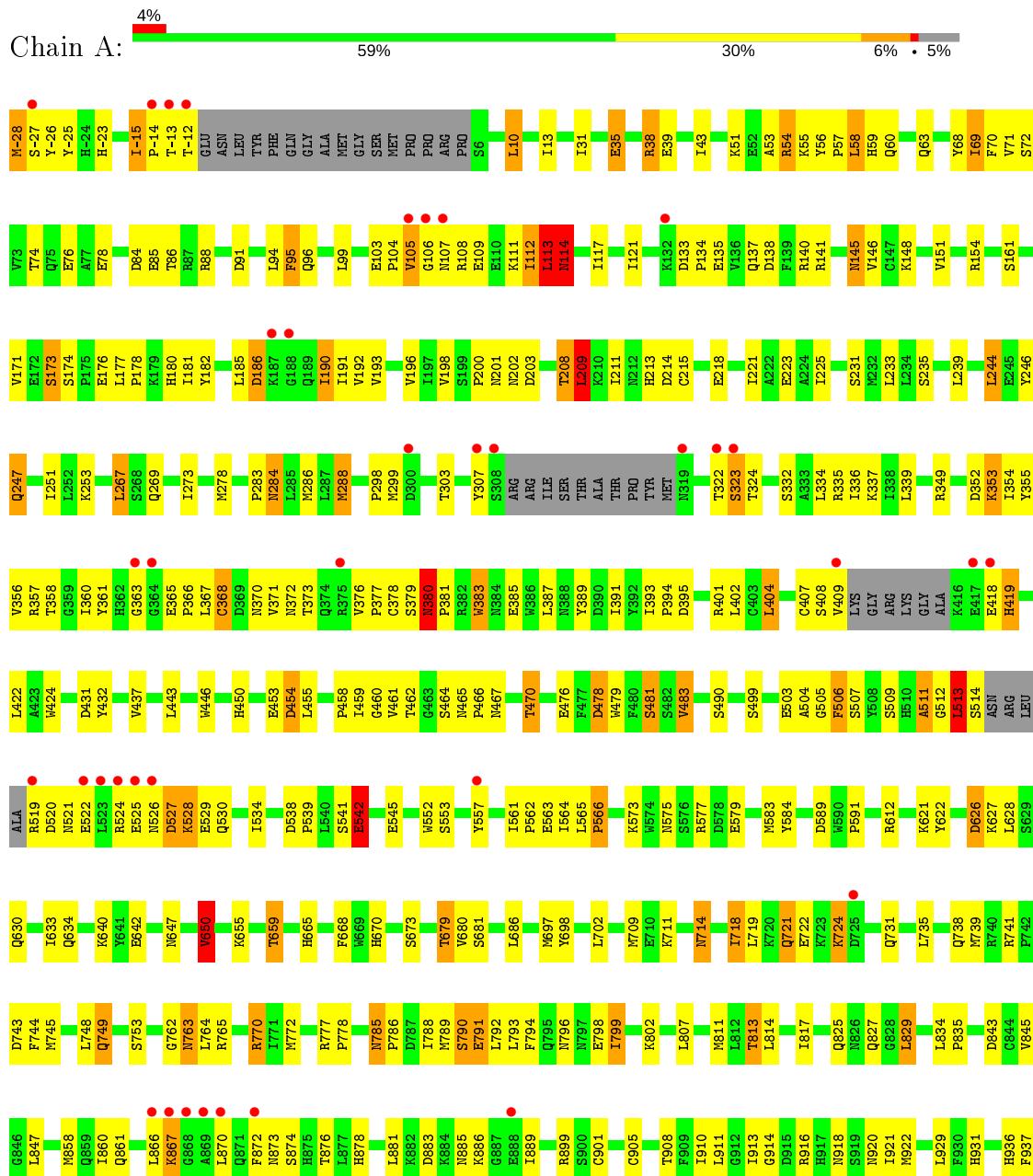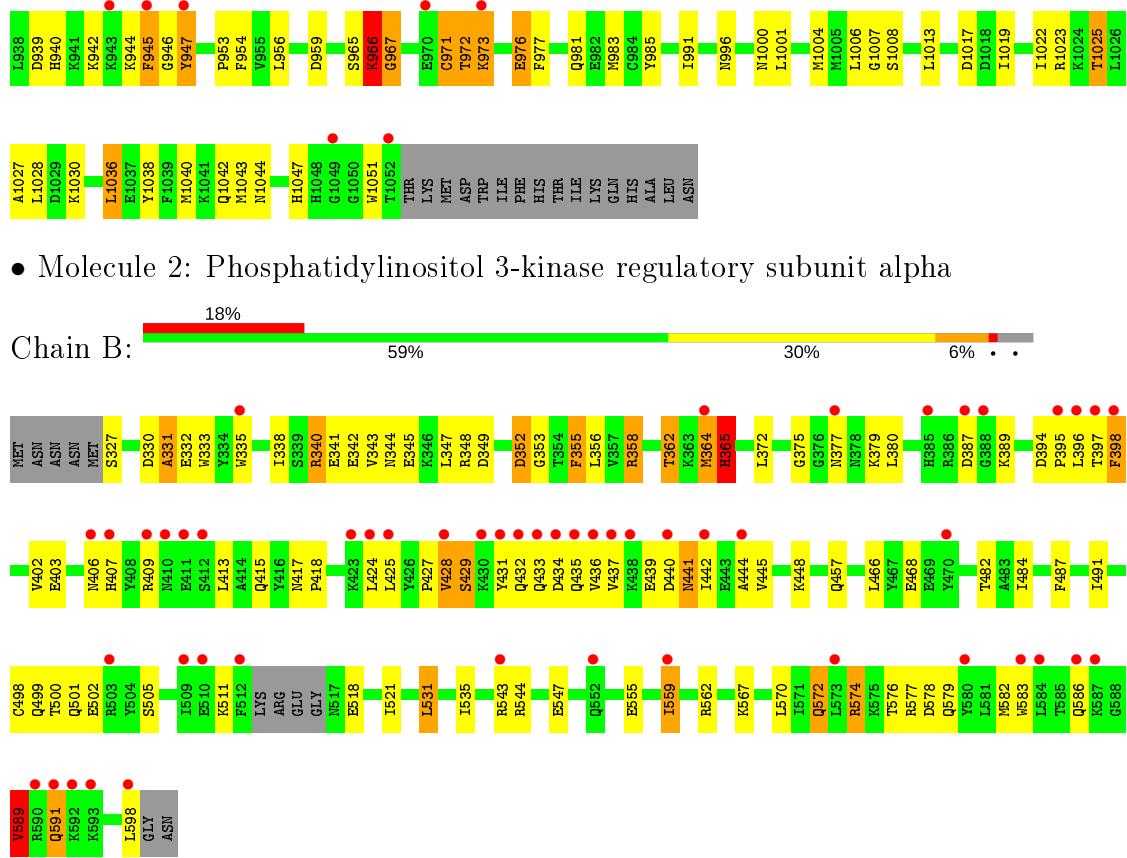
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	114.69Å 116.20Å 149.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.79 – 2.96 37.77 – 2.96	Depositor EDS
% Data completeness (in resolution range)	99.1 (37.79-2.96) 99.2 (37.77-2.96)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.21 (at 2.95Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.191 , 0.272 0.194 , 0.276	Depositor DCC
R_{free} test set	2122 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	77.2	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 90.9	EDS
L-test for twinning [2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10848	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.60	0/8746	0.84	9/11820 (0.1%)
2	B	0.47	0/2320	0.69	0/3109
All	All	0.58	0/11066	0.81	9/14929 (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	2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	650	VAL	CB-CA-C	-6.28	99.47	111.40
1	A	513	LEU	CA-CB-CG	6.12	129.36	115.30
1	A	10	LEU	CA-CB-CG	5.75	128.54	115.30
1	A	612	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	A	829	LEU	CA-CB-CG	5.74	128.51	115.30
1	A	239	LEU	CA-CB-CG	5.70	128.40	115.30
1	A	177	LEU	CA-CB-CG	5.59	128.17	115.30
1	A	209	LEU	CA-CB-CG	5.39	127.71	115.30
1	A	749	GLN	C-N-CA	-5.04	111.72	122.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	LEU	Peptide
1	A	114[B]	ASN	Peptide

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	8549	0	8513	300	0
2	B	2281	0	2258	76	0
3	A	17	0	0	1	0
3	B	1	0	0	0	0
All	All	10848	0	10771	361	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 (361) 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:749:GLN:O	1:A:762:GLY:HA2	1.42	1.16
1:A:-14:PRO:HG3	1:A:186:ASP:HB3	1.42	1.00
1:A:298:PRO:HG2	1:A:697:MET:HG3	1.41	0.99
1:A:509:SER:HB2	1:A:513:LEU:HD22	1.41	0.99
1:A:356:VAL:HB	1:A:372:ASN:HD21	1.29	0.98
1:A:799:ILE:HD11	1:A:847:LEU:HD22	1.47	0.96
1:A:360:ILE:O	1:A:366:PRO:HD2	1.66	0.96
1:A:942:LYS:HB2	1:A:946:GLY:HA3	1.49	0.93
1:A:367:LEU:HD22	1:A:389:TYR:HB3	1.52	0.92
1:A:137:GLN:HE22	1:A:140:ARG:HH11	1.16	0.90
1:A:721:GLN:O	1:A:722:GLU:HB2	1.72	0.90
1:A:945:PHE:HB3	2:B:598:LEU:HD22	1.54	0.89
2:B:355:PHE:CE1	2:B:427:PRO:HA	2.08	0.88
1:A:284:ASN:OD1	1:A:792:LEU:CD1	2.22	0.88
1:A:31:ILE:HD11	2:B:531:LEU:HD13	1.56	0.88
1:A:642:GLU:HG2	1:A:647:ASN:CG	1.94	0.86
1:A:640:LYS:HE2	1:A:680:VAL:HG11	1.57	0.86
1:A:525:GLU:HB2	1:A:528:LYS:HG2	1.57	0.85
1:A:749:GLN:HE21	1:A:764:LEU:H	1.18	0.85
1:A:878:HIS:NE2	1:A:966:LYS:O	2.11	0.84
1:A:910:ILE:HA	1:A:1025:THR:CG2	2.09	0.82
1:A:-28:MET:C	1:A:-26:TYR:H	1.82	0.82
1:A:541:SER:HB2	2:B:340:ARG:NH2	1.96	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:341:GLU:O	2:B:345:GLU:HG2	1.80	0.81
1:A:284:ASN:OD1	1:A:792:LEU:HD12	1.83	0.79
1:A:367:LEU:CD2	1:A:389:TYR:HB3	2.13	0.79
1:A:552:TRP:HZ3	1:A:583:MET:HE3	1.48	0.79
1:A:770:ARG:HG3	1:A:772:MET:HE1	1.64	0.79
1:A:956:LEU:H	1:A:1047:HIS:HE1	1.30	0.78
1:A:910:ILE:HA	1:A:1025:THR:HG21	1.63	0.78
1:A:192:VAL:HG13	1:A:283:PRO:HB2	1.66	0.78
2:B:578:ASP:O	2:B:582:MET:HG2	1.83	0.78
1:A:284:ASN:OD1	1:A:792:LEU:HD11	1.84	0.77
1:A:731:GLN:HE22	1:A:777:ARG:HE	1.30	0.77
1:A:-28:MET:N	1:A:-25:TYR:H	1.82	0.77
1:A:942:LYS:HB2	1:A:946:GLY:CA	2.15	0.76
1:A:749:GLN:O	1:A:762:GLY:CA	2.31	0.76
1:A:453:GLU:HB2	2:B:348:ARG:HH21	1.51	0.76
2:B:355:PHE:HE1	2:B:427:PRO:HA	1.49	0.75
1:A:111:LYS:O	1:A:114[A]:ASN:HB2	1.85	0.74
1:A:154:ARG:O	1:A:161:SER:HB3	1.88	0.74
2:B:445:VAL:HG21	2:B:583:TRP:CZ3	2.23	0.73
2:B:343:VAL:HG21	2:B:358:ARG:HD3	1.70	0.73
1:A:762:GLY:O	1:A:763:ASN:HB2	1.88	0.73
1:A:367:LEU:HD13	1:A:368:CYS:O	1.87	0.72
2:B:432:GLN:HG2	2:B:579:GLN:HG2	1.69	0.72
1:A:356:VAL:HB	1:A:372:ASN:ND2	2.04	0.72
1:A:94:LEU:O	1:A:95:PHE:CB	2.36	0.72
1:A:353:LYS:HA	1:A:377:PRO:HB2	1.71	0.72
1:A:-28:MET:C	1:A:-26:TYR:N	2.43	0.72
1:A:965:SER:HA	1:A:976:GLU:HG3	1.73	0.71
1:A:106:GLY:O	1:A:108:ARG:N	2.23	0.71
1:A:956:LEU:H	1:A:1047:HIS:CE1	2.09	0.71
1:A:731:GLN:NE2	1:A:777:ARG:HE	1.88	0.71
1:A:633:ILE:HD11	1:A:811:MET:HE2	1.73	0.70
2:B:340:ARG:O	2:B:344:ASN:ND2	2.24	0.70
1:A:395:ASP:OD1	1:A:577:ARG:HG2	1.91	0.70
1:A:182:TYR:O	1:A:185:LEU:HB2	1.92	0.69
1:A:552:TRP:HZ3	1:A:583:MET:CE	2.04	0.69
1:A:1038:TYR:O	1:A:1042:GLN:HG2	1.92	0.69
1:A:885:ASN:HB3	1:A:889:ILE:HG22	1.76	0.68
1:A:322:THR:O	1:A:323:SER:HB2	1.94	0.67
1:A:372:ASN:HB3	1:A:387:LEU:HD21	1.77	0.67
1:A:103:GLU:HG3	1:A:104:PRO:HD2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:ILE:HD13	1:A:402:LEU:HD22	1.76	0.66
1:A:944:LYS:HD2	2:B:457:GLN:HG2	1.76	0.66
2:B:333:TRP:HA	2:B:429:SER:OG	1.96	0.65
2:B:544:ARG:O	2:B:547:GLU:HG2	1.97	0.65
1:A:251:ILE:HD12	1:A:288:MET:HB3	1.80	0.64
1:A:908:THR:HG21	1:A:954:PHE:HB2	1.80	0.64
1:A:1027:ALA:HB1	1:A:1030:LYS:HD2	1.78	0.64
2:B:330:ASP:O	2:B:332:GLU:N	2.30	0.63
1:A:770:ARG:HG3	1:A:772:MET:CE	2.27	0.63
1:A:719:LEU:HD22	1:A:731:GLN:HG2	1.79	0.63
1:A:542:GLU:HG2	2:B:380:LEU:HD22	1.79	0.63
2:B:441:ASN:HB3	2:B:444:ALA:HB3	1.78	0.63
1:A:-28:MET:H3	1:A:-25:TYR:H	1.46	0.63
1:A:198:VAL:H	1:A:201:ASN:HD22	1.47	0.63
1:A:509:SER:CB	1:A:513:LEU:HD22	2.23	0.63
1:A:200:PRO:CD	1:A:201:ASN:HA	2.28	0.63
2:B:387:ASP:C	2:B:389:LYS:H	2.03	0.62
1:A:283:PRO:C	1:A:284:ASN:HD22	2.03	0.62
1:A:354:ILE:HD11	1:A:381:PRO:HB3	1.82	0.62
1:A:749:GLN:HG2	1:A:763:ASN:H	1.65	0.62
1:A:965:SER:O	1:A:967:GLY:N	2.31	0.62
1:A:94:LEU:O	1:A:95:PHE:HB3	1.99	0.61
1:A:51:LYS:HG2	1:A:54:ARG:HH21	1.64	0.61
1:A:911:LEU:O	1:A:937:PHE:O	2.18	0.61
2:B:487:PHE:O	2:B:491:ILE:HG13	2.00	0.61
1:A:910:ILE:O	1:A:1025:THR:HG21	2.00	0.61
2:B:577:ARG:HG2	2:B:577:ARG:O	1.99	0.61
1:A:200:PRO:N	1:A:201:ASN:HA	2.15	0.61
1:A:910:ILE:HA	1:A:1025:THR:HG23	1.83	0.61
1:A:721:GLN:O	1:A:722:GLU:CB	2.47	0.60
1:A:117:ILE:O	1:A:121:ILE:HG13	2.01	0.60
1:A:621:LYS:HB3	1:A:622:TYR:HD1	1.65	0.60
1:A:799:ILE:CD1	1:A:847:LEU:HD22	2.27	0.60
1:A:977:PHE:CE1	1:A:981:GLN:NE2	2.69	0.60
1:A:284:ASN:N	1:A:284:ASN:HD22	1.99	0.60
1:A:137:GLN:HE22	1:A:140:ARG:NH1	1.93	0.60
1:A:454:ASP:HA	2:B:349:ASP:OD1	2.01	0.59
1:A:111:LYS:O	1:A:114[A]:ASN:CB	2.50	0.59
2:B:445:VAL:HG21	2:B:583:TRP:HZ3	1.63	0.59
1:A:878:HIS:CE1	1:A:966:LYS:O	2.56	0.59
2:B:330:ASP:C	2:B:332:GLU:H	2.05	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:518:GLU:HG2	2:B:521:ILE:HD12	1.84	0.59
2:B:394:ASP:N	2:B:395:PRO:HD2	2.18	0.59
1:A:530:GLN:O	1:A:534:ILE:HG13	2.03	0.59
1:A:267:LEU:HD13	1:A:273:ILE:HG13	1.84	0.58
1:A:772:MET:HA	1:A:772:MET:HE2	1.85	0.58
1:A:977:PHE:HE1	1:A:981:GLN:NE2	2.01	0.58
1:A:778:PRO:HB3	1:A:802:LYS:HG3	1.86	0.58
2:B:343:VAL:CG2	2:B:358:ARG:HD3	2.33	0.58
1:A:520:ASP:O	1:A:522:GLU:N	2.36	0.58
1:A:709:MET:HE1	1:A:847:LEU:HD21	1.86	0.58
1:A:54:ARG:HG2	1:A:59:HIS:CE1	2.38	0.57
1:A:910:ILE:CA	1:A:1025:THR:HG21	2.32	0.57
1:A:401:ARG:NH2	1:A:458:PRO:O	2.36	0.57
1:A:524:ARG:HD3	1:A:557:TYR:CE1	2.40	0.57
1:A:965:SER:OG	1:A:971:CYS:HB3	2.05	0.57
1:A:527:ASP:C	1:A:529:GLU:H	2.08	0.56
1:A:714:ASN:O	1:A:718:ILE:HG13	2.05	0.56
1:A:561:ILE:O	1:A:564:ILE:HG22	2.04	0.56
2:B:355:PHE:CD1	2:B:427:PRO:HA	2.40	0.56
1:A:-15:ILE:HB	1:A:-14:PRO:HD3	1.87	0.56
1:A:138:ASP:OD1	1:A:141:ARG:NH2	2.39	0.55
2:B:355:PHE:HE1	2:B:427:PRO:CA	2.18	0.55
1:A:-28:MET:H2	1:A:-25:TYR:H	1.53	0.55
1:A:360:ILE:C	1:A:366:PRO:HD2	2.26	0.55
1:A:745:MET:O	1:A:749:GLN:HB2	2.06	0.55
2:B:343:VAL:HG21	2:B:358:ARG:HH11	1.72	0.55
1:A:910:ILE:HD13	1:A:991:ILE:HG21	1.89	0.55
1:A:91:ASP:OD1	1:A:711:LYS:NZ	2.40	0.55
1:A:655:LYS:O	1:A:659:THR:HB	2.06	0.55
1:A:647:ASN:ND2	1:A:650:VAL:H	2.04	0.55
1:A:178:PRO:HD2	1:A:181:ILE:HD12	1.87	0.55
2:B:582:MET:O	2:B:586:GLN:HG2	2.06	0.55
1:A:772:MET:HA	1:A:772:MET:CE	2.37	0.55
2:B:372:LEU:HD11	2:B:413:LEU:HD13	1.87	0.55
1:A:193:VAL:HG22	1:A:208:THR:HG22	1.89	0.55
1:A:642:GLU:HG2	1:A:647:ASN:OD1	2.07	0.54
1:A:817:ILE:HG22	1:A:835:PRO:HB3	1.90	0.54
1:A:372:ASN:HB2	1:A:385:GLU:OE2	2.07	0.54
1:A:332:SER:O	1:A:393:ILE:HG12	2.08	0.54
1:A:479:TRP:CE2	1:A:481:SER:HA	2.43	0.54
1:A:171:VAL:HG13	1:A:269:GLN:HG2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:LEU:O	1:A:383:TRP:O	2.26	0.54
1:A:972:THR:HB	1:A:973:LYS:HG2	1.90	0.54
1:A:542:GLU:OE2	2:B:340:ARG:HD3	2.07	0.53
2:B:498:CYS:HB3	2:B:531:LEU:HG	1.89	0.53
1:A:541:SER:HB2	2:B:340:ARG:HH21	1.72	0.53
1:A:565:LEU:HB3	1:A:566:PRO:HD3	1.89	0.53
1:A:334:LEU:HA	1:A:393:ILE:HD11	1.90	0.53
1:A:573:LYS:HB2	1:A:579:GLU:OE1	2.09	0.53
1:A:353:LYS:HG3	1:A:377:PRO:HG3	1.89	0.53
1:A:467:ASN:O	1:A:470:THR:OG1	2.27	0.53
1:A:785:ASN:HD22	1:A:786:PRO:HD2	1.73	0.53
1:A:827:GLN:HG3	3:A:1115:HOH:O	2.08	0.53
1:A:718:ILE:O	1:A:721:GLN:O	2.26	0.52
1:A:10:LEU:HB3	1:A:13:ILE:HD11	1.91	0.52
1:A:446:TRP:CZ3	1:A:679:THR:HG22	2.44	0.52
2:B:362:THR:HG22	2:B:364:MET:H	1.74	0.52
2:B:572:GLN:O	2:B:576:THR:HG23	2.09	0.52
1:A:525:GLU:HB2	1:A:528:LYS:CG	2.36	0.52
2:B:440:ASP:HA	2:B:583:TRP:HH2	1.74	0.52
1:A:108:ARG:O	1:A:112:ILE:HG13	2.10	0.52
1:A:358:THR:HG22	1:A:404:LEU:HB3	1.91	0.52
1:A:908:THR:HG23	1:A:953:PRO:HB2	1.92	0.52
1:A:213:HIS:CE1	1:A:214:ASP:HB3	2.45	0.51
1:A:562:PRO:HG3	1:A:591:PRO:HG2	1.90	0.51
1:A:621:LYS:HB3	1:A:622:TYR:CD1	2.45	0.51
1:A:765:ARG:CZ	1:A:796:ASN:HD21	2.22	0.51
1:A:43:ILE:HG13	1:A:85:GLU:O	2.09	0.51
1:A:916:ARG:HH12	1:A:920:ASN:HB2	1.74	0.51
1:A:96:GLN:OE1	1:A:96:GLN:HA	2.11	0.51
1:A:1043:MET:O	1:A:1047:HIS:HD2	1.94	0.51
2:B:338:ILE:HB	2:B:342:GLU:HG3	1.92	0.51
1:A:744:PHE:HD2	1:A:748:LEU:HD12	1.76	0.51
1:A:642:GLU:HG2	1:A:647:ASN:CB	2.40	0.51
2:B:535:ILE:HG22	2:B:535:ILE:O	2.10	0.51
1:A:353:LYS:HG3	1:A:377:PRO:CG	2.41	0.50
1:A:552:TRP:CZ3	1:A:583:MET:CE	2.90	0.50
1:A:1019:ILE:HG22	1:A:1019:ILE:O	2.10	0.50
1:A:552:TRP:CZ3	1:A:583:MET:HE3	2.38	0.50
1:A:192:VAL:HG12	1:A:193:VAL:N	2.26	0.50
2:B:466:LEU:HD21	2:B:562:ARG:NH1	2.25	0.50
1:A:739:MET:O	1:A:745:MET:CE	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ILE:HD13	1:A:246:TYR:HB3	1.94	0.50
1:A:354:ILE:HA	1:A:407:CYS:O	2.11	0.50
1:A:113:LEU:O	1:A:114[B]:ASN:CG	2.51	0.49
2:B:439:GLU:OE2	2:B:448:LYS:NZ	2.37	0.49
1:A:-28:MET:O	1:A:-26:TYR:N	2.40	0.49
1:A:813:THR:HG22	1:A:814:LEU:N	2.27	0.49
2:B:433:GLN:HG2	2:B:583:TRP:CD1	2.46	0.49
1:A:985:TYR:CZ	1:A:1040:MET:HG2	2.48	0.49
1:A:1044:ASN:ND2	1:A:1051:TRP:O	2.45	0.49
1:A:84:ASP:OD1	1:A:86:THR:OG1	2.31	0.49
1:A:108:ARG:HD3	1:A:111:LYS:HD2	1.94	0.49
1:A:324:THR:HG22	1:A:483:VAL:HG22	1.95	0.49
1:A:538:ASP:HB2	1:A:539:PRO:CD	2.42	0.49
2:B:518:GLU:HA	2:B:521:ILE:HD12	1.94	0.49
1:A:985:TYR:OH	1:A:1040:MET:HG2	2.13	0.49
1:A:361:TYR:CE2	1:A:365:GLU:HB3	2.48	0.49
1:A:53:ALA:O	1:A:55:LYS:N	2.46	0.49
1:A:640:LYS:HG2	1:A:680:VAL:CG1	2.43	0.48
2:B:333:TRP:HA	2:B:429:SER:HG	1.78	0.48
1:A:503:GLU:O	1:A:505:GLY:N	2.46	0.48
2:B:441:ASN:CB	2:B:444:ALA:HB3	2.42	0.48
1:A:813:THR:CG2	1:A:814:LEU:N	2.75	0.48
1:A:39:GLU:O	1:A:88:ARG:HG2	2.13	0.48
1:A:53:ALA:C	1:A:55:LYS:H	2.16	0.48
1:A:665:HIS:ND1	1:A:698:TYR:OH	2.41	0.48
2:B:466:LEU:HD21	2:B:562:ARG:HH12	1.79	0.48
1:A:542:GLU:HG2	2:B:380:LEU:CD2	2.43	0.47
1:A:70:PHE:CD1	1:A:99:LEU:HB3	2.49	0.47
1:A:945:PHE:CD1	2:B:598:LEU:HB3	2.49	0.47
1:A:137:GLN:NE2	1:A:140:ARG:HD3	2.30	0.47
1:A:916:ARG:NH1	1:A:920:ASN:HB2	2.29	0.47
1:A:431:ASP:C	1:A:431:ASP:OD1	2.52	0.47
1:A:538:ASP:HA	1:A:996:ASN:ND2	2.29	0.47
1:A:913:ILE:HD12	1:A:914:GLY:O	2.14	0.47
1:A:901:CYS:HA	1:A:929:LEU:HD22	1.95	0.47
1:A:858:MET:HG2	1:A:858:MET:O	2.15	0.47
2:B:377:ASN:HB3	2:B:379:LYS:NZ	2.30	0.47
1:A:244:LEU:HD12	1:A:247:GLN:HE22	1.79	0.47
1:A:789:MET:O	1:A:790:SER:C	2.53	0.46
1:A:503:GLU:HA	1:A:506:PHE:CE2	2.49	0.46
1:A:709:MET:CE	1:A:847:LEU:HD21	2.45	0.46

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:372:LEU:HB2	2:B:379:LYS:HB2	1.97	0.46
1:A:944:LYS:HB2	1:A:944:LYS:HE2	1.79	0.46
1:A:253:LYS:HD3	1:A:286:MET:HE1	1.98	0.46
1:A:724:LYS:HG3	1:A:724:LYS:H	1.60	0.46
1:A:944:LYS:HD2	2:B:457:GLN:CG	2.44	0.46
1:A:109:GLU:O	1:A:113:LEU:HD13	2.16	0.46
1:A:640:LYS:HG2	1:A:680:VAL:HG12	1.98	0.46
1:A:173:SER:HB3	1:A:626:ASP:OD2	2.16	0.46
1:A:985:TYR:HB3	1:A:1036:LEU:HD21	1.98	0.46
1:A:360:ILE:HG22	1:A:366:PRO:HG2	1.96	0.46
2:B:511:LYS:N	2:B:511:LYS:HD2	2.31	0.46
1:A:1023:ARG:HA	1:A:1028:LEU:HD12	1.97	0.45
1:A:190:ILE:HD11	1:A:213:HIS:HA	1.97	0.45
1:A:337:LYS:HD3	1:A:339:LEU:HD11	1.97	0.45
1:A:542:GLU:OE2	2:B:340:ARG:CD	2.64	0.45
1:A:628:LEU:O	1:A:628:LEU:HD12	2.16	0.45
1:A:971:CYS:O	1:A:973:LYS:N	2.49	0.45
1:A:360:ILE:HD13	1:A:367:LEU:HD21	1.97	0.45
1:A:13:ILE:C	1:A:13:ILE:HD12	2.36	0.45
1:A:424:TRP:CH2	1:A:460:GLY:HA3	2.52	0.45
1:A:76:GLU:O	1:A:78:GLU:N	2.48	0.45
1:A:191:ILE:HA	1:A:209:LEU:O	2.17	0.45
1:A:735:LEU:O	1:A:739:MET:HG3	2.17	0.45
1:A:936:HIS:HB3	1:A:940:HIS:HB3	1.98	0.45
1:A:367:LEU:HD23	1:A:391:ILE:CG2	2.47	0.45
1:A:901:CYS:O	1:A:905:CYS:HB2	2.17	0.45
1:A:352:ASP:HB3	1:A:353:LYS:HE3	1.99	0.45
1:A:35:GLU:O	1:A:35:GLU:HG3	2.17	0.45
1:A:843:ASP:O	1:A:845:VAL:HG23	2.17	0.45
1:A:942:LYS:C	1:A:944:LYS:N	2.71	0.45
1:A:145:ASN:OD1	1:A:145:ASN:N	2.49	0.45
1:A:738:GLN:HE22	1:A:741:ARG:HH21	1.65	0.45
1:A:408:SER:OG	1:A:422:LEU:HD21	2.17	0.44
1:A:453:GLU:HG2	2:B:567:LYS:NZ	2.31	0.44
1:A:785:ASN:HD22	1:A:786:PRO:CD	2.30	0.44
1:A:108:ARG:HH22	1:A:303:THR:HG21	1.82	0.44
1:A:419:HIS:HB3	1:A:455:LEU:HD11	2.00	0.44
1:A:799:ILE:HD13	1:A:847:LEU:HB3	2.00	0.44
2:B:427:PRO:O	2:B:428:VAL:C	2.55	0.44
1:A:218:GLU:HA	1:A:221:ILE:HD12	1.99	0.44
1:A:670:HIS:O	1:A:673:SER:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:739:MET:O	1:A:745:MET:HE3	2.17	0.44
1:A:353:LYS:HG3	1:A:377:PRO:CB	2.47	0.44
1:A:511:ALA:HB3	2:B:417:ASN:HD22	1.83	0.44
1:A:524:ARG:HD2	1:A:529:GLU:OE2	2.18	0.44
1:A:899:ARG:NH1	1:A:983:MET:HE3	2.32	0.44
2:B:355:PHE:O	2:B:356:LEU:HB3	2.18	0.44
1:A:873:ASN:HB3	1:A:876:THR:HG23	2.00	0.43
2:B:441:ASN:O	2:B:442:ILE:HB	2.18	0.43
1:A:1001:LEU:HD23	1:A:1001:LEU:HA	1.87	0.43
1:A:71:VAL:HG22	1:A:72:SER:N	2.33	0.43
1:A:68:TYR:O	1:A:69:ILE:HD12	2.18	0.43
2:B:589:VAL:HG12	2:B:591:GLN:HG3	2.00	0.43
1:A:-28:MET:HB3	1:A:-26:TYR:HD2	1.83	0.43
1:A:503:GLU:C	1:A:505:GLY:H	2.22	0.43
2:B:439:GLU:O	2:B:445:VAL:HG23	2.19	0.43
1:A:180:HIS:CE1	1:A:825:GLN:HG3	2.54	0.43
1:A:883:ASP:HA	1:A:886:LYS:HE3	1.99	0.43
1:A:971:CYS:C	1:A:973:LYS:N	2.71	0.43
2:B:394:ASP:O	2:B:396:LEU:N	2.43	0.43
2:B:409:ARG:HA	2:B:424:LEU:HB2	2.01	0.43
2:B:555:GLU:O	2:B:559:ILE:HG12	2.19	0.43
1:A:512:GLY:O	1:A:514:SER:N	2.52	0.43
1:A:791:GLU:CD	1:A:791:GLU:H	2.22	0.43
1:A:916:ARG:HA	1:A:920:ASN:OD1	2.19	0.43
2:B:570:LEU:O	2:B:574:ARG:HB2	2.18	0.43
1:A:233:LEU:HD23	1:A:233:LEU:HA	1.84	0.43
1:A:298:PRO:CG	1:A:697:MET:HG3	2.29	0.43
2:B:343:VAL:HG12	2:B:347:LEU:HD12	2.01	0.43
1:A:1000:ASN:O	1:A:1004:MET:HG3	2.19	0.42
1:A:53:ALA:C	1:A:55:LYS:N	2.71	0.42
1:A:542:GLU:CD	1:A:542:GLU:N	2.72	0.42
1:A:718:ILE:H	1:A:718:ILE:HG13	1.69	0.42
1:A:1019:ILE:CG2	1:A:1019:ILE:O	2.67	0.42
1:A:-14:PRO:CG	1:A:186:ASP:HB3	2.31	0.42
1:A:244:LEU:HD12	1:A:247:GLN:NE2	2.34	0.42
1:A:355:TYR:HD2	1:A:371:VAL:HB	1.85	0.42
1:A:380:ASN:HA	1:A:381:PRO:HD3	1.74	0.42
1:A:527:ASP:O	1:A:529:GLU:N	2.51	0.42
1:A:861:GLN:HE22	1:A:918:ASN:ND2	2.17	0.42
2:B:327:SER:O	2:B:331:ALA:N	2.52	0.42
1:A:63:GLN:HB2	1:A:68:TYR:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:402:VAL:O	2:B:406:ASN:ND2	2.51	0.42
1:A:193:VAL:HG22	1:A:208:THR:CG2	2.50	0.42
1:A:151:VAL:HA	1:A:154:ARG:HD3	2.02	0.42
1:A:524:ARG:HD3	1:A:557:TYR:CZ	2.54	0.42
1:A:793:LEU:HG	1:A:794:PHE:CD2	2.55	0.42
2:B:335:TRP:N	2:B:335:TRP:CD1	2.87	0.42
1:A:200:PRO:HD2	1:A:201:ASN:HA	2.00	0.42
1:A:446:TRP:CZ2	1:A:465:ASN:HA	2.54	0.42
1:A:526:ASN:O	1:A:529:GLU:HG2	2.19	0.42
2:B:394:ASP:C	2:B:396:LEU:H	2.20	0.42
1:A:200:PRO:HG2	1:A:202:ASN:H	1.84	0.42
1:A:971:CYS:O	1:A:972:THR:C	2.58	0.42
1:A:866:LEU:HG	1:A:867:LYS:H	1.84	0.41
1:A:939:ASP:O	1:A:942:LYS:HG2	2.19	0.41
2:B:398:PHE:HD1	2:B:403:GLU:HG3	1.84	0.41
1:A:146:VAL:HG13	1:A:655:LYS:HB2	2.02	0.41
2:B:499:GLN:O	2:B:500:THR:C	2.58	0.41
1:A:1006:LEU:HD23	1:A:1013:LEU:HB3	2.02	0.41
1:A:465:ASN:HA	1:A:466:PRO:HD3	1.96	0.41
1:A:647:ASN:HD21	1:A:650:VAL:H	1.67	0.41
1:A:337:LYS:HA	1:A:385:GLU:O	2.20	0.41
1:A:409:VAL:HA	1:A:418:GLU:HB2	2.02	0.41
1:A:527:ASP:C	1:A:529:GLU:N	2.73	0.41
1:A:686:LEU:HD23	1:A:686:LEU:HA	1.94	0.41
2:B:502:GLU:HA	2:B:505:SER:OG	2.20	0.41
1:A:443:LEU:HD12	1:A:464:SER:HB3	2.02	0.41
1:A:38:ARG:NH2	1:A:743:ASP:OD2	2.54	0.41
1:A:278:MET:HA	1:A:278:MET:CE	2.51	0.41
1:A:353:LYS:HA	1:A:377:PRO:CB	2.47	0.41
1:A:209:LEU:HD11	1:A:223:GLU:HB3	2.03	0.41
1:A:355:TYR:CD2	1:A:371:VAL:HB	2.56	0.41
1:A:946:GLY:O	1:A:947:TYR:C	2.59	0.41
1:A:916:ARG:HB3	1:A:921:ILE:HD11	2.03	0.41
2:B:407:HIS:CD2	2:B:407:HIS:C	2.95	0.41
1:A:634:GLN:HG2	1:A:1001:LEU:HD22	2.02	0.41
1:A:57:PRO:O	1:A:58:LEU:HB2	2.21	0.41
2:B:364:MET:O	2:B:365:HIS:HD2	2.03	0.41
1:A:668:PHE:CD2	1:A:702:LEU:HD22	2.56	0.40
1:A:921:ILE:HG12	1:A:931:HIS:CE1	2.56	0.40
1:A:94:LEU:O	1:A:95:PHE:HB2	2.19	0.40
1:A:192:VAL:HG12	1:A:193:VAL:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:GLU:HG3	1:A:432:TYR:CG	2.56	0.40
1:A:56:TYR:HB3	1:A:57:PRO:HD2	2.03	0.40
1:A:60:GLN:H	1:A:60:GLN:CD	2.24	0.40
1:A:361:TYR:HA	1:A:366:PRO:CD	2.51	0.40
1:A:393:ILE:N	1:A:394:PRO:CD	2.85	0.40
2:B:387:ASP:C	2:B:389:LYS:N	2.72	0.40
1:A:105:VAL:HG12	1:A:106:GLY:H	1.85	0.40
1:A:133:ASP:HA	1:A:134:PRO:HD3	1.95	0.40
1:A:-28:MET:N	1:A:-23:HIS:H	2.19	0.40
1:A:251:ILE:HD11	1:A:288:MET:HG2	2.03	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	1035/1096 (94%)	895 (86%)	99 (10%)	41 (4%)	3	14
2	B	264/279 (95%)	208 (79%)	41 (16%)	15 (6%)	1	8
All	All	1299/1375 (94%)	1103 (85%)	140 (11%)	56 (4%)	3	12

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	PHE
1	A	107	ASN
1	A	114[A]	ASN
1	A	114[B]	ASN
1	A	478	ASP
1	A	504	ALA
1	A	511	ALA
1	A	513	LEU

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Mol	Chain	Res	Type
1	A	521	ASN
1	A	966	LYS
2	B	331	ALA
2	B	352	ASP
2	B	398	PHE
1	A	58	LEU
1	A	481	SER
1	A	528	LYS
1	A	791	GLU
1	A	867	LYS
1	A	947	TYR
1	A	972	THR
2	B	365	HIS
2	B	375	GLY
2	B	428	VAL
2	B	429	SER
2	B	437	VAL
2	B	589	VAL
1	A	54	ARG
1	A	323	SER
1	A	379	SER
1	A	507	SER
1	A	542	GLU
1	A	967	GLY
2	B	340	ARG
2	B	353	GLY
2	B	418	PRO
2	B	431	TYR
1	A	235	SER
1	A	376	VAL
1	A	419	HIS
1	A	450	HIS
1	A	454	ASP
1	A	506	PHE
1	A	1008	SER
2	B	591	GLN
1	A	-27	SER
1	A	186	ASP
1	A	307	TYR
1	A	378	CYS
1	A	763	ASN
1	A	945	PHE

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Mol	Chain	Res	Type
1	A	176	GLU
1	A	1007	GLY
1	A	380	ASN
1	A	363	GLY
2	B	436	VAL
1	A	105	VAL

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	957/999 (96%)	862 (90%)	95 (10%)	8	27
2	B	250/259 (96%)	228 (91%)	22 (9%)	10	33
All	All	1207/1258 (96%)	1090 (90%)	117 (10%)	8	28

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-28	MET
1	A	-15	ILE
1	A	-13	THR
1	A	-12	THR
1	A	35	GLU
1	A	38	ARG
1	A	69	ILE
1	A	74	THR
1	A	112	ILE
1	A	113	LEU
1	A	145	ASN
1	A	148	LYS
1	A	173	SER
1	A	174	SER
1	A	190	ILE
1	A	196	VAL
1	A	203	ASP

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Mol	Chain	Res	Type
1	A	208	THR
1	A	209	LEU
1	A	211	ILE
1	A	215	CYS
1	A	231	SER
1	A	244	LEU
1	A	247	GLN
1	A	267	LEU
1	A	284	ASN
1	A	288	MET
1	A	299	MET
1	A	335	ARG
1	A	349	ARG
1	A	353	LYS
1	A	357	ARG
1	A	368	CYS
1	A	370	ASN
1	A	373	THR
1	A	380	ASN
1	A	383	TRP
1	A	404	LEU
1	A	437	VAL
1	A	459	ILE
1	A	461	VAL
1	A	462	THR
1	A	470	THR
1	A	476	GLU
1	A	478	ASP
1	A	483	VAL
1	A	490	SER
1	A	499	SER
1	A	519	ARG
1	A	527	ASP
1	A	542	GLU
1	A	545	GLU
1	A	553	SER
1	A	563	GLU
1	A	566	PRO
1	A	575	ASN
1	A	584	TYR
1	A	589	ASP
1	A	626	ASP

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Mol	Chain	Res	Type
1	A	627	LYS
1	A	630	GLN
1	A	650	VAL
1	A	659	THR
1	A	679	THR
1	A	681	SER
1	A	714	ASN
1	A	718	ILE
1	A	721	GLN
1	A	724	LYS
1	A	753	SER
1	A	770	ARG
1	A	785	ASN
1	A	788	ILE
1	A	790	SER
1	A	798	GLU
1	A	799	ILE
1	A	807	LEU
1	A	813	THR
1	A	829	LEU
1	A	834	LEU
1	A	860	ILE
1	A	870	LEU
1	A	872	PHE
1	A	874	SER
1	A	881	LEU
1	A	922	MET
1	A	959	ASP
1	A	966	LYS
1	A	971	CYS
1	A	973	LYS
1	A	976	GLU
1	A	1017	ASP
1	A	1022	ILE
1	A	1025	THR
1	A	1036	LEU
2	B	352	ASP
2	B	355	PHE
2	B	358	ARG
2	B	362	THR
2	B	364	MET
2	B	365	HIS

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Mol	Chain	Res	Type
2	B	397	THR
2	B	415	GLN
2	B	425	LEU
2	B	434	ASP
2	B	435	GLN
2	B	441	ASN
2	B	468	GLU
2	B	482	THR
2	B	484	ILE
2	B	501	GLN
2	B	531	LEU
2	B	543	ARG
2	B	559	ILE
2	B	572	GLN
2	B	574	ARG
2	B	589	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-22	HIS
1	A	59	HIS
1	A	137	GLN
1	A	247	GLN
1	A	345	ASN
1	A	374	GLN
1	A	575	ASN
1	A	605	ASN
1	A	647	ASN
1	A	670	HIS
1	A	731	GLN
1	A	749	GLN
1	A	785	ASN
1	A	796	ASN
1	A	861	GLN
1	A	917	HIS
1	A	931	HIS
1	A	936	HIS
1	A	996	ASN
1	A	1047	HIS
2	B	365	HIS
2	B	407	HIS

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Mol	Chain	Res	Type
2	B	415	GLN
2	B	417	ASN
2	B	432	GLN
2	B	453	ASN
2	B	475	GLN
2	B	488	ASN
2	B	564	ASN
2	B	591	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	1044/1096 (95%)	0.08	44 (4%)	36	23	39, 76, 130, 176	0
2	B	268/279 (96%)	0.94	51 (19%)	1	0	82, 126, 174, 189	0
All	All	1312/1375 (95%)	0.25	95 (7%)	15	8	39, 83, 154, 189	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	524	ARG	7.0
1	A	322	THR	6.7
2	B	430	LYS	6.3
2	B	423	LYS	5.4
2	B	436	VAL	5.2
2	B	590	ARG	5.1
1	A	523	LEU	5.1
2	B	425	LEU	4.8
2	B	395	PRO	4.7
2	B	587	LYS	4.6
1	A	525	GLU	4.6
2	B	437	VAL	4.4
2	B	592	LYS	4.3
1	A	522	GLU	4.3
1	A	409	VAL	4.3
1	A	519	ARG	4.1
2	B	412	SER	4.1
2	B	409	ARG	4.0
2	B	364	MET	4.0
2	B	593	LYS	4.0
2	B	410	ASN	3.8
2	B	435	GLN	3.8
2	B	433	GLN	3.7
1	A	867	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	-12	THR	3.7
1	A	308	SER	3.6
2	B	584	LEU	3.5
1	A	943	LYS	3.5
1	A	375	ARG	3.5
2	B	434	ASP	3.4
1	A	947	TYR	3.4
2	B	411	GLU	3.2
2	B	591	GLN	3.2
2	B	397	THR	3.2
1	A	526	ASN	3.2
2	B	398	PHE	3.2
1	A	-13	THR	3.2
1	A	945	PHE	3.1
1	A	187	LYS	3.0
2	B	470	TYR	3.0
1	A	1049	GLY	3.0
1	A	363	GLY	3.0
2	B	598	LEU	2.9
2	B	431	TYR	2.9
2	B	580	TYR	2.9
2	B	424	LEU	2.9
2	B	438	LYS	2.8
2	B	442	ILE	2.8
1	A	725	ASP	2.8
2	B	559	ILE	2.8
1	A	557	TYR	2.8
1	A	-14	PRO	2.8
2	B	583	TRP	2.7
2	B	509	ILE	2.7
1	A	872	PHE	2.7
1	A	323	SER	2.6
1	A	132	LYS	2.6
1	A	107	ASN	2.6
1	A	105	VAL	2.6
1	A	869	ALA	2.6
1	A	364	GLY	2.6
1	A	868	GLY	2.6
2	B	432	GLN	2.6
2	B	586	GLN	2.6
2	B	543	ARG	2.6
1	A	307	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	-27	SER	2.5
2	B	503	ARG	2.5
1	A	973	LYS	2.5
1	A	888	GLU	2.4
2	B	440	ASP	2.4
1	A	970	GLU	2.4
2	B	385	HIS	2.3
2	B	512	PHE	2.3
2	B	444	ALA	2.3
2	B	396	LEU	2.3
1	A	300	ASP	2.2
2	B	387	ASP	2.2
2	B	552	GLN	2.2
1	A	1052	THR	2.2
1	A	866	LEU	2.2
1	A	417	GLU	2.2
2	B	335	TRP	2.2
1	A	319	ASN	2.1
1	A	870	LEU	2.1
2	B	377	ASN	2.1
2	B	406	ASN	2.1
1	A	106	GLY	2.1
2	B	428	VAL	2.1
1	A	418	GLU	2.1
1	A	188	GLY	2.1
2	B	573	LEU	2.1
2	B	407	HIS	2.1
2	B	388	GLY	2.0
2	B	510	GLU	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 carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.