



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 10:31 AM EDT

PDB ID : 2RF9 / pdb_00002rf9
Title : Crystal structure of the complex between the EGFR kinase domain and a Mig6 peptide
Authors : Zhang, X.; Pickin, K.A.; Bose, R.; Jura, N.; Cole, P.A.; Kuriyan, J.
Deposited on : 2007-09-28
Resolution : 3.50 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

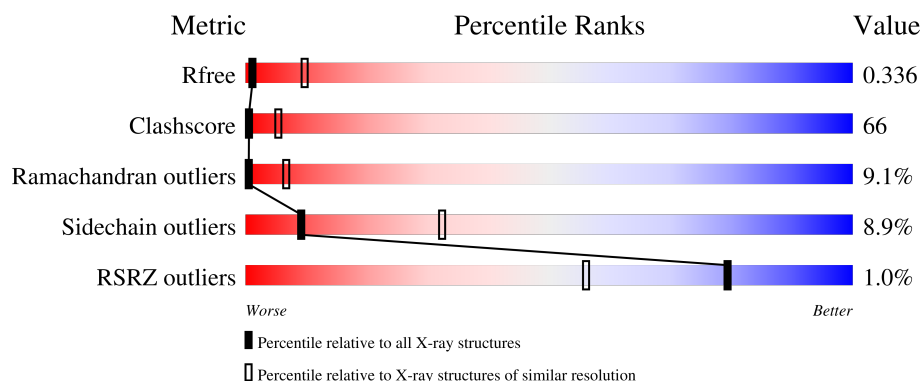
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	330	
1	B	330	
2	C	65	
2	D	65	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4435 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 Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2068	1336	345	372	15			
1	B	269	Total	C	N	O	S	0	0	0
			2010	1298	334	363	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	669	GLY	-	expression tag	UNP P00533
A	670	ALA	-	expression tag	UNP P00533
A	671	MET	-	expression tag	UNP P00533
B	669	GLY	-	expression tag	UNP P00533
B	670	ALA	-	expression tag	UNP P00533
B	671	MET	-	expression tag	UNP P00533

- Molecule 2 is a protein called ERBB receptor feedback inhibitor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	27	Total	C	N	O	S	0	0	0
			183	119	27	36	1			
2	D	26	Total	C	N	O	S	0	0	0
			174	113	26	34	1			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	310	GLY	-	expression tag	UNP Q9UJM3
C	311	PRO	-	expression tag	UNP Q9UJM3
C	312	LEU	-	expression tag	UNP Q9UJM3
C	313	GLY	-	expression tag	UNP Q9UJM3
C	314	SER	-	expression tag	UNP Q9UJM3
D	310	GLY	-	expression tag	UNP Q9UJM3

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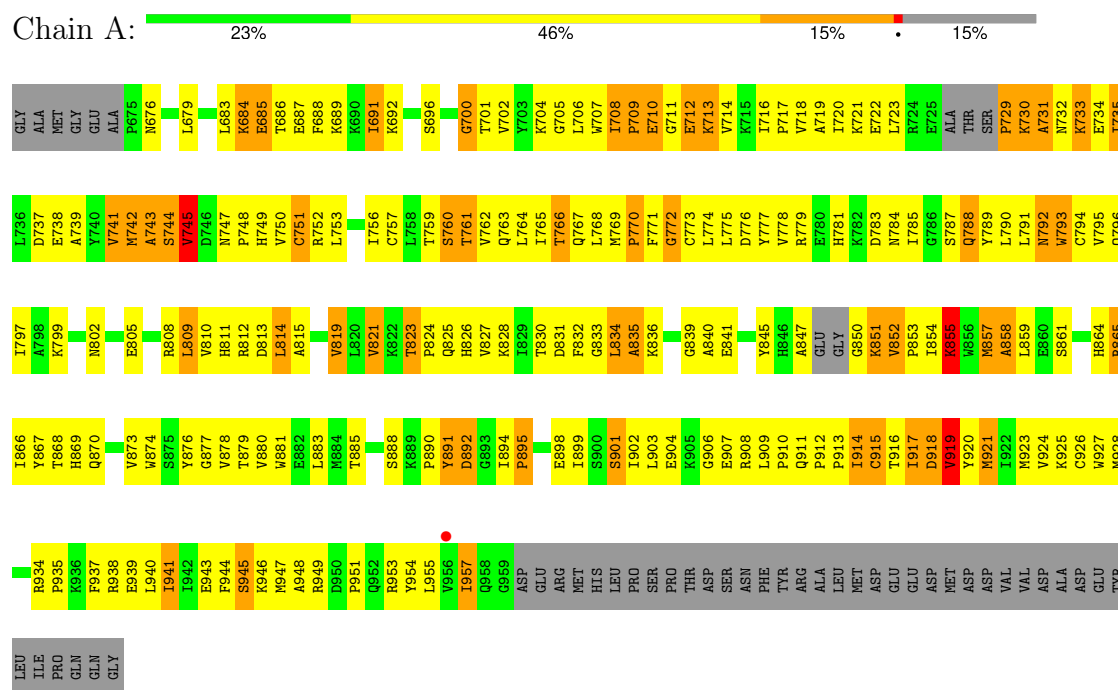
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Chain	Residue	Modelled	Actual	Comment	Reference
D	311	PRO	-	expression tag	UNP Q9UJM3
D	312	LEU	-	expression tag	UNP Q9UJM3
D	313	GLY	-	expression tag	UNP Q9UJM3
D	314	SER	-	expression tag	UNP Q9UJM3

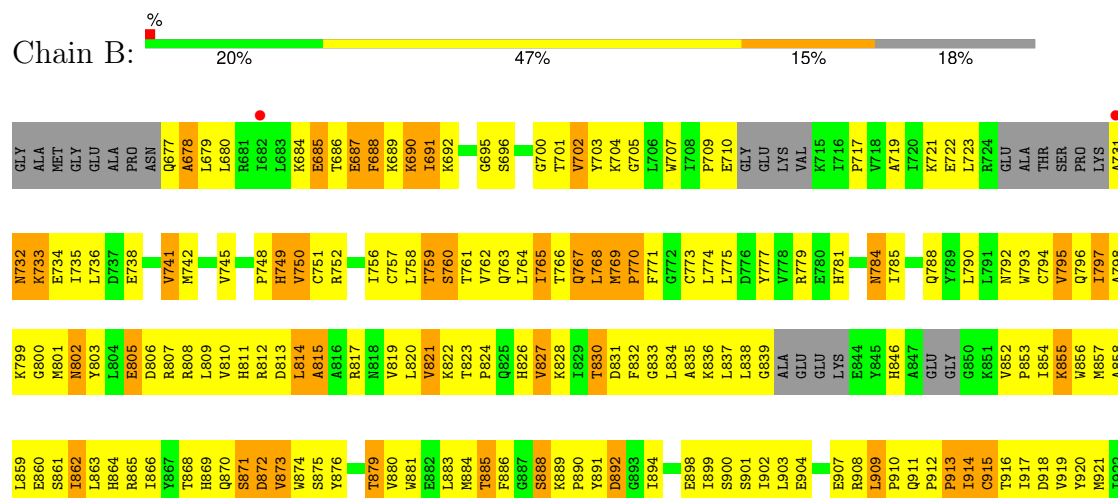
3 Residue-property plots

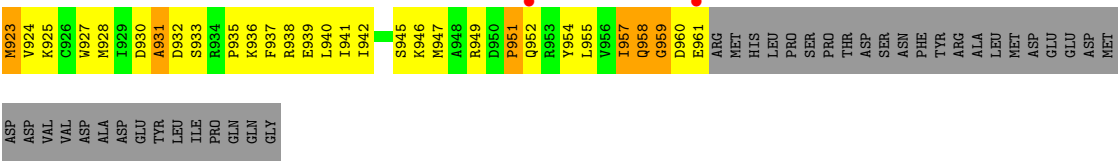
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Epidermal growth factor receptor

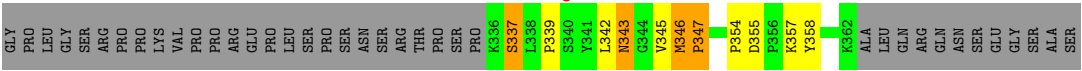
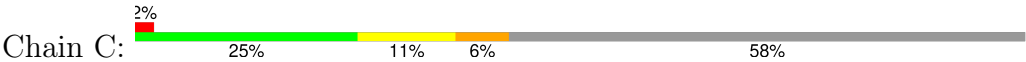


• Molecule 1: Epidermal growth factor receptor





● Molecule 2: ERBB receptor feedback inhibitor 1



● Molecule 2: ERBB receptor feedback inhibitor 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	188.76Å 42.65Å 99.73Å 90.00° 109.12° 90.00°	Depositor
Resolution (Å)	47.11 – 3.50 47.11 – 3.50	Depositor EDS
% Data completeness (in resolution range)	84.5 (47.11-3.50) 84.5 (47.11-3.50)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 3.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.272 , 0.329 0.275 , 0.336	Depositor DCC
R_{free} test set	495 reflections (5.45%)	wwPDB-VP
Wilson B-factor (Å ²)	70.1	Xtriage
Anisotropy	0.699	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 115.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	4435	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.45% 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	0.62	0/2114	1.18	19/2887 (0.7%)
1	B	0.60	0/2054	1.18	22/2800 (0.8%)
2	C	0.86	0/190	1.35	4/264 (1.5%)
2	D	0.73	0/181	1.39	6/251 (2.4%)
All	All	0.63	0/4539	1.20	51/6202 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	731	ALA	N-CA-C	-9.85	101.46	113.19
1	B	760	SER	N-CA-C	-9.82	100.98	113.16
1	B	822	LYS	N-CA-C	-9.57	100.81	111.14
1	A	700	GLY	N-CA-C	9.16	120.65	111.95
1	A	760	SER	N-CA-C	-8.74	103.14	112.93
1	A	741	VAL	N-CA-C	-8.25	104.72	111.81
1	A	832	PHE	N-CA-C	-7.86	100.71	111.56
1	A	772	GLY	N-CA-C	7.70	119.33	111.56
1	B	872	ASP	N-CA-C	-7.63	102.56	111.03
1	B	936	LYS	N-CA-C	-7.60	100.50	110.53
1	B	931	ALA	N-CA-C	6.99	118.97	111.36
2	C	346	MET	CA-C-N	6.81	124.63	119.66
2	C	346	MET	C-N-CA	6.81	124.63	119.66
1	B	817	ARG	N-CA-C	-6.68	103.25	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	355	ASP	CA-C-N	6.67	126.37	119.56
2	D	355	ASP	C-N-CA	6.67	126.37	119.56
1	A	743	ALA	N-CA-C	-6.66	105.78	114.04
2	C	347	PRO	N-CA-C	6.61	116.82	110.47
1	B	723	LEU	N-CA-C	6.52	120.17	109.94
1	A	684	LYS	N-CA-C	-6.33	99.70	109.76
1	A	729	PRO	N-CA-CB	6.16	109.78	103.00
1	A	733	LYS	N-CA-C	-6.14	104.59	111.28
1	A	915	CYS	N-CA-C	6.13	118.73	108.73
1	A	894	ILE	N-CA-C	5.88	113.37	107.55
1	B	915	CYS	N-CA-C	5.87	118.23	109.25
1	B	805	GLU	N-CA-C	-5.80	105.09	111.82
1	B	830	THR	N-CA-C	5.77	118.87	109.06
2	D	346	MET	CA-C-N	5.76	126.32	120.38
2	D	346	MET	C-N-CA	5.76	126.32	120.38
1	A	821	VAL	N-CA-C	5.74	116.06	107.51
1	B	733	LYS	N-CA-C	-5.67	105.62	112.54
1	B	923	MET	N-CA-C	-5.67	104.73	111.03
1	B	765	ILE	N-CA-C	5.66	116.15	107.77
1	A	919	VAL	N-CA-C	-5.62	105.14	110.42
2	D	342	LEU	CA-C-N	5.59	132.21	121.54
2	D	342	LEU	C-N-CA	5.59	132.21	121.54
1	B	802	ASN	N-CA-C	-5.55	104.86	111.03
1	A	745	VAL	N-CA-C	5.51	116.92	108.71
1	A	939	GLU	N-CA-C	5.49	117.69	111.11
1	A	945	SER	N-CA-C	-5.45	106.71	113.19
1	B	862	ILE	CB-CA-C	-5.39	104.86	111.92
1	B	689	LYS	N-CA-C	5.38	117.67	108.90
1	B	749	HIS	N-CA-C	5.31	117.67	110.88
1	B	814	LEU	N-CA-C	-5.29	103.91	110.41
2	C	337	SER	N-CA-C	5.27	118.78	108.18
1	B	932	ASP	N-CA-C	-5.22	106.88	113.20
1	B	958	GLN	N-CA-C	5.19	117.22	109.59
1	A	855	LYS	N-CA-C	5.15	119.04	112.34
1	B	871	SER	N-CA-C	-5.12	106.14	112.38
1	A	921	MET	N-CA-C	5.11	118.29	111.75
1	B	888	SER	N-CA-C	-5.03	102.47	109.96

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	891	TYR	Sidechain

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	2068	0	1961	271	0
1	B	2010	0	1902	271	0
2	C	183	0	152	22	0
2	D	174	0	138	28	0
All	All	4435	0	4153	570	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 66.

All (570) 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)
2:D:341:TYR:CE2	2:D:347:PRO:HD2	1.80	1.17
1:A:880:VAL:HB	1:A:923:MET:HE3	1.34	1.09
2:D:341:TYR:HE2	2:D:347:PRO:HD2	0.95	1.09
2:D:339:PRO:CB	2:D:341:TYR:HE1	1.71	1.03
1:A:907:GLU:O	1:A:908:ARG:HD3	1.57	1.03
1:B:808:ARG:HH11	1:B:839:GLY:HA2	1.23	1.03
2:D:339:PRO:HB3	2:D:341:TYR:HE1	1.27	0.98
2:D:341:TYR:HE2	2:D:347:PRO:CD	1.78	0.96
1:A:859:LEU:HD13	1:A:903:LEU:HD23	1.47	0.95
1:B:696:SER:HB2	1:B:701:THR:HG22	1.49	0.93
1:A:739:ALA:HA	1:A:742:MET:HB3	1.50	0.93
2:D:339:PRO:HB2	2:D:341:TYR:CE1	2.04	0.93
1:A:864:HIS:O	1:A:866:ILE:HG13	1.68	0.92
2:D:341:TYR:CE2	2:D:347:PRO:CD	2.52	0.91
2:D:339:PRO:CB	2:D:341:TYR:CE1	2.54	0.91
1:A:775:LEU:HG	1:A:779:ARG:HE	1.36	0.89
1:A:812:ARG:HG3	1:A:867:TYR:CD2	2.08	0.89
1:A:928:MET:HE3	2:C:357:LYS:CB	2.06	0.86
1:B:781:HIS:O	1:B:785:ILE:HG13	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:696:SER:HA	1:B:701:THR:HA	1.58	0.86
1:B:902:ILE:HB	1:B:907:GLU:HG3	1.56	0.86
1:B:707:TRP:CE2	1:B:709:PRO:HG3	2.11	0.86
1:A:795:VAL:HG22	1:A:944:PHE:HB3	1.59	0.85
1:B:880:VAL:HG12	1:B:884:MET:HE2	1.57	0.85
1:B:880:VAL:O	1:B:884:MET:HG2	1.75	0.85
1:B:696:SER:CB	1:B:701:THR:HG22	2.06	0.84
1:A:729:PRO:C	1:A:731:ALA:H	1.85	0.84
1:A:873:VAL:HG12	1:A:926:CYS:HB3	1.59	0.84
1:B:876:TYR:O	1:B:880:VAL:HG23	1.77	0.83
1:B:881:TRP:HB2	1:B:923:MET:HE1	1.58	0.83
1:A:757:CYS:HB3	1:A:763:GLN:HB2	1.59	0.83
1:A:688:PHE:HA	1:A:706:LEU:O	1.79	0.83
1:B:815:ALA:O	1:B:819:VAL:HG23	1.80	0.82
1:A:687:GLU:O	1:A:707:TRP:HD1	1.63	0.82
1:B:777:TYR:OH	1:B:824:PRO:HG3	1.80	0.81
1:A:721:LYS:HZ1	1:A:830:THR:HG21	1.46	0.80
1:B:758:LEU:HD23	1:B:762:VAL:HG23	1.61	0.80
1:A:947:MET:HA	1:A:954:TYR:CE1	2.16	0.80
1:A:948:ALA:O	1:A:951:PRO:HD3	1.82	0.80
1:A:702:VAL:HG22	1:A:721:LYS:HA	1.61	0.80
1:A:830:THR:HG22	1:A:831:ASP:H	1.46	0.80
1:A:880:VAL:HB	1:A:923:MET:CE	2.11	0.80
1:A:899:ILE:O	1:A:903:LEU:HB2	1.81	0.80
1:B:808:ARG:NH1	1:B:839:GLY:HA2	1.97	0.80
1:A:839:GLY:O	1:A:841:GLU:N	2.15	0.80
1:B:707:TRP:NE1	1:B:709:PRO:HG3	1.98	0.79
1:B:757:CYS:HB3	1:B:763:GLN:HB2	1.64	0.79
1:B:954:TYR:O	1:B:955:LEU:HD23	1.82	0.79
1:A:733:LYS:HE3	1:A:737:ASP:OD2	1.83	0.79
1:A:909:LEU:HD13	1:A:927:TRP:CH2	2.18	0.78
1:B:939:GLU:HA	1:B:942:ILE:HD12	1.65	0.78
1:B:769:MET:HG3	1:B:820:LEU:HD13	1.66	0.78
1:B:919:VAL:HG21	1:B:955:LEU:HD21	1.66	0.77
1:B:881:TRP:CB	1:B:923:MET:HE1	2.15	0.77
1:A:772:GLY:O	1:A:821:VAL:HG23	1.84	0.77
1:B:794:CYS:HA	1:B:797:ILE:HD12	1.65	0.76
1:A:721:LYS:NZ	1:A:830:THR:HG21	2.01	0.76
1:A:812:ARG:CZ	1:A:834:LEU:O	2.33	0.76
1:B:691:ILE:HB	1:B:704:LYS:O	1.86	0.75
1:B:881:TRP:CA	1:B:923:MET:HE1	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:911:GLN:NE2	2:C:339:PRO:HG3	2.02	0.75
1:B:702:VAL:CG2	1:B:721:LYS:HG2	2.16	0.75
1:A:753:LEU:HD11	1:A:764:LEU:HD22	1.68	0.75
1:A:702:VAL:HG13	1:A:720:ILE:O	1.87	0.74
1:B:775:LEU:HD11	1:B:779:ARG:HE	1.52	0.74
1:B:853:PRO:O	1:B:857:MET:HE3	1.86	0.74
1:B:773:CYS:SG	1:B:775:LEU:HB3	2.28	0.74
1:B:793:TRP:O	1:B:797:ILE:HG13	1.85	0.74
1:A:760:SER:O	1:A:761:THR:HG23	1.87	0.74
1:B:930:ASP:O	1:B:933:SER:HB3	1.87	0.73
1:A:909:LEU:N	1:A:909:LEU:HD12	2.04	0.73
1:A:881:TRP:N	1:A:923:MET:HE1	2.04	0.73
1:B:795:VAL:HG12	1:B:799:LYS:HE3	1.71	0.72
1:A:753:LEU:HD12	1:A:766:THR:HG23	1.71	0.72
1:B:688:PHE:HA	1:B:707:TRP:HA	1.70	0.72
1:B:947:MET:HA	1:B:954:TYR:CE1	2.25	0.72
1:A:696:SER:HB3	1:A:701:THR:HG23	1.70	0.72
1:A:830:THR:HG22	1:A:831:ASP:N	2.05	0.71
1:B:814:LEU:HD12	1:B:815:ALA:H	1.56	0.71
1:B:738:GLU:O	1:B:741:VAL:HG23	1.90	0.71
1:B:855:LYS:HZ2	1:B:889:LYS:HE2	1.54	0.71
1:B:684:LYS:C	1:B:686:THR:H	1.98	0.70
1:A:859:LEU:HD13	1:A:903:LEU:CD2	2.21	0.70
1:B:885:THR:HB	1:B:888:SER:HB2	1.71	0.70
1:A:788:GLN:CD	1:A:792:ASN:HD21	2.00	0.70
1:B:899:ILE:O	1:B:903:LEU:HD13	1.91	0.70
1:A:795:VAL:O	1:A:799:LYS:HG3	1.92	0.70
1:A:876:TYR:O	1:A:880:VAL:HG23	1.91	0.70
1:B:957:ILE:HD12	1:B:957:ILE:N	2.07	0.70
1:A:696:SER:HA	1:A:701:THR:HA	1.73	0.70
1:A:722:GLU:O	1:A:722:GLU:HG2	1.92	0.70
1:A:787:SER:HA	1:A:955:LEU:HD12	1.74	0.70
1:A:792:ASN:O	1:A:793:TRP:C	2.34	0.70
2:D:339:PRO:HB3	2:D:341:TYR:CE1	2.20	0.69
1:A:880:VAL:CB	1:A:923:MET:HE3	2.19	0.69
1:A:916:THR:HG23	1:A:954:TYR:O	1.92	0.69
1:A:689:LYS:O	1:A:705:GLY:HA3	1.92	0.69
1:A:789:TYR:HA	1:A:792:ASN:HD22	1.58	0.69
1:B:741:VAL:HG11	1:B:809:LEU:HD21	1.74	0.69
1:B:771:PHE:HE2	1:B:823:THR:HA	1.56	0.69
1:A:775:LEU:CG	1:A:779:ARG:HE	2.06	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:721:LYS:O	1:A:763:GLN:HA	1.93	0.68
1:B:874:TRP:CE3	1:B:927:TRP:HA	2.29	0.68
1:A:789:TYR:O	1:A:792:ASN:HB2	1.94	0.68
1:B:869:HIS:O	1:B:872:ASP:HB2	1.93	0.68
1:B:909:LEU:H	1:B:909:LEU:HD12	1.59	0.68
1:B:814:LEU:HD23	1:B:876:TYR:HA	1.74	0.68
1:B:855:LYS:HE2	1:B:891:TYR:HB2	1.75	0.68
1:B:917:ILE:O	1:B:921:MET:HG2	1.93	0.68
1:A:785:ILE:HD13	1:A:793:TRP:HH2	1.59	0.67
1:A:809:LEU:CD1	1:A:810:VAL:H	2.08	0.67
1:A:729:PRO:O	1:A:731:ALA:N	2.28	0.67
1:A:770:PRO:HG2	1:A:771:PHE:H	1.60	0.67
1:A:775:LEU:HG	1:A:779:ARG:NE	2.08	0.66
1:A:790:LEU:HD23	1:A:793:TRP:CZ3	2.29	0.66
1:B:809:LEU:HD22	1:B:837:LEU:HD13	1.77	0.66
1:B:919:VAL:HA	1:B:947:MET:HE1	1.76	0.66
1:B:710:GLU:HG2	1:B:710:GLU:O	1.95	0.66
1:B:762:VAL:HG22	1:B:763:GLN:N	2.11	0.66
1:A:919:VAL:HA	1:A:947:MET:HE1	1.78	0.66
1:A:734:GLU:O	1:A:735:ILE:C	2.37	0.66
1:A:687:GLU:O	1:A:707:TRP:HA	1.96	0.66
1:A:722:GLU:HA	1:A:763:GLN:HG2	1.78	0.66
1:A:753:LEU:HD21	1:A:764:LEU:CD2	2.27	0.65
1:A:791:LEU:O	1:A:794:CYS:HB2	1.96	0.65
1:A:912:PRO:HB2	1:A:915:CYS:SG	2.37	0.65
1:B:911:GLN:HA	1:B:920:TYR:CE1	2.32	0.65
1:A:687:GLU:O	1:A:707:TRP:CD1	2.49	0.65
1:A:791:LEU:HD21	1:A:955:LEU:HD21	1.79	0.65
2:D:344:GLY:O	2:D:345:VAL:C	2.39	0.65
1:B:745:VAL:HA	1:B:803:TYR:OH	1.97	0.65
1:A:911:GLN:CD	2:C:339:PRO:HG3	2.22	0.64
1:A:709:PRO:HB2	1:A:712:GLU:HB2	1.78	0.64
1:A:815:ALA:O	1:A:819:VAL:HG23	1.96	0.64
1:A:937:PHE:O	1:A:938:ARG:C	2.40	0.64
2:D:341:TYR:HD2	2:D:345:VAL:O	1.80	0.63
1:A:730:LYS:C	1:A:732:ASN:H	2.04	0.63
1:A:908:ARG:HB3	1:A:927:TRP:CE3	2.34	0.63
1:B:864:HIS:O	1:B:866:ILE:HG13	1.98	0.63
1:B:873:VAL:O	1:B:876:TYR:HB3	1.97	0.63
1:B:910:PRO:HG3	2:D:347:PRO:O	1.98	0.63
1:A:909:LEU:HD12	1:A:909:LEU:H	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:859:LEU:HG	1:B:863:LEU:HG	1.79	0.63
1:B:901:SER:HA	1:B:904:GLU:OE1	1.99	0.63
1:A:910:PRO:HG3	2:C:346:MET:HE3	1.81	0.63
1:A:917:ILE:HG12	2:C:337:SER:HB2	1.79	0.63
1:B:930:ASP:HB3	1:B:933:SER:CB	2.28	0.63
1:A:788:GLN:HE21	1:A:788:GLN:HA	1.62	0.62
1:A:785:ILE:HD13	1:A:793:TRP:CH2	2.34	0.62
1:A:792:ASN:O	1:A:795:VAL:N	2.31	0.62
1:A:812:ARG:HG3	1:A:867:TYR:CE2	2.35	0.62
1:A:917:ILE:HG12	2:C:337:SER:CB	2.30	0.62
1:B:917:ILE:HG22	2:D:337:SER:HB2	1.81	0.62
1:A:712:GLU:O	1:A:714:VAL:N	2.33	0.62
1:B:788:GLN:HE21	1:B:792:ASN:HD21	1.48	0.61
1:B:731:ALA:C	1:B:733:LYS:H	2.07	0.61
1:B:876:TYR:CE2	1:B:940:LEU:HD13	2.35	0.61
1:A:799:LYS:O	1:A:802:ASN:HB3	2.00	0.61
1:A:732:ASN:HA	1:A:735:ILE:HG12	1.82	0.61
1:B:930:ASP:HB3	1:B:933:SER:HB2	1.83	0.61
1:A:854:ILE:HA	1:A:857:MET:SD	2.41	0.60
1:A:747:ASN:OD1	1:A:749:HIS:N	2.34	0.60
1:A:919:VAL:HG22	1:A:954:TYR:HB3	1.82	0.60
1:B:907:GLU:O	1:B:908:ARG:NH1	2.34	0.60
1:B:909:LEU:HD12	1:B:909:LEU:N	2.16	0.60
1:B:721:LYS:O	1:B:763:GLN:HA	2.01	0.60
1:B:925:LYS:O	1:B:928:MET:HG3	2.02	0.60
2:C:345:VAL:HG23	2:C:345:VAL:O	2.02	0.60
1:B:852:VAL:N	1:B:853:PRO:HD3	2.16	0.59
1:B:947:MET:HA	1:B:954:TYR:HE1	1.65	0.59
1:B:702:VAL:HG13	1:B:703:TYR:N	2.16	0.59
1:B:796:GLN:O	1:B:799:LYS:HB2	2.03	0.59
1:A:712:GLU:C	1:A:714:VAL:H	2.08	0.59
1:A:805:GLU:HG3	1:A:869:HIS:ND1	2.18	0.59
1:B:758:LEU:CD2	1:B:762:VAL:HG23	2.30	0.59
1:B:909:LEU:HD13	1:B:927:TRP:CH2	2.37	0.59
1:A:770:PRO:HG2	1:A:771:PHE:CD1	2.38	0.59
1:A:857:MET:HE2	1:A:861:SER:HB3	1.83	0.59
2:C:355:ASP:OD1	2:C:357:LYS:N	2.29	0.59
1:A:753:LEU:HD21	1:A:764:LEU:HD22	1.83	0.59
1:B:870:GLN:HG3	1:B:931:ALA:O	2.02	0.59
1:B:917:ILE:CG2	2:D:337:SER:HB2	2.33	0.59
1:A:943:GLU:O	1:A:947:MET:HG3	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:876:TYR:HE2	1:A:940:LEU:HD22	1.68	0.58
1:B:912:PRO:HD2	1:B:915:CYS:HB2	1.85	0.58
1:B:745:VAL:CG2	1:B:752:ARG:HA	2.34	0.58
1:B:811:HIS:O	1:B:812:ARG:HB2	2.02	0.58
1:A:910:PRO:HB3	2:C:347:PRO:O	2.02	0.58
1:B:898:GLU:O	1:B:901:SER:N	2.37	0.58
1:B:917:ILE:O	1:B:917:ILE:HG13	2.04	0.58
1:A:881:TRP:CD2	1:A:909:LEU:HD23	2.39	0.58
1:B:805:GLU:HG3	1:B:869:HIS:ND1	2.19	0.58
1:B:837:LEU:HD12	1:B:838:LEU:H	1.69	0.58
1:B:700:GLY:O	1:B:701:THR:HG23	2.04	0.58
1:B:741:VAL:HG11	1:B:809:LEU:CD2	2.32	0.58
1:B:769:MET:HG3	1:B:820:LEU:CD1	2.33	0.58
1:B:946:LYS:O	1:B:949:ARG:N	2.36	0.58
1:A:723:LEU:HD23	1:A:723:LEU:H	1.69	0.57
1:B:937:PHE:O	1:B:941:ILE:HG13	2.04	0.57
1:B:764:LEU:O	1:B:765:ILE:HD13	2.03	0.57
1:A:909:LEU:H	1:A:909:LEU:CD1	2.17	0.57
1:A:742:MET:HE3	1:A:831:ASP:CG	2.30	0.57
1:A:809:LEU:HD13	1:A:810:VAL:H	1.70	0.57
1:B:766:THR:O	1:B:768:LEU:N	2.37	0.57
1:B:861:SER:HA	1:B:866:ILE:O	2.04	0.57
1:B:912:PRO:HB2	1:B:915:CYS:SG	2.45	0.57
1:B:767:GLN:O	1:B:768:LEU:C	2.47	0.57
1:A:864:HIS:O	1:A:865:ARG:C	2.48	0.57
1:B:707:TRP:O	1:B:709:PRO:HD3	2.05	0.57
1:A:921:MET:O	1:A:925:LYS:HB2	2.04	0.57
1:B:919:VAL:HG22	1:B:947:MET:SD	2.45	0.56
1:B:759:THR:OG1	1:B:760:SER:N	2.38	0.56
1:B:898:GLU:O	1:B:899:ILE:C	2.49	0.56
1:B:731:ALA:O	1:B:733:LYS:N	2.35	0.56
1:A:741:VAL:C	1:A:743:ALA:H	2.14	0.56
1:A:739:ALA:HB1	1:A:753:LEU:HD23	1.87	0.55
1:B:900:SER:O	1:B:904:GLU:HG3	2.06	0.55
1:A:916:THR:C	1:A:918:ASP:H	2.14	0.55
1:A:845:TYR:HE2	1:A:847:ALA:HB2	1.72	0.55
1:A:709:PRO:O	1:A:710:GLU:C	2.49	0.55
1:B:870:GLN:HA	1:B:873:VAL:HG23	1.89	0.55
1:A:700:GLY:HA3	1:A:723:LEU:HA	1.88	0.55
1:A:711:GLY:O	1:A:712:GLU:C	2.49	0.55
1:B:722:GLU:O	1:B:722:GLU:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:911:GLN:HA	1:A:920:TYR:CE1	2.42	0.54
1:A:874:TRP:HZ2	1:A:903:LEU:HD11	1.73	0.54
1:A:756:ILE:HD12	1:A:764:LEU:HD21	1.88	0.54
1:B:957:ILE:HG22	1:B:958:GLN:H	1.72	0.54
1:A:729:PRO:C	1:A:731:ALA:N	2.54	0.54
1:B:805:GLU:HG3	1:B:869:HIS:CE1	2.43	0.54
1:A:783:ASP:O	1:A:784:ASN:ND2	2.41	0.54
1:B:873:VAL:O	1:B:876:TYR:N	2.39	0.54
1:A:691:ILE:HG22	1:A:692:LYS:N	2.22	0.54
1:A:788:GLN:HA	1:A:788:GLN:NE2	2.23	0.54
1:B:799:LYS:HA	1:B:941:ILE:HD13	1.90	0.53
1:A:732:ASN:HA	1:A:735:ILE:CG1	2.39	0.53
1:A:914:ILE:O	1:A:955:LEU:HA	2.09	0.53
1:B:684:LYS:C	1:B:686:THR:N	2.62	0.53
1:A:890:PRO:C	1:A:891:TYR:CD1	2.87	0.53
1:A:921:MET:HE3	1:A:925:LYS:HE3	1.90	0.53
1:A:730:LYS:C	1:A:732:ASN:N	2.62	0.53
1:A:750:VAL:O	1:A:752:ARG:N	2.41	0.53
1:A:898:GLU:O	1:A:902:ILE:HG12	2.08	0.53
1:A:788:GLN:HG3	1:A:789:TYR:N	2.23	0.53
1:A:858:ALA:HA	1:A:874:TRP:CD2	2.43	0.53
1:B:808:ARG:O	1:B:837:LEU:HD12	2.08	0.53
1:B:881:TRP:HB2	1:B:923:MET:CE	2.36	0.53
1:A:762:VAL:C	1:A:763:GLN:HG3	2.34	0.53
1:B:880:VAL:HB	1:B:923:MET:HE3	1.90	0.53
1:A:874:TRP:C	1:A:874:TRP:CD1	2.87	0.53
1:B:687:GLU:O	1:B:688:PHE:HB3	2.08	0.53
1:B:807:ARG:O	1:B:809:LEU:HD23	2.09	0.53
1:B:790:LEU:HA	1:B:793:TRP:CE3	2.44	0.52
1:B:937:PHE:CD2	1:B:940:LEU:HD12	2.43	0.52
1:A:751:CYS:O	1:A:752:ARG:C	2.53	0.52
1:A:777:TYR:OH	1:A:824:PRO:HG3	2.09	0.52
1:A:789:TYR:CA	1:A:792:ASN:HD22	2.21	0.52
1:A:908:ARG:HB3	1:A:927:TRP:HE3	1.74	0.52
1:B:814:LEU:O	1:B:815:ALA:HB2	2.09	0.52
1:B:732:ASN:O	1:B:736:LEU:HG	2.09	0.52
1:B:890:PRO:HB2	1:B:891:TYR:HD1	1.74	0.52
1:B:733:LYS:HA	1:B:736:LEU:HD12	1.91	0.52
1:B:790:LEU:HD23	1:B:793:TRP:CZ3	2.45	0.52
1:A:688:PHE:HD2	1:A:720:ILE:HD11	1.74	0.52
1:B:813:ASP:CG	1:B:813:ASP:O	2.51	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:947:MET:HA	1:B:954:TYR:CD1	2.45	0.52
1:A:704:LYS:HA	1:A:719:ALA:HA	1.92	0.52
1:A:709:PRO:HD2	1:A:714:VAL:O	2.09	0.52
1:A:911:GLN:NE2	2:C:339:PRO:CG	2.73	0.52
1:B:794:CYS:HA	1:B:797:ILE:CD1	2.35	0.52
1:B:823:THR:OG1	1:B:824:PRO:HD2	2.09	0.52
1:B:748:PRO:O	1:B:828:LYS:HE2	2.09	0.51
1:A:941:ILE:O	1:A:945:SER:N	2.31	0.51
1:A:946:LYS:O	1:A:949:ARG:N	2.43	0.51
1:B:881:TRP:CE2	1:B:885:THR:HG21	2.45	0.51
1:B:891:TYR:O	1:B:894:ILE:HB	2.10	0.51
1:B:902:ILE:HB	1:B:907:GLU:CG	2.35	0.51
1:A:734:GLU:O	1:A:737:ASP:N	2.44	0.51
1:B:858:ALA:HA	1:B:874:TRP:CE2	2.45	0.51
1:A:909:LEU:HB2	1:A:927:TRP:HH2	1.75	0.51
1:B:702:VAL:HG22	1:B:721:LYS:HG2	1.91	0.51
1:B:938:ARG:O	1:B:942:ILE:HG13	2.11	0.51
1:B:947:MET:HG2	1:B:954:TYR:CE1	2.46	0.51
1:A:809:LEU:HD12	1:A:810:VAL:H	1.75	0.51
1:A:909:LEU:N	1:A:909:LEU:CD1	2.71	0.51
1:A:790:LEU:HA	1:A:793:TRP:CE3	2.46	0.51
1:A:947:MET:HA	1:A:954:TYR:HE1	1.72	0.51
2:C:342:LEU:O	2:C:343:ASN:CB	2.58	0.51
1:A:912:PRO:O	1:A:915:CYS:HB2	2.10	0.51
1:A:823:THR:HG23	1:A:826:HIS:N	2.26	0.51
1:A:890:PRO:O	1:A:891:TYR:HD1	1.94	0.51
1:B:834:LEU:O	1:B:836:LYS:HE3	2.11	0.51
1:B:777:TYR:HH	1:B:824:PRO:HG3	1.75	0.50
1:B:815:ALA:HA	1:B:879:THR:HG23	1.93	0.50
1:A:768:LEU:HD12	1:A:769:MET:H	1.77	0.50
1:A:790:LEU:HD23	1:A:793:TRP:HZ3	1.73	0.50
1:A:907:GLU:C	1:A:908:ARG:HD3	2.33	0.50
1:A:938:ARG:O	1:A:941:ILE:HG13	2.11	0.50
1:B:795:VAL:O	1:B:799:LYS:HG3	2.11	0.50
1:A:739:ALA:HA	1:A:742:MET:CB	2.33	0.50
1:B:798:ALA:O	1:B:802:ASN:N	2.43	0.50
1:A:790:LEU:CD2	1:A:793:TRP:HZ3	2.25	0.50
1:A:823:THR:C	1:A:825:GLN:N	2.68	0.50
1:B:793:TRP:CD1	1:B:827:VAL:HG21	2.46	0.50
1:A:917:ILE:HG12	2:C:337:SER:OG	2.11	0.50
1:B:794:CYS:O	1:B:795:VAL:C	2.53	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:890:PRO:HB2	1:B:891:TYR:CD1	2.46	0.50
1:A:712:GLU:C	1:A:714:VAL:N	2.69	0.50
1:B:812:ARG:HH21	1:B:836:LYS:HE3	1.77	0.50
1:B:719:ALA:O	1:B:765:ILE:HA	2.12	0.50
1:B:854:ILE:C	1:B:856:TRP:H	2.20	0.50
1:B:912:PRO:HG2	1:B:915:CYS:SG	2.52	0.50
1:B:921:MET:O	1:B:925:LYS:HE3	2.12	0.50
1:B:930:ASP:CG	1:B:933:SER:HB2	2.37	0.50
1:B:858:ALA:HA	1:B:874:TRP:CD2	2.47	0.50
1:B:876:TYR:HA	1:B:879:THR:OG1	2.12	0.50
1:B:894:ILE:HD11	2:D:348:PRO:HB3	1.94	0.50
1:A:831:ASP:CG	1:A:833:GLY:H	2.20	0.49
1:B:858:ALA:HB1	1:B:860:GLU:OE1	2.12	0.49
1:A:775:LEU:HD21	1:A:779:ARG:HH21	1.76	0.49
1:B:820:LEU:O	1:B:827:VAL:HG12	2.12	0.49
1:B:912:PRO:HD2	1:B:915:CYS:CB	2.41	0.49
1:B:917:ILE:HG22	2:D:337:SER:CB	2.42	0.49
1:A:753:LEU:HA	1:A:766:THR:CG2	2.43	0.49
1:A:753:LEU:HA	1:A:766:THR:HG22	1.93	0.49
1:A:787:SER:OG	1:A:951:PRO:HB2	2.13	0.49
1:A:934:ARG:HB3	1:A:935:PRO:CD	2.43	0.49
1:B:735:ILE:HD12	1:B:833:GLY:CA	2.42	0.49
1:B:793:TRP:HD1	1:B:827:VAL:CG2	2.25	0.49
1:A:743:ALA:C	1:A:745:VAL:H	2.21	0.49
1:A:845:TYR:HB3	1:A:867:TYR:HB2	1.95	0.49
1:A:879:THR:O	1:A:883:LEU:HG	2.12	0.49
1:B:793:TRP:O	1:B:796:GLN:HB2	2.12	0.49
1:B:958:GLN:O	1:B:959:GLY:O	2.30	0.49
1:B:939:GLU:O	1:B:940:LEU:C	2.55	0.49
1:A:781:HIS:HB3	1:A:784:ASN:HB2	1.95	0.49
1:B:891:TYR:O	1:B:892:ASP:C	2.56	0.49
1:B:902:ILE:O	1:B:907:GLU:HB2	2.13	0.49
1:B:821:VAL:HA	1:B:827:VAL:HG12	1.95	0.49
1:B:885:THR:CB	1:B:888:SER:HB2	2.43	0.49
1:A:909:LEU:HB2	1:A:927:TRP:CH2	2.48	0.49
1:B:919:VAL:HG21	1:B:955:LEU:CD2	2.40	0.49
1:A:683:LEU:HD11	1:A:765:ILE:HG13	1.95	0.48
1:A:946:LYS:O	1:A:947:MET:C	2.54	0.48
1:B:814:LEU:HD23	1:B:876:TYR:CA	2.43	0.48
1:A:741:VAL:O	1:A:744:SER:N	2.45	0.48
1:B:748:PRO:HB2	1:B:826:HIS:NE2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:846:HIS:HA	1:B:865:ARG:O	2.13	0.48
1:A:874:TRP:CZ2	1:A:903:LEU:HD21	2.48	0.48
1:B:835:ALA:O	1:B:836:LYS:HD3	2.13	0.48
1:A:790:LEU:HD23	1:A:793:TRP:CE3	2.49	0.48
1:A:830:THR:CG2	1:A:831:ASP:H	2.18	0.48
1:A:854:ILE:O	1:A:857:MET:HG3	2.13	0.48
1:B:873:VAL:O	1:B:874:TRP:C	2.55	0.48
1:A:775:LEU:CD2	1:A:779:ARG:HE	2.26	0.48
1:B:794:CYS:SG	1:B:880:VAL:HG13	2.53	0.48
1:B:939:GLU:O	1:B:942:ILE:N	2.47	0.48
1:A:787:SER:O	1:A:788:GLN:C	2.56	0.48
1:A:852:VAL:O	1:A:853:PRO:C	2.57	0.48
1:B:691:ILE:HG13	1:B:705:GLY:HA2	1.96	0.48
1:B:762:VAL:HG22	1:B:763:GLN:H	1.75	0.48
1:B:868:THR:H	1:B:871:SER:CB	2.26	0.48
1:B:872:ASP:O	1:B:873:VAL:C	2.57	0.48
1:B:685:GLU:HA	1:B:688:PHE:CZ	2.48	0.48
1:A:792:ASN:O	1:A:794:CYS:N	2.47	0.48
1:A:880:VAL:O	1:A:881:TRP:C	2.56	0.48
1:B:677:GLN:O	1:B:678:ALA:HB2	2.13	0.48
1:B:930:ASP:CB	1:B:933:SER:HB2	2.44	0.48
1:A:891:TYR:O	1:A:892:ASP:C	2.56	0.48
1:A:912:PRO:HD3	1:A:920:TYR:CD1	2.49	0.48
1:B:880:VAL:CG1	1:B:884:MET:HE2	2.38	0.48
1:B:741:VAL:CG1	1:B:809:LEU:HD21	2.43	0.47
1:B:775:LEU:CD1	1:B:779:ARG:HE	2.23	0.47
1:B:959:GLY:C	1:B:961:GLU:H	2.21	0.47
1:A:898:GLU:HA	1:A:901:SER:OG	2.14	0.47
1:B:695:GLY:O	1:B:702:VAL:N	2.47	0.47
1:B:868:THR:H	1:B:871:SER:HB3	1.79	0.47
1:B:881:TRP:N	1:B:923:MET:HE1	2.29	0.47
1:A:688:PHE:HD2	1:A:720:ILE:CD1	2.27	0.47
1:A:795:VAL:HG12	1:A:799:LYS:HE3	1.96	0.47
1:A:823:THR:CG2	1:A:826:HIS:HB2	2.45	0.47
1:A:944:PHE:C	1:A:946:LYS:H	2.22	0.47
2:D:341:TYR:N	2:D:341:TYR:CD1	2.82	0.47
1:A:741:VAL:C	1:A:743:ALA:N	2.70	0.47
1:A:810:VAL:O	1:A:835:ALA:HA	2.14	0.47
1:A:753:LEU:HD21	1:A:764:LEU:HD21	1.97	0.47
1:A:759:THR:C	1:A:761:THR:H	2.23	0.47
1:B:879:THR:O	1:B:883:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:909:LEU:HD13	1:B:927:TRP:CZ3	2.50	0.47
1:A:752:ARG:O	1:A:766:THR:HG22	2.14	0.47
1:B:735:ILE:HD12	1:B:833:GLY:HA2	1.95	0.47
1:B:762:VAL:CG2	1:B:763:GLN:N	2.77	0.47
1:B:947:MET:HG2	1:B:954:TYR:CD1	2.49	0.47
1:B:870:GLN:HA	1:B:873:VAL:CG2	2.45	0.47
1:A:708:ILE:O	1:A:710:GLU:N	2.48	0.46
1:B:731:ALA:C	1:B:733:LYS:N	2.73	0.46
2:D:341:TYR:CD2	2:D:347:PRO:CD	2.97	0.46
1:A:776:ASP:O	1:A:779:ARG:HB2	2.15	0.46
1:B:799:LYS:HA	1:B:941:ILE:CD1	2.45	0.46
1:B:814:LEU:HD23	1:B:876:TYR:HB2	1.96	0.46
1:B:957:ILE:N	1:B:957:ILE:CD1	2.76	0.46
1:B:745:VAL:O	1:B:745:VAL:HG23	2.16	0.46
2:D:354:PRO:O	2:D:355:ASP:C	2.56	0.46
1:A:811:HIS:O	1:A:812:ARG:HB3	2.15	0.46
1:A:718:VAL:HG21	1:A:765:ILE:HG23	1.98	0.46
1:A:823:THR:C	1:A:825:GLN:H	2.22	0.46
1:B:801:MET:HE1	1:B:872:ASP:OD2	2.15	0.46
1:A:707:TRP:CE3	1:A:716:ILE:HD12	2.51	0.46
1:A:721:LYS:NZ	1:A:830:THR:CG2	2.75	0.46
1:B:823:THR:HG22	1:B:826:HIS:HB3	1.96	0.46
1:B:742:MET:HA	1:B:745:VAL:HG13	1.97	0.46
1:B:891:TYR:OH	1:B:909:LEU:HD11	2.16	0.46
1:A:811:HIS:CE1	1:A:813:ASP:O	2.69	0.46
1:B:864:HIS:HB2	1:B:866:ILE:CD1	2.46	0.46
1:A:809:LEU:CD1	1:A:835:ALA:HB1	2.46	0.46
1:A:904:GLU:C	1:A:906:GLY:H	2.25	0.45
1:B:796:GLN:O	1:B:799:LYS:N	2.48	0.45
1:B:864:HIS:HB2	1:B:866:ILE:HD12	1.96	0.45
1:B:884:MET:HE3	1:B:919:VAL:HG11	1.98	0.45
1:B:889:LYS:HG2	1:B:890:PRO:N	2.31	0.45
1:B:764:LEU:HD23	1:B:764:LEU:HA	1.74	0.45
1:B:793:TRP:HD1	1:B:827:VAL:HG21	1.81	0.45
1:A:734:GLU:O	1:A:738:GLU:N	2.35	0.45
1:A:778:VAL:HG12	1:A:785:ILE:CD1	2.45	0.45
1:B:745:VAL:HG21	1:B:752:ARG:HA	1.97	0.45
1:B:749:HIS:HA	1:B:828:LYS:HG2	1.97	0.45
1:B:803:TYR:O	1:B:806:ASP:HB2	2.16	0.45
1:B:830:THR:HG22	1:B:831:ASP:O	2.16	0.45
1:B:925:LYS:HE3	1:B:925:LYS:HB2	1.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:803:TYR:HA	1:B:806:ASP:HB2	1.98	0.45
1:A:874:TRP:CD1	1:A:874:TRP:O	2.70	0.45
1:A:777:TYR:C	1:A:779:ARG:H	2.24	0.45
1:A:814:LEU:HD12	1:A:815:ALA:N	2.32	0.45
1:B:687:GLU:O	1:B:688:PHE:CB	2.64	0.45
1:A:768:LEU:HD12	1:A:769:MET:N	2.32	0.45
1:A:911:GLN:HE21	2:C:339:PRO:HD3	1.82	0.45
1:A:917:ILE:CG1	2:C:337:SER:HB2	2.47	0.45
1:B:719:ALA:O	1:B:765:ILE:HD13	2.17	0.45
1:A:708:ILE:O	1:A:708:ILE:HG23	2.17	0.44
1:A:940:LEU:O	1:A:944:PHE:HD2	2.00	0.44
1:A:787:SER:N	1:A:957:ILE:CD1	2.81	0.44
1:A:830:THR:CG2	1:A:831:ASP:N	2.75	0.44
1:A:876:TYR:CE2	1:A:940:LEU:HD13	2.52	0.44
1:A:924:VAL:O	2:C:358:TYR:HE2	1.99	0.44
1:B:690:LYS:O	1:B:690:LYS:HE3	2.18	0.44
1:B:798:ALA:HA	1:B:801:MET:HB2	1.98	0.44
2:C:343:ASN:C	2:C:345:VAL:H	2.24	0.44
1:A:774:LEU:HD12	1:A:774:LEU:O	2.18	0.44
1:B:748:PRO:HB2	1:B:826:HIS:CE1	2.53	0.44
1:B:854:ILE:C	1:B:856:TRP:N	2.72	0.44
2:D:341:TYR:CD2	2:D:347:PRO:HD3	2.52	0.44
1:A:696:SER:CB	1:A:701:THR:HG23	2.43	0.44
1:B:880:VAL:HA	1:B:883:LEU:CD1	2.48	0.44
1:B:913:PRO:HD3	2:D:346:MET:SD	2.57	0.44
1:A:684:LYS:O	1:A:686:THR:N	2.42	0.44
1:B:700:GLY:O	1:B:701:THR:CG2	2.66	0.44
1:B:821:VAL:HG13	1:B:827:VAL:HG13	2.00	0.44
1:B:891:TYR:O	1:B:892:ASP:O	2.36	0.44
1:A:753:LEU:CD1	1:A:764:LEU:HD22	2.43	0.44
1:B:881:TRP:CZ2	1:B:885:THR:HG21	2.53	0.44
1:B:891:TYR:CZ	1:B:909:LEU:HG	2.53	0.44
1:A:796:GLN:O	1:A:797:ILE:C	2.61	0.43
1:B:770:PRO:HG2	1:B:771:PHE:H	1.82	0.43
1:A:741:VAL:O	1:A:743:ALA:N	2.51	0.43
1:A:855:LYS:HG2	1:A:899:ILE:HG13	2.00	0.43
1:B:810:VAL:O	1:B:811:HIS:C	2.62	0.43
1:B:874:TRP:CZ3	1:B:927:TRP:HA	2.53	0.43
1:A:756:ILE:HG13	1:A:763:GLN:O	2.19	0.43
1:A:775:LEU:O	1:A:779:ARG:HD2	2.17	0.43
1:B:796:GLN:OE1	1:B:827:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:853:PRO:C	1:B:857:MET:HE3	2.42	0.43
1:A:685:GLU:O	1:A:686:THR:HG23	2.18	0.43
1:A:711:GLY:O	1:A:713:LYS:N	2.51	0.43
1:A:811:HIS:O	1:A:812:ARG:CB	2.66	0.43
1:A:944:PHE:C	1:A:946:LYS:N	2.77	0.43
1:B:912:PRO:HA	1:B:913:PRO:HD3	1.90	0.43
1:A:707:TRP:O	1:A:709:PRO:HD3	2.19	0.43
1:A:716:ILE:HA	1:A:717:PRO:HD3	1.66	0.43
1:B:759:THR:C	1:B:761:THR:H	2.26	0.43
1:B:935:PRO:HA	1:B:939:GLU:OE1	2.19	0.43
1:A:707:TRP:N	1:A:716:ILE:O	2.49	0.43
1:A:773:CYS:HA	1:A:819:VAL:O	2.19	0.43
1:A:788:GLN:NE2	1:A:788:GLN:CA	2.80	0.43
1:B:796:GLN:O	1:B:797:ILE:C	2.62	0.43
1:B:749:HIS:C	1:B:750:VAL:CG2	2.92	0.43
1:B:916:THR:C	1:B:918:ASP:H	2.27	0.43
1:B:924:VAL:O	1:B:927:TRP:N	2.40	0.43
1:A:879:THR:O	1:A:880:VAL:C	2.62	0.42
1:A:940:LEU:O	1:A:944:PHE:HB2	2.18	0.42
1:B:799:LYS:O	1:B:800:GLY:C	2.62	0.42
1:B:810:VAL:O	1:B:810:VAL:HG12	2.18	0.42
1:B:864:HIS:C	1:B:866:ILE:HG13	2.43	0.42
1:B:903:LEU:HG	1:B:908:ARG:HH12	1.85	0.42
1:B:941:ILE:O	1:B:945:SER:OG	2.35	0.42
1:A:748:PRO:HB2	1:A:826:HIS:NE2	2.34	0.42
1:A:787:SER:CB	1:A:951:PRO:HB2	2.49	0.42
1:A:916:THR:C	1:A:918:ASP:N	2.75	0.42
1:B:691:ILE:HG22	1:B:692:LYS:N	2.34	0.42
1:B:911:GLN:HA	1:B:920:TYR:CD1	2.54	0.42
1:B:951:PRO:HG2	1:B:952:GLN:H	1.84	0.42
2:D:339:PRO:HB2	2:D:341:TYR:CD1	2.51	0.42
1:A:777:TYR:CE1	1:A:781:HIS:CD2	3.08	0.42
1:A:791:LEU:O	1:A:795:VAL:HG23	2.19	0.42
2:D:341:TYR:C	2:D:343:ASN:H	2.26	0.42
1:A:906:GLY:HA2	1:A:908:ARG:NH1	2.34	0.42
1:A:722:GLU:CA	1:A:763:GLN:HG2	2.47	0.42
1:A:813:ASP:HB2	1:A:852:VAL:HG22	2.02	0.42
1:A:876:TYR:CD2	1:A:940:LEU:HD13	2.54	0.42
1:A:953:ARG:O	1:A:953:ARG:HG2	2.19	0.42
1:B:831:ASP:CG	1:B:832:PHE:H	2.27	0.42
1:A:764:LEU:HD23	1:A:764:LEU:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:788:GLN:C	1:A:792:ASN:ND2	2.78	0.42
1:B:700:GLY:C	1:B:701:THR:HG23	2.44	0.42
1:B:702:VAL:CG1	1:B:703:TYR:N	2.77	0.42
1:B:881:TRP:CZ3	1:B:888:SER:O	2.73	0.42
2:C:354:PRO:HB2	2:D:339:PRO:HA	2.02	0.42
1:A:777:TYR:CD1	1:A:781:HIS:CD2	3.07	0.42
1:A:788:GLN:O	1:A:792:ASN:ND2	2.52	0.42
2:C:354:PRO:O	2:C:355:ASP:C	2.61	0.42
1:A:890:PRO:O	1:A:891:TYR:CD1	2.71	0.42
1:B:770:PRO:HG2	1:B:771:PHE:N	2.34	0.42
1:B:788:GLN:HE21	1:B:792:ASN:ND2	2.14	0.42
1:B:946:LYS:O	1:B:947:MET:C	2.63	0.42
1:A:749:HIS:C	1:A:750:VAL:HG23	2.44	0.41
1:A:819:VAL:CG1	1:A:828:LYS:O	2.68	0.41
1:A:874:TRP:O	1:A:874:TRP:HD1	2.03	0.41
1:B:916:THR:HG23	1:B:954:TYR:O	2.19	0.41
1:A:819:VAL:HG12	1:A:828:LYS:O	2.19	0.41
1:B:870:GLN:O	1:B:873:VAL:HB	2.20	0.41
1:A:785:ILE:HG21	1:A:790:LEU:HG	2.03	0.41
1:B:914:ILE:O	1:B:914:ILE:HG13	2.20	0.41
1:B:912:PRO:CG	1:B:915:CYS:SG	3.09	0.41
1:A:859:LEU:HD12	1:A:859:LEU:HA	1.71	0.41
1:A:876:TYR:CE1	1:A:880:VAL:CG2	3.04	0.41
1:A:878:VAL:O	1:A:881:TRP:HB3	2.19	0.41
1:A:920:TYR:CE2	1:A:924:VAL:HG21	2.56	0.41
1:B:831:ASP:CG	1:B:832:PHE:N	2.79	0.41
1:B:690:LYS:O	1:B:690:LYS:HD2	2.21	0.41
1:B:748:PRO:O	1:B:828:LYS:HG2	2.21	0.41
1:A:877:GLY:O	1:A:923:MET:CE	2.69	0.41
1:A:885:THR:HB	1:A:888:SER:OG	2.21	0.41
1:B:815:ALA:CA	1:B:879:THR:HG23	2.50	0.41
1:B:912:PRO:C	1:B:914:ILE:H	2.29	0.41
1:A:770:PRO:CG	1:A:771:PHE:H	2.31	0.41
1:A:957:ILE:H	1:A:957:ILE:HG13	1.77	0.41
2:D:341:TYR:CE2	2:D:347:PRO:HD3	2.52	0.41
2:D:341:TYR:CD2	2:D:345:VAL:O	2.68	0.41
2:D:346:MET:HA	2:D:347:PRO:HD2	1.81	0.41
1:A:788:GLN:CG	1:A:789:TYR:N	2.83	0.41
1:A:881:TRP:CZ2	2:C:346:MET:HE1	2.56	0.41
1:A:917:ILE:HG23	2:C:337:SER:O	2.21	0.41
1:B:784:ASN:HD22	1:B:784:ASN:HA	1.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:909:LEU:H	1:B:909:LEU:CD1	2.32	0.41
1:A:796:GLN:HA	1:A:799:LYS:HD2	2.04	0.40
1:A:916:THR:HA	2:C:337:SER:O	2.21	0.40
1:B:756:ILE:O	1:B:756:ILE:HG23	2.20	0.40
2:D:341:TYR:N	2:D:341:TYR:HD1	2.18	0.40
1:A:868:THR:C	1:A:870:GLN:N	2.76	0.40
1:A:890:PRO:O	1:A:891:TYR:HB2	2.22	0.40
1:B:742:MET:HA	1:B:745:VAL:CG1	2.51	0.40
1:B:771:PHE:HD2	1:B:821:VAL:O	2.04	0.40
1:B:774:LEU:O	1:B:777:TYR:HB3	2.21	0.40
1:B:790:LEU:HD23	1:B:793:TRP:HZ3	1.86	0.40
1:A:850:GLY:O	1:A:851:LYS:HB3	2.22	0.40
1:B:793:TRP:CD1	1:B:827:VAL:CG2	3.02	0.40
1:B:884:MET:C	1:B:886:PHE:H	2.30	0.40
2:C:346:MET:HA	2:C:347:PRO:HD2	1.96	0.40
1:A:777:TYR:C	1:A:779:ARG:N	2.78	0.40
1:A:890:PRO:C	1:A:891:TYR:HD1	2.28	0.40
1:B:881:TRP:HA	1:B:923:MET:HE1	2.01	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	274/330 (83%)	188 (69%)	57 (21%)	29 (11%)	0	5
1	B	259/330 (78%)	183 (71%)	54 (21%)	22 (8%)	0	7
2	C	25/65 (38%)	21 (84%)	3 (12%)	1 (4%)	2	19
2	D	24/65 (37%)	15 (62%)	8 (33%)	1 (4%)	2	19
All	All	582/790 (74%)	407 (70%)	122 (21%)	53 (9%)	0	7

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	713	LYS
1	A	730	LYS
1	A	751	CYS
1	A	788	GLN
1	A	835	ALA
1	A	840	ALA
1	A	851	LYS
1	B	678	ALA
1	B	679	LEU
1	B	767	GLN
1	B	892	ASP
1	B	959	GLY
2	C	343	ASN
2	D	345	VAL
1	A	685	GLU
1	A	712	GLU
1	A	767	GLN
1	A	770	PRO
1	A	836	LYS
1	A	895	PRO
1	B	691	ILE
1	B	732	ASN
1	B	873	VAL
1	A	710	GLU
1	A	735	ILE
1	A	792	ASN
1	A	808	ARG
1	A	852	VAL
1	A	858	ALA
1	A	892	ASP
1	B	688	PHE
1	B	768	LEU
1	B	815	ALA
1	B	855	LYS
1	A	679	LEU
1	A	742	MET
1	A	744	SER
1	A	793	TRP
1	B	687	GLU
1	B	770	PRO
1	A	676	ASN
1	A	709	PRO
1	A	855	LYS

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Mol	Chain	Res	Type
1	B	680	LEU
1	B	685	GLU
1	B	885	THR
1	B	951	PRO
1	B	960	ASP
1	B	717	PRO
1	B	797	ILE
1	B	913	PRO
1	A	917	ILE
1	A	691	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	203/288 (70%)	183 (90%)	20 (10%)	7	29
1	B	200/288 (69%)	182 (91%)	18 (9%)	9	32
2	C	18/58 (31%)	18 (100%)	0	100	100
2	D	16/58 (28%)	15 (94%)	1 (6%)	16	42
All	All	437/692 (63%)	398 (91%)	39 (9%)	9	32

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	708	ILE
1	A	745	VAL
1	A	761	THR
1	A	766	THR
1	A	809	LEU
1	A	814	LEU
1	A	819	VAL
1	A	823	THR
1	A	827	VAL
1	A	834	LEU
1	A	857	MET

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Mol	Chain	Res	Type
1	A	865	ARG
1	A	895	PRO
1	A	901	SER
1	A	913	PRO
1	A	914	ILE
1	A	918	ASP
1	A	919	VAL
1	A	941	ILE
1	A	957	ILE
1	B	690	LYS
1	B	702	VAL
1	B	734	GLU
1	B	741	VAL
1	B	750	VAL
1	B	751	CYS
1	B	759	THR
1	B	769	MET
1	B	784	ASN
1	B	795	VAL
1	B	821	VAL
1	B	827	VAL
1	B	862	ILE
1	B	875	SER
1	B	879	THR
1	B	909	LEU
1	B	914	ILE
1	B	957	ILE
2	D	346	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	788	GLN
1	A	792	ASN
1	A	802	ASN
1	A	811	HIS
1	A	911	GLN
1	B	749	HIS
1	B	781	HIS
1	B	784	ASN
1	B	788	GLN
1	B	802	ASN

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Mol	Chain	Res	Type
1	B	811	HIS
1	B	825	GLN
1	B	911	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 [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(Å ²)	Q<0.9
1	A	280/330 (84%)	0.15	1 (0%) 88 72	24, 62, 106, 126	0
1	B	269/330 (81%)	0.23	4 (1%) 72 47	41, 71, 102, 111	0
2	C	27/65 (41%)	0.65	1 (3%) 45 25	71, 84, 98, 100	0
2	D	26/65 (40%)	0.42	0 100 100	68, 83, 92, 102	0
All	All	602/790 (76%)	0.22	6 (0%) 79 56	24, 70, 102, 126	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	961	GLU	2.9
1	B	952	GLN	2.8
1	B	731	ALA	2.4
2	C	340	SER	2.3
1	A	956	VAL	2.0
1	B	682	ILE	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.