



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:10 AM GMT

PDB ID : 1ZYC  
Title : Crystal Structure of eIF2alpha Protein Kinase GCN2: Wild-Type in Apo Form.  
Authors : Padyana, A.K.; Qiu, H.; Roll-Mecak, A.; Hinnebusch, A.G.; Burley, S.K.  
Deposited on : 2005-06-09  
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

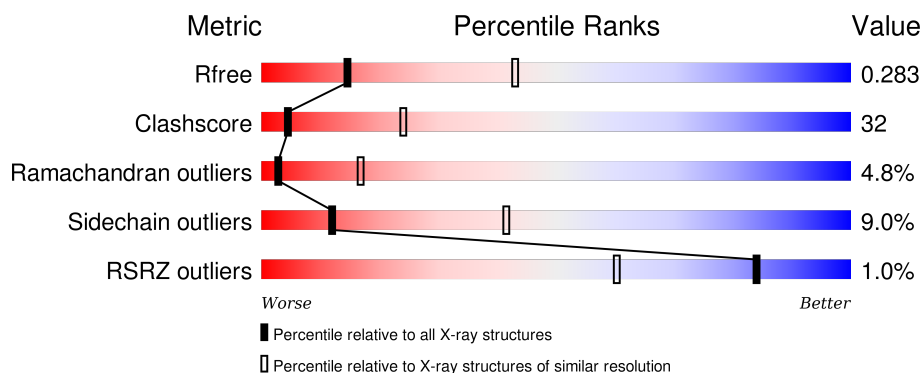
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	303	<div> <div></div> <div>42%37%8%14%</div> </div>
1	B	303	<div> <div>%</div> <div>42%34%8%16%</div> </div>
1	C	303	<div> <div></div> <div>38%43%7%11%</div> </div>
1	D	303	<div> <div>2%</div> <div>36%40%8%16%</div> </div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 8601 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 Serine/threonine-protein kinase GCN2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	5	0	0
			2153	1378	375	391	9			
1	B	254	Total	C	N	O	S	0	0	0
			2091	1341	364	377	9			
1	C	271	Total	C	N	O	S	0	0	0
			2235	1435	388	403	9			
1	D	256	Total	C	N	O	S	0	0	0
			2108	1352	366	381	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	592	SER	-	CLONING ARTIFACT	UNP P15442
A	593	LEU	-	CLONING ARTIFACT	UNP P15442
B	592	SER	-	CLONING ARTIFACT	UNP P15442
B	593	LEU	-	CLONING ARTIFACT	UNP P15442
C	592	SER	-	CLONING ARTIFACT	UNP P15442
C	593	LEU	-	CLONING ARTIFACT	UNP P15442
D	592	SER	-	CLONING ARTIFACT	UNP P15442
D	593	LEU	-	CLONING ARTIFACT	UNP P15442

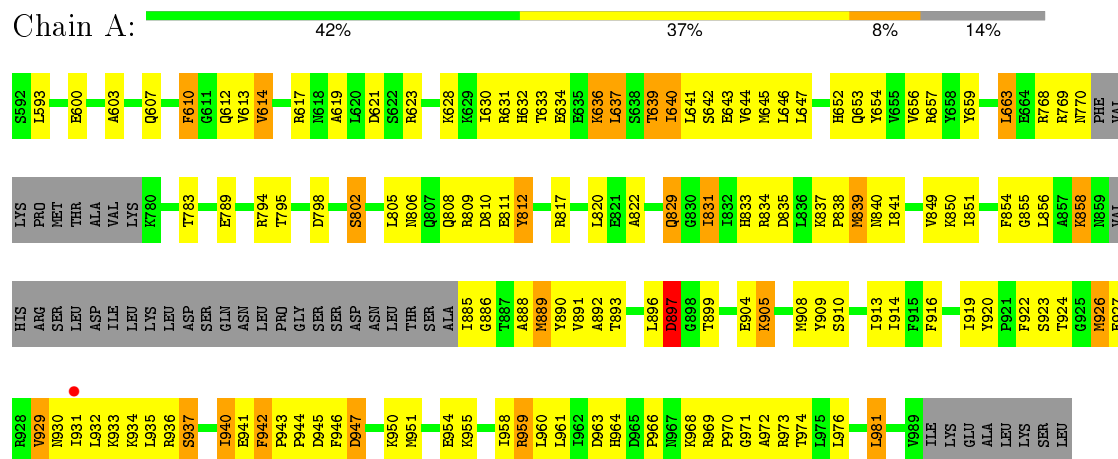
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	O	0	0
			3	3		
2	B	6	Total	O	0	0
			6	6		
2	C	5	Total	O	0	0
			5	5		

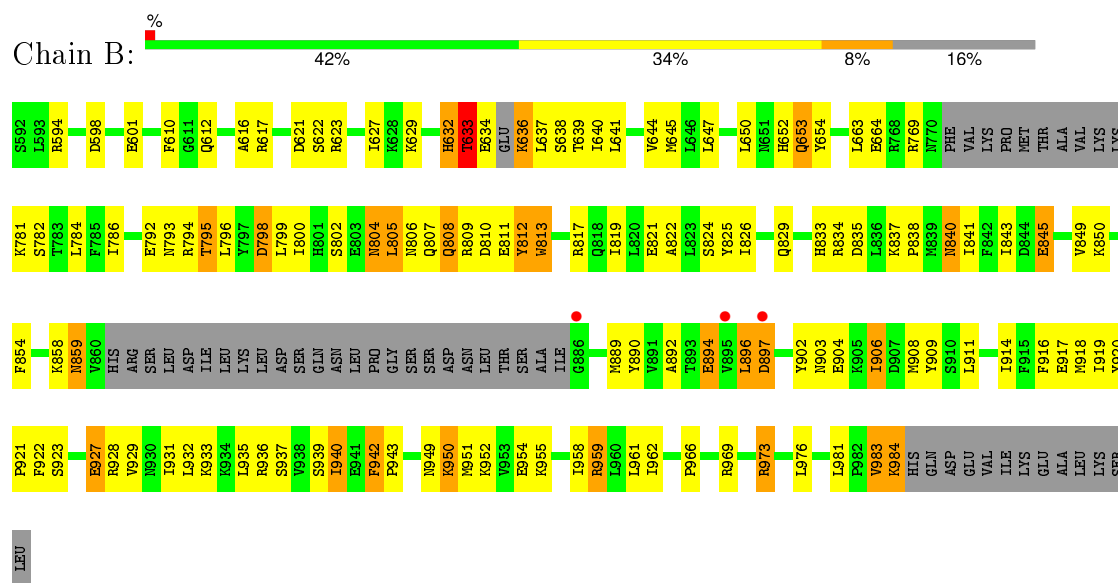
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Serine/threonine-protein kinase GCN2

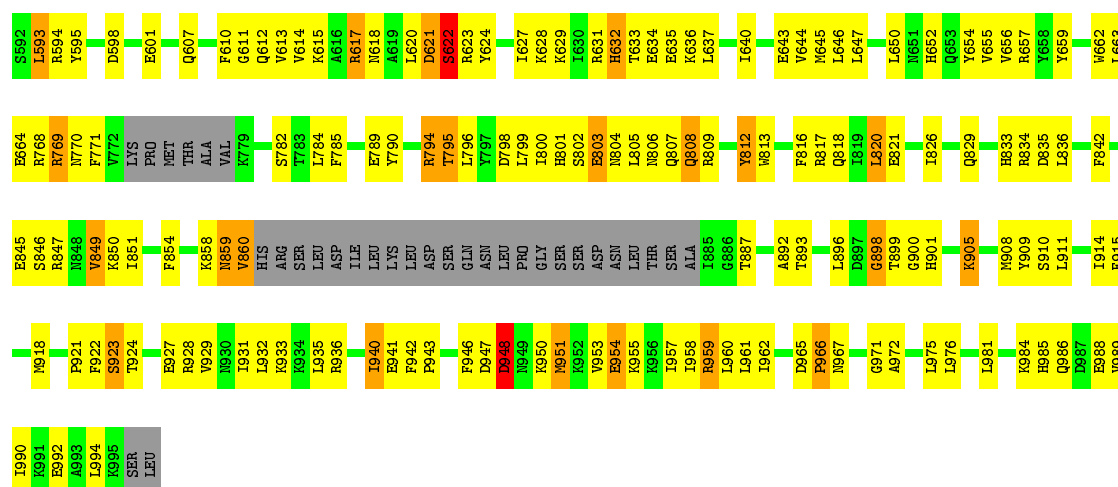


#### • Molecule 1: Serine/threonine-protein kinase GCN2

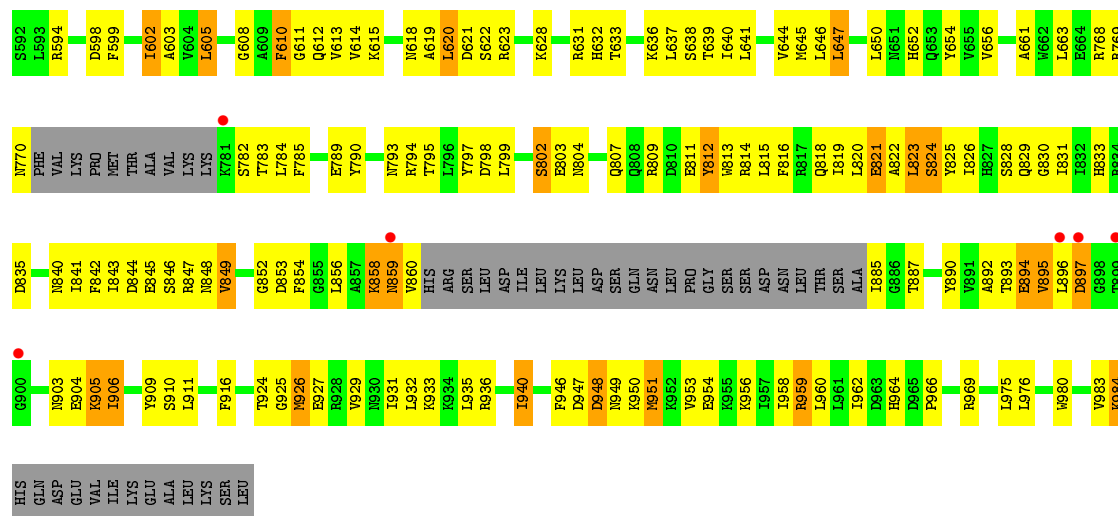


#### • Molecule 1: Serine/threonine-protein kinase GCN2





● Molecule 1: Serine/threonine-protein kinase GCN2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.89Å 95.70Å 175.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.99 – 3.00 41.99 – 2.81	Depositor EDS
% Data completeness (in resolution range)	94.6 (41.99-3.00) 93.1 (41.99-2.81)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 2.81Å)	Xtriage
Refinement program	CNX 2000.1	Depositor
R, $R_{free}$	0.234 , 0.299 0.226 , 0.283	Depositor DCC
$R_{free}$ test set	562 reflections (2.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	81.8	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 68.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 31126 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8601	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.32% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.46	0/2196	0.71	1/2956 (0.0%)
1	B	0.45	0/2132	0.76	4/2869 (0.1%)
1	C	0.46	0/2279	0.71	2/3066 (0.1%)
1	D	0.46	0/2150	0.70	0/2895
All	All	0.46	0/8757	0.72	7/11786 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	633	THR	N-CA-C	11.42	141.84	111.00
1	C	898	GLY	N-CA-C	-8.85	90.99	113.10
1	C	820	LEU	CA-CB-CG	-6.17	101.10	115.30
1	B	859	ASN	N-CA-C	5.95	127.07	111.00
1	A	858	LYS	N-CA-C	5.81	126.68	111.00
1	B	633	THR	CB-CA-C	-5.11	97.80	111.60
1	B	633	THR	C-N-CA	5.04	134.29	121.70

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2153	0	2160	133	0
1	B	2091	0	2104	144	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2235	0	2259	158	0
1	D	2108	0	2122	142	0
2	A	3	0	0	0	0
2	B	6	0	0	1	0
2	C	5	0	0	0	0
All	All	8601	0	8645	559	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 32.

All (559) 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:D:924:THR:HG22	1:D:926:MET:H	1.09	1.14
1:B:769:ARG:HB3	1:B:769:ARG:HH11	1.22	1.00
1:B:769:ARG:NH1	1:B:769:ARG:HB3	1.78	0.97
1:D:858:LYS:HD2	1:D:858:LYS:H	1.34	0.92
1:C:657:ARG:HB2	1:C:789:GLU:HB2	1.52	0.92
1:C:593:LEU:HD23	1:C:664:GLU:HB3	1.48	0.92
1:C:940:ILE:HG13	1:C:959:ARG:HH22	1.36	0.91
1:C:976:LEU:HA	1:C:981:LEU:HD12	1.52	0.91
1:B:769:ARG:HG3	1:B:782:SER:HA	1.51	0.91
1:D:959:ARG:O	1:D:959:ARG:HD3	1.71	0.90
1:A:806:ASN:HB2	1:A:919:ILE:O	1.73	0.89
1:B:909:TYR:HB2	1:B:969:ARG:HH11	1.41	0.85
1:A:885:ILE:HD11	1:A:888:ALA:HB3	1.58	0.85
1:B:983:VAL:O	1:B:984:LYS:HB2	1.76	0.84
1:A:932:LEU:HA	1:A:935:LEU:HD12	1.60	0.84
1:B:929:VAL:O	1:B:933:LYS:HB2	1.78	0.84
1:B:634:GLU:O	1:B:637:LEU:HB2	1.78	0.83
1:B:932:LEU:HA	1:B:935:LEU:HD12	1.62	0.81
1:B:805:LEU:HA	1:B:808:GLN:HE22	1.45	0.81
1:B:798:ASP:O	1:B:802:SER:HB3	1.79	0.81
1:B:909:TYR:HB2	1:B:969:ARG:NH1	1.96	0.80
1:B:633:THR:O	1:B:781:LYS:HG2	1.80	0.80
1:A:940:ILE:HG21	1:A:959:ARG:NH2	1.96	0.80
1:D:893:THR:HG21	1:D:964:HIS:ND1	1.97	0.79
1:B:894:GLU:OE2	1:B:966:PRO:HB3	1.84	0.77
1:A:652:HIS:CD2	1:A:653:GLN:H	2.02	0.77
1:C:976:LEU:HA	1:C:981:LEU:CD1	2.14	0.77
1:A:940:ILE:HG21	1:A:959:ARG:HH22	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:859:ASN:O	1:C:860:VAL:HG13	1.84	0.76
1:A:628:LYS:HD3	1:A:630:ILE:HD11	1.65	0.76
1:D:951:MET:HG3	1:D:954:GLU:HG3	1.67	0.76
1:B:894:GLU:OE1	1:B:906:ILE:HG22	1.86	0.75
1:C:928:ARG:NH1	1:C:932:LEU:HD11	2.01	0.75
1:D:599:PHE:CE2	1:D:618:ASN:HB2	2.21	0.75
1:D:924:THR:HG22	1:D:926:MET:N	1.95	0.75
1:B:809:ARG:HA	1:B:812:TYR:CE2	2.22	0.75
1:D:847:ARG:HB3	1:D:847:ARG:HH11	1.51	0.74
1:B:958:ILE:O	1:B:962:ILE:HG12	1.87	0.74
1:D:858:LYS:HD2	1:D:858:LYS:N	2.03	0.73
1:C:806:ASN:ND2	1:C:921:PRO:HB3	2.05	0.72
1:A:910:SER:O	1:A:914:ILE:HG13	1.88	0.72
1:D:903:ASN:O	1:D:906:ILE:HG22	1.89	0.72
1:D:605:LEU:HD21	1:D:615:LYS:HB2	1.69	0.72
1:A:940:ILE:HG13	1:A:959:ARG:HH12	1.55	0.72
1:C:601:GLU:OE1	1:C:614:VAL:HG21	1.90	0.71
1:B:769:ARG:HG3	1:B:782:SER:CA	2.20	0.71
1:C:922:PHE:CD2	1:C:928:ARG:HG3	2.26	0.71
1:A:923:SER:HB3	1:A:927:GLU:OE2	1.91	0.71
1:D:893:THR:HG21	1:D:964:HIS:CE1	2.26	0.71
1:B:845:GLU:CD	1:B:845:GLU:H	1.92	0.71
1:A:657:ARG:HH22	1:B:594:ARG:HD2	1.55	0.71
1:A:839:MET:HE3	1:A:839:MET:H	1.56	0.71
1:D:608:GLY:HA3	1:D:611:GLY:O	1.91	0.71
1:D:615:LYS:HG3	1:D:790:TYR:CE1	2.26	0.70
1:B:637:LEU:HD21	1:B:663:LEU:HD21	1.73	0.70
1:D:905:LYS:HE2	1:D:969:ARG:O	1.91	0.70
1:D:650:LEU:HD11	1:D:831:ILE:HD12	1.74	0.70
1:B:769:ARG:CG	1:B:782:SER:HA	2.22	0.70
1:B:799:LEU:HD11	1:B:843:ILE:HG13	1.73	0.69
1:B:894:GLU:OE2	1:B:969:ARG:NH2	2.26	0.69
1:C:946:PHE:CE2	1:C:955:LYS:HD2	2.27	0.69
1:A:926:MET:HA	1:A:929:VAL:HG23	1.75	0.69
1:C:806:ASN:HB2	1:C:921:PRO:HD3	1.74	0.68
1:D:840:ASN:HD22	1:D:853:ASP:HB2	1.59	0.68
1:C:799:LEU:HB3	1:C:805:LEU:HD22	1.74	0.68
1:A:805:LEU:HG	1:A:805:LEU:O	1.92	0.68
1:C:806:ASN:CG	1:C:921:PRO:HB3	2.14	0.68
1:D:605:LEU:H	1:D:605:LEU:HD12	1.56	0.68
1:D:959:ARG:C	1:D:959:ARG:HD3	2.13	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:653:GLN:O	1:A:850:LYS:HE3	1.94	0.67
1:A:973:ARG:NH1	1:A:976:LEU:HD13	2.09	0.67
1:C:771:PHE:CE2	1:D:830:GLY:HA3	2.30	0.67
1:A:811:GLU:OE2	1:A:811:GLU:HA	1.95	0.67
1:B:940:ILE:HD13	1:B:959:ARG:NH1	2.10	0.67
1:C:959:ARG:HD3	1:C:959:ARG:O	1.94	0.67
1:B:796:LEU:HA	1:B:799:LEU:HD13	1.78	0.66
1:B:955:LYS:O	1:B:959:ARG:HB2	1.96	0.66
1:D:892:ALA:HA	1:D:909:TYR:CD2	2.30	0.66
1:C:985:HIS:HD2	1:C:986:GLN:H	1.43	0.66
1:B:903:ASN:O	1:B:906:ILE:HG23	1.96	0.66
1:C:923:SER:OG	1:C:924:THR:HG23	1.95	0.66
1:D:640:ILE:O	1:D:644:VAL:HG23	1.95	0.66
1:B:806:ASN:ND2	1:B:921:PRO:HB3	2.10	0.66
1:A:942:PHE:HB3	1:A:943:PRO:HD2	1.78	0.66
1:B:616:ALA:HB3	1:B:627:ILE:HD13	1.78	0.65
1:B:805:LEU:HA	1:B:808:GLN:NE2	2.11	0.65
1:B:809:ARG:HA	1:B:812:TYR:CZ	2.32	0.65
1:B:769:ARG:CB	1:B:769:ARG:HH11	2.02	0.65
1:A:886:GLY:O	1:A:889:MET:HB2	1.97	0.65
1:B:652:HIS:HB2	1:B:825:TYR:CE2	2.31	0.65
1:B:640:ILE:O	1:B:644:VAL:HG23	1.96	0.65
1:A:971:GLY:O	1:A:974:THR:HB	1.97	0.65
1:D:940:ILE:HD11	1:D:964:HIS:CD2	2.32	0.64
1:D:847:ARG:HB3	1:D:847:ARG:NH1	2.12	0.64
1:C:833:HIS:HD2	1:C:835:ASP:H	1.45	0.64
1:D:916:PHE:HB2	1:D:958:ILE:HD13	1.80	0.64
1:A:940:ILE:CG2	1:A:959:ARG:HH22	2.10	0.64
1:C:953:VAL:C	1:C:955:LYS:H	2.02	0.63
1:A:839:MET:CE	1:A:839:MET:H	2.10	0.63
1:C:768:ARG:O	1:C:769:ARG:HD2	1.98	0.63
1:B:973:ARG:HE	1:B:973:ARG:HA	1.64	0.63
1:C:928:ARG:HH12	1:C:932:LEU:HD11	1.64	0.63
1:A:893:THR:HG21	1:A:964:HIS:CD2	2.34	0.63
1:A:795:THR:HG21	1:A:839:MET:O	1.99	0.63
1:D:610:PHE:N	1:D:610:PHE:HD2	1.96	0.63
1:D:903:ASN:O	1:D:905:LYS:N	2.32	0.62
1:D:815:LEU:HD22	1:D:849:VAL:HG12	1.81	0.62
1:C:613:VAL:CG2	1:C:628:LYS:HD2	2.30	0.62
1:A:795:THR:HB	1:A:838:PRO:O	1.99	0.62
1:B:961:LEU:O	1:B:969:ARG:HD3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:816:PHE:CE2	1:C:820:LEU:HD11	2.34	0.62
1:A:896:LEU:O	1:A:897:ASP:HB2	1.99	0.62
1:B:664:GLU:O	1:B:782:SER:HB3	1.99	0.62
1:C:633:THR:OG1	1:C:636:LYS:HB2	1.99	0.62
1:B:641:LEU:O	1:B:645:MET:HG2	1.99	0.61
1:A:943:PRO:HG2	1:A:946:PHE:HB2	1.81	0.61
1:D:641:LEU:O	1:D:645:MET:HG2	2.00	0.61
1:D:903:ASN:ND2	1:D:905:LYS:HB2	2.15	0.61
1:C:771:PHE:HE2	1:D:830:GLY:HA3	1.65	0.61
1:C:946:PHE:O	1:C:948:ASP:N	2.34	0.61
1:D:647:LEU:HD12	1:D:831:ILE:HD13	1.82	0.61
1:A:641:LEU:HA	1:A:644:VAL:HG12	1.81	0.61
1:C:652:HIS:HD2	1:C:654:TYR:H	1.48	0.61
1:A:632:HIS:CD2	1:A:633:THR:H	2.19	0.61
1:C:985:HIS:CD2	1:C:986:GLN:H	2.19	0.61
1:D:798:ASP:O	1:D:802:SER:HB2	2.00	0.61
1:C:851:ILE:HD12	1:C:851:ILE:N	2.16	0.61
1:B:919:ILE:HG13	1:B:920:TYR:N	2.16	0.61
1:B:804:ASN:HD22	1:B:807:GLN:HB2	1.66	0.61
1:C:652:HIS:CD2	1:C:654:TYR:H	2.19	0.61
1:B:799:LEU:CD1	1:B:843:ILE:HG13	2.31	0.60
1:B:805:LEU:HD22	1:B:812:TYR:HB3	1.83	0.60
1:C:957:ILE:O	1:C:960:LEU:N	2.32	0.60
1:A:932:LEU:O	1:A:935:LEU:N	2.34	0.60
1:D:613:VAL:HG22	1:D:628:LYS:HG3	1.83	0.60
1:A:833:HIS:O	1:A:834:ARG:HB2	2.01	0.60
1:C:656:VAL:HG13	1:C:789:GLU:HB3	1.83	0.60
1:B:634:GLU:O	1:B:637:LEU:CB	2.50	0.60
1:C:613:VAL:HG22	1:C:628:LYS:HD2	1.84	0.60
1:D:951:MET:HG3	1:D:954:GLU:CG	2.32	0.60
1:D:799:LEU:HA	1:D:803:GLU:HG3	1.84	0.59
1:D:610:PHE:N	1:D:610:PHE:CD2	2.68	0.59
1:A:892:ALA:HA	1:A:909:TYR:CD2	2.36	0.59
1:A:899:THR:HG22	1:A:899:THR:O	2.03	0.59
1:B:650:LEU:HD22	1:B:825:TYR:CE2	2.37	0.59
1:A:645:MET:SD	1:B:641:LEU:HD22	2.42	0.59
1:D:768:ARG:HG2	1:D:782:SER:OG	2.02	0.59
1:D:602:ILE:HG22	1:D:603:ALA:N	2.17	0.59
1:B:902:TYR:HB2	1:B:906:ILE:HG21	1.85	0.59
1:C:922:PHE:CE2	1:C:928:ARG:HG3	2.38	0.59
1:C:909:TYR:HA	1:C:961:LEU:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:796:LEU:O	1:C:800:ILE:HG13	2.02	0.58
1:B:633:THR:HB	1:B:637:LEU:HD13	1.85	0.58
1:C:634:GLU:HG3	1:C:782:SER:OG	2.02	0.58
1:B:637:LEU:C	1:B:639:THR:H	2.07	0.58
1:C:615:LYS:HD3	1:C:790:TYR:CE1	2.37	0.58
1:C:812:TYR:C	1:C:812:TYR:CD1	2.77	0.58
1:B:981:LEU:N	1:B:981:LEU:HD12	2.19	0.58
1:A:641:LEU:O	1:A:645:MET:HG2	2.03	0.58
1:A:961:LEU:O	1:A:969:ARG:HD2	2.03	0.58
1:A:909:TYR:HA	1:A:961:LEU:O	2.04	0.57
1:C:632:HIS:CE1	1:C:636:LYS:HG2	2.39	0.57
1:B:896:LEU:O	1:B:897:ASP:C	2.41	0.57
1:C:931:ILE:HD12	1:C:943:PRO:HB3	1.86	0.57
1:D:815:LEU:HD22	1:D:849:VAL:CG1	2.34	0.57
1:C:957:ILE:O	1:C:960:LEU:HB2	2.04	0.57
1:D:631:ARG:HD2	1:D:783:THR:HG22	1.85	0.57
1:D:896:LEU:O	1:D:897:ASP:HB2	2.03	0.57
1:D:841:ILE:O	1:D:841:ILE:HG22	2.05	0.57
1:A:631:ARG:CB	1:A:783:THR:HG22	2.35	0.57
1:D:947:ASP:CG	1:D:950:LYS:HB3	2.25	0.57
1:D:823:LEU:O	1:D:826:ILE:N	2.37	0.57
1:C:976:LEU:HD23	1:C:981:LEU:HD11	1.86	0.56
1:D:840:ASN:HD22	1:D:853:ASP:CB	2.18	0.56
1:C:986:GLN:O	1:C:989:VAL:HB	2.05	0.56
1:D:809:ARG:HA	1:D:812:TYR:CE2	2.39	0.56
1:D:925:GLY:O	1:D:929:VAL:HG23	2.06	0.56
1:B:908:MET:O	1:B:961:LEU:HD22	2.05	0.56
1:B:889:MET:HG2	1:B:932:LEU:HD12	1.87	0.56
1:B:966:PRO:O	1:B:969:ARG:HB2	2.06	0.56
1:B:799:LEU:HD12	1:B:799:LEU:N	2.19	0.56
1:C:812:TYR:C	1:C:812:TYR:HD1	2.09	0.56
1:B:838:PRO:HD3	1:B:890:TYR:CE2	2.40	0.56
1:D:816:PHE:CE1	1:D:911:LEU:HD11	2.40	0.56
1:B:984:LYS:HA	1:B:984:LYS:NZ	2.21	0.56
1:D:852:GLY:O	1:D:853:ASP:HB2	2.04	0.56
1:B:645:MET:HA	1:B:645:MET:HE2	1.86	0.56
1:D:844:ASP:C	1:D:846:SER:H	2.10	0.56
1:D:894:GLU:OE1	1:D:966:PRO:HB3	2.06	0.56
1:D:618:ASN:HB3	1:D:621:ASP:OD1	2.07	0.55
1:C:985:HIS:CD2	1:C:986:GLN:N	2.74	0.55
1:D:983:VAL:O	1:D:984:LYS:CB	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:ASP:OD2	1:A:623:ARG:HB2	2.06	0.55
1:C:932:LEU:O	1:C:935:LEU:N	2.36	0.55
1:C:617:ARG:HH11	1:C:617:ARG:HG3	1.71	0.55
1:A:617:ARG:NH2	1:C:893:THR:HG22	2.21	0.55
1:D:820:LEU:HB2	1:D:976:LEU:HD21	1.88	0.55
1:D:903:ASN:HD21	1:D:905:LYS:HB2	1.72	0.55
1:D:594:ARG:O	1:D:598:ASP:HB2	2.07	0.55
1:A:645:MET:HB3	1:B:663:LEU:HB2	1.88	0.55
1:B:633:THR:O	1:B:781:LYS:CG	2.54	0.55
1:C:657:ARG:HB3	1:C:659:TYR:CE2	2.41	0.55
1:C:769:ARG:C	1:C:771:PHE:H	2.10	0.55
1:B:811:GLU:HA	1:B:811:GLU:OE2	2.07	0.55
1:C:657:ARG:HE	1:C:659:TYR:HE2	1.53	0.55
1:C:769:ARG:O	1:C:771:PHE:N	2.40	0.55
1:C:621:ASP:C	1:C:621:ASP:OD1	2.45	0.55
1:B:627:ILE:N	1:B:627:ILE:HD12	2.23	0.54
1:C:800:ILE:HG22	1:C:801:HIS:HD2	1.72	0.54
1:A:768:ARG:HD2	1:B:829:GLN:O	2.07	0.54
1:A:839:MET:CE	1:A:839:MET:N	2.70	0.54
1:A:632:HIS:CD2	1:A:633:THR:HG23	2.42	0.54
1:B:922:PHE:CE2	1:B:931:ILE:HD12	2.42	0.54
1:C:923:SER:HB3	1:C:927:GLU:HG3	1.90	0.54
1:A:808:GLN:O	1:A:811:GLU:N	2.41	0.54
1:D:811:GLU:HA	1:D:811:GLU:OE1	2.07	0.54
1:A:919:ILE:HG13	1:A:920:TYR:N	2.23	0.54
1:B:805:LEU:CA	1:B:808:GLN:HE22	2.19	0.54
1:B:795:THR:HG23	1:B:798:ASP:OD1	2.08	0.54
1:B:819:ILE:HG21	1:B:911:LEU:HD13	1.90	0.54
1:D:814:ARG:NH1	1:D:847:ARG:O	2.33	0.54
1:C:800:ILE:HG22	1:C:801:HIS:CD2	2.43	0.54
1:B:784:LEU:C	1:B:784:LEU:HD23	2.28	0.53
1:C:935:LEU:HD12	1:C:941:GLU:O	2.07	0.53
1:B:769:ARG:CD	1:B:782:SER:HA	2.39	0.53
1:D:983:VAL:O	1:D:984:LYS:HB3	2.09	0.53
1:B:800:ILE:HD13	1:B:917:GLU:HB3	1.90	0.53
1:C:946:PHE:CD2	1:C:955:LYS:HD2	2.44	0.53
1:A:632:HIS:HB3	1:A:637:LEU:HD13	1.91	0.53
1:D:612:GLN:HE21	1:D:614:VAL:CG1	2.21	0.53
1:B:769:ARG:HG3	1:B:782:SER:CB	2.39	0.53
1:A:933:LYS:HB2	1:A:933:LYS:NZ	2.23	0.53
1:A:934:LYS:HD2	1:A:941:GLU:OE1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:605:LEU:H	1:D:605:LEU:CD1	2.17	0.53
1:C:645:MET:CE	1:D:641:LEU:HD22	2.39	0.53
1:D:804:ASN:HB3	1:D:807:GLN:NE2	2.23	0.53
1:D:983:VAL:O	1:D:984:LYS:HG2	2.09	0.52
1:A:885:ILE:HG12	1:A:886:GLY:N	2.24	0.52
1:A:817:ARG:NH1	1:A:981:LEU:HB3	2.23	0.52
1:C:640:ILE:O	1:C:644:VAL:HG23	2.08	0.52
1:A:909:TYR:CE2	1:A:913:ILE:HD11	2.45	0.52
1:C:950:LYS:HE3	1:C:951:MET:HE2	1.90	0.52
1:A:653:GLN:HG3	1:A:654:TYR:CD2	2.45	0.52
1:B:845:GLU:CD	1:B:845:GLU:N	2.61	0.52
1:B:647:LEU:HD21	1:B:854:PHE:CD2	2.44	0.52
1:D:816:PHE:HE1	1:D:911:LEU:HD11	1.74	0.52
1:B:835:ASP:OD2	1:B:837:LYS:HE2	2.09	0.52
1:D:799:LEU:HD11	1:D:843:ILE:HG13	1.92	0.52
1:A:628:LYS:HD3	1:A:630:ILE:CD1	2.38	0.52
1:C:595:TYR:HE1	1:C:627:ILE:CD1	2.23	0.52
1:D:940:ILE:HD13	1:D:959:ARG:NH1	2.25	0.52
1:A:637:LEU:O	1:A:640:ILE:HG12	2.10	0.52
1:B:904:GLU:N	1:B:904:GLU:OE2	2.40	0.51
1:B:799:LEU:HD12	1:B:799:LEU:H	1.75	0.51
1:C:769:ARG:C	1:C:771:PHE:N	2.64	0.51
1:A:841:ILE:O	1:A:841:ILE:HG22	2.09	0.51
1:A:930:ASN:O	1:A:933:LYS:N	2.43	0.51
1:A:934:LYS:O	1:A:937:SER:HB3	2.11	0.51
1:A:922:PHE:CZ	1:A:932:LEU:HD11	2.45	0.51
1:C:931:ILE:O	1:C:935:LEU:HD13	2.11	0.51
1:C:836:LEU:HB3	1:C:910:SER:OG	2.10	0.51
1:C:908:MET:HE1	1:C:972:ALA:HA	1.93	0.51
1:B:645:MET:HA	1:B:645:MET:CE	2.41	0.51
1:A:837:LYS:HB2	1:A:837:LYS:NZ	2.25	0.51
1:C:940:ILE:HG13	1:C:959:ARG:NH2	2.18	0.51
1:C:656:VAL:HG23	1:C:851:ILE:O	2.10	0.50
1:D:783:THR:OG1	1:D:785:PHE:CE1	2.62	0.50
1:C:794:ARG:NH1	1:C:847:ARG:HH21	2.08	0.50
1:B:942:PHE:CD2	1:B:942:PHE:N	2.79	0.50
1:A:628:LYS:CD	1:A:630:ILE:HD11	2.39	0.50
1:A:632:HIS:CD2	1:A:636:LYS:HG3	2.46	0.50
1:C:621:ASP:O	1:C:622:SER:HB2	2.10	0.50
1:D:894:GLU:OE1	1:D:969:ARG:NH2	2.45	0.50
1:D:605:LEU:CD1	1:D:613:VAL:HG12	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:841:ILE:O	1:B:841:ILE:HG22	2.11	0.50
1:B:610:PHE:CD2	1:B:610:PHE:N	2.79	0.50
1:A:908:MET:HE2	1:A:972:ALA:N	2.26	0.50
1:B:942:PHE:HD2	1:B:942:PHE:N	2.09	0.50
1:A:942:PHE:N	1:A:942:PHE:CD1	2.79	0.50
1:B:632:HIS:CD2	1:B:632:HIS:O	2.64	0.50
1:C:915:PHE:O	1:C:918:MET:HB2	2.11	0.50
1:B:652:HIS:CD2	1:B:654:TYR:H	2.30	0.50
1:A:634:GLU:HA	1:A:634:GLU:OE2	2.12	0.50
1:D:799:LEU:HD22	1:D:847:ARG:NH2	2.27	0.50
1:B:804:ASN:O	1:B:808:GLN:NE2	2.44	0.50
1:B:612:GLN:O	1:B:629:LYS:HG2	2.11	0.50
1:C:820:LEU:HB2	1:C:976:LEU:HD21	1.92	0.49
1:A:812:TYR:CZ	1:A:919:ILE:HG22	2.47	0.49
1:B:837:LYS:H	1:B:840:ASN:HD21	1.60	0.49
1:B:954:GLU:O	1:B:958:ILE:HD12	2.12	0.49
1:A:942:PHE:H	1:A:942:PHE:HD1	1.60	0.49
1:D:858:LYS:CD	1:D:858:LYS:H	2.15	0.49
1:B:923:SER:HB2	1:B:927:GLU:OE2	2.12	0.49
1:A:942:PHE:HD1	1:A:942:PHE:N	2.11	0.49
1:A:888:ALA:HA	1:A:891:VAL:HG13	1.93	0.49
1:B:817:ARG:O	1:B:821:GLU:HG2	2.12	0.49
1:B:634:GLU:OE2	1:B:781:LYS:N	2.45	0.49
1:B:973:ARG:HH11	1:B:976:LEU:CD1	2.26	0.48
1:D:823:LEU:O	1:D:824:SER:C	2.50	0.48
1:B:914:ILE:O	1:B:918:MET:HG3	2.12	0.48
1:D:947:ASP:C	1:D:949:ASN:H	2.16	0.48
1:C:953:VAL:C	1:C:955:LYS:N	2.66	0.48
1:C:953:VAL:HG13	1:C:954:GLU:N	2.28	0.48
1:C:655:VAL:HG22	1:C:826:ILE:HD11	1.96	0.48
1:C:965:ASP:C	1:C:967:ASN:H	2.16	0.48
1:A:619:ALA:CB	1:C:899:THR:HG21	2.43	0.48
1:D:638:SER:HA	1:D:641:LEU:HG	1.96	0.48
1:A:908:MET:CE	1:A:972:ALA:N	2.76	0.48
1:C:607:GLN:OE1	1:C:612:GLN:HB3	2.13	0.48
1:C:976:LEU:HD23	1:C:981:LEU:CD1	2.44	0.48
1:D:661:ALA:HA	1:D:785:PHE:O	2.13	0.48
1:C:950:LYS:HE3	1:C:951:MET:CE	2.44	0.48
1:C:662:TRP:O	1:C:784:LEU:HD12	2.13	0.48
1:D:903:ASN:O	1:D:906:ILE:CG2	2.60	0.48
1:C:618:ASN:HB3	1:C:621:ASP:OD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:892:ALA:HA	1:C:909:TYR:CD2	2.49	0.48
1:B:822:ALA:O	1:B:826:ILE:HG13	2.14	0.48
1:A:607:GLN:HG3	1:A:612:GLN:HG2	1.95	0.48
1:C:611:GLY:HA3	1:C:629:LYS:O	2.13	0.48
1:C:798:ASP:O	1:C:802:SER:N	2.46	0.48
1:B:892:ALA:HB1	1:B:969:ARG:HH12	1.78	0.47
1:D:795:THR:OG1	1:D:797:TYR:HB3	2.13	0.47
1:B:916:PHE:CE2	1:B:935:LEU:HD11	2.50	0.47
1:D:804:ASN:HB3	1:D:807:GLN:CD	2.35	0.47
1:A:932:LEU:HD12	1:A:932:LEU:N	2.29	0.47
1:A:849:VAL:CG1	1:A:850:LYS:N	2.77	0.47
1:D:947:ASP:O	1:D:949:ASN:N	2.47	0.47
1:A:631:ARG:HB2	1:A:783:THR:HG22	1.96	0.47
1:B:632:HIS:CG	1:B:632:HIS:O	2.67	0.47
1:D:932:LEU:O	1:D:936:ARG:HG2	2.13	0.47
1:A:940:ILE:CB	1:A:959:ARG:HH22	2.27	0.47
1:D:631:ARG:O	1:D:632:HIS:HB2	2.14	0.47
1:D:956:LYS:NZ	1:D:980:TRP:CD2	2.83	0.47
1:C:795:THR:HA	1:C:842:PHE:HA	1.96	0.47
1:D:652:HIS:HB2	1:D:825:TYR:CE2	2.50	0.47
1:D:893:THR:O	1:D:895:VAL:N	2.48	0.47
1:B:637:LEU:O	1:B:639:THR:N	2.45	0.47
1:C:645:MET:HE3	1:D:641:LEU:HD22	1.96	0.47
1:A:849:VAL:HG12	1:A:850:LYS:N	2.30	0.47
1:C:935:LEU:HD11	1:C:942:PHE:HA	1.97	0.47
1:D:924:THR:HG22	1:D:925:GLY:N	2.29	0.47
1:C:650:LEU:CD2	1:C:829:GLN:HG3	2.45	0.47
1:B:955:LYS:HA	1:B:958:ILE:HD12	1.97	0.47
1:D:960:LEU:O	1:D:969:ARG:HG3	2.15	0.47
1:C:817:ARG:O	1:C:821:GLU:HG2	2.15	0.47
1:A:963:ASP:OD1	1:A:968:LYS:HB2	2.15	0.46
1:D:619:ALA:O	1:D:621:ASP:N	2.48	0.46
1:D:844:ASP:O	1:D:846:SER:N	2.47	0.46
1:D:647:LEU:CD1	1:D:831:ILE:HD13	2.45	0.46
1:D:890:TYR:O	1:D:910:SER:HB3	2.15	0.46
1:B:920:TYR:CE2	1:B:943:PRO:HG3	2.51	0.46
1:C:957:ILE:HA	1:C:960:LEU:HD12	1.97	0.46
1:C:923:SER:OG	1:C:924:THR:N	2.45	0.46
1:B:819:ILE:CD1	1:B:841:ILE:HD13	2.45	0.46
1:B:821:GLU:O	1:B:824:SER:HB3	2.15	0.46
1:A:951:MET:HB3	1:A:954:GLU:CG	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:937:SER:C	1:B:939:SER:H	2.17	0.46
1:D:844:ASP:C	1:D:846:SER:N	2.68	0.46
1:D:654:TYR:CD1	1:D:818:GLN:HB3	2.51	0.46
1:A:603:ALA:O	1:A:614:VAL:HB	2.15	0.46
1:C:984:LYS:HE2	1:C:988:GLU:OE1	2.16	0.46
1:C:595:TYR:HE1	1:C:627:ILE:HD13	1.81	0.46
1:B:833:HIS:O	1:B:834:ARG:HB2	2.15	0.46
1:A:809:ARG:HA	1:A:812:TYR:CE2	2.51	0.46
1:B:932:LEU:O	1:B:936:ARG:HG3	2.16	0.46
1:B:942:PHE:CZ	1:B:959:ARG:HG2	2.51	0.46
1:A:959:ARG:HG2	1:A:959:ARG:HH21	1.80	0.46
1:A:959:ARG:HG2	1:A:959:ARG:NH2	2.31	0.46
1:C:621:ASP:OD1	1:C:623:ARG:N	2.49	0.46
1:C:804:ASN:N	1:C:804:ASN:ND2	2.62	0.46
1:B:892:ALA:HB2	1:B:909:TYR:CB	2.46	0.46
1:D:946:PHE:CE2	1:D:951:MET:HB3	2.51	0.46
1:D:613:VAL:CG2	1:D:628:LYS:HG3	2.46	0.46
1:D:633:THR:O	1:D:637:LEU:HG	2.16	0.46
1:A:798:ASP:O	1:A:802:SER:HB2	2.16	0.46
1:B:951:MET:HA	1:B:954:GLU:HG2	1.98	0.45
1:A:654:TYR:CB	1:A:822:ALA:HB2	2.46	0.45
1:A:794:ARG:HA	1:A:798:ASP:OD2	2.15	0.45
1:A:839:MET:HE2	1:A:839:MET:N	2.30	0.45
1:C:640:ILE:HA	1:C:643:GLU:OE1	2.17	0.45
1:B:858:LYS:HG2	1:B:902:TYR:OH	2.17	0.45
1:D:615:LYS:NZ	1:D:790:TYR:CZ	2.85	0.45
1:D:953:VAL:O	1:D:956:LYS:N	2.47	0.45
1:C:618:ASN:OD1	1:C:620:LEU:N	2.49	0.45
1:B:621:ASP:C	1:B:623:ARG:H	2.20	0.45
1:C:851:ILE:CD1	1:C:851:ILE:N	2.78	0.45
1:D:621:ASP:O	1:D:622:SER:OG	2.26	0.45
1:C:909:TYR:OH	1:C:936:ARG:HG2	2.16	0.45
1:C:617:ARG:NH1	1:C:617:ARG:HG3	2.32	0.45
1:A:805:LEU:O	1:A:812:TYR:HD2	2.00	0.45
1:A:645:MET:CB	1:B:663:LEU:HB2	2.47	0.45
1:B:937:SER:C	1:B:939:SER:N	2.70	0.45
1:C:953:VAL:O	1:C:955:LYS:N	2.49	0.45
1:B:652:HIS:HB2	1:B:825:TYR:CD2	2.52	0.45
1:B:621:ASP:O	1:B:623:ARG:N	2.50	0.45
1:B:973:ARG:HE	1:B:973:ARG:CA	2.28	0.45
1:D:769:ARG:O	1:D:770:ASN:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:818:GLN:OE1	1:C:849:VAL:HG13	2.17	0.45
1:B:950:LYS:C	1:B:952:LYS:H	2.19	0.45
1:D:924:THR:CG2	1:D:925:GLY:N	2.80	0.45
1:C:621:ASP:OD1	1:C:623:ARG:HG3	2.17	0.45
1:A:654:TYR:HB3	1:A:822:ALA:HB2	1.98	0.44
1:D:599:PHE:CD2	1:D:618:ASN:HB2	2.51	0.44
1:B:929:VAL:O	1:B:929:VAL:HG12	2.17	0.44
1:A:835:ASP:O	1:A:840:ASN:ND2	2.51	0.44
1:B:812:TYR:CZ	1:B:919:ILE:HG22	2.53	0.44
1:C:807:GLN:O	1:C:809:ARG:N	2.50	0.44
1:D:816:PHE:HE1	1:D:911:LEU:CD1	2.31	0.44
1:B:813:TRP:HA	1:B:813:TRP:CE3	2.51	0.44
1:B:637:LEU:HG	1:B:641:LEU:HG	1.98	0.44
1:D:650:LEU:CD2	1:D:829:GLN:HG3	2.48	0.44
1:C:621:ASP:OD1	1:C:623:ARG:CG	2.65	0.44
1:B:632:HIS:NE2	1:B:636:LYS:CE	2.80	0.44
1:C:929:VAL:O	1:C:929:VAL:HG12	2.17	0.44
1:C:615:LYS:HE2	1:C:624:TYR:CD2	2.52	0.44
1:D:833:HIS:HD2	1:D:835:ASP:C	2.21	0.44
1:C:990:ILE:C	1:C:992:GLU:H	2.21	0.44
1:D:927:GLU:O	1:D:931:ILE:HG13	2.17	0.44
1:B:919:ILE:HG13	1:B:920:TYR:H	1.82	0.44
1:A:963:ASP:O	1:A:969:ARG:NH1	2.50	0.44
1:A:631:ARG:O	1:A:632:HIS:HB2	2.18	0.44
1:A:916:PHE:HB2	1:A:958:ILE:HD13	1.99	0.44
1:D:950:LYS:HE3	1:D:951:MET:SD	2.58	0.44
1:D:975:LEU:HD23	1:D:975:LEU:HA	1.89	0.44
1:D:770:ASN:N	1:D:770:ASN:HD22	2.16	0.44
1:A:600:GLU:HB2	1:C:898:GLY:O	2.17	0.44
1:C:851:ILE:CD1	1:C:851:ILE:H	2.30	0.43
1:D:656:VAL:HG13	1:D:789:GLU:HB3	1.99	0.43
1:D:842:PHE:O	1:D:849:VAL:HA	2.18	0.43
1:C:909:TYR:CD1	1:C:962:ILE:HA	2.53	0.43
1:C:965:ASP:O	1:C:967:ASN:N	2.51	0.43
1:B:637:LEU:CD2	1:B:663:LEU:HD21	2.45	0.43
1:A:652:HIS:CG	1:A:653:GLN:H	2.36	0.43
1:C:806:ASN:HA	1:C:918:MET:O	2.19	0.43
1:D:650:LEU:HD11	1:D:831:ILE:CD1	2.47	0.43
1:C:933:LYS:NZ	1:C:933:LYS:HB2	2.34	0.43
1:B:806:ASN:HB2	1:B:919:ILE:O	2.18	0.43
1:C:647:LEU:HD11	1:C:854:PHE:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:909:TYR:HA	1:B:961:LEU:O	2.18	0.43
1:B:809:ARG:NH1	1:B:954:GLU:OE2	2.52	0.43
1:B:973:ARG:HB3	2:B:8:HOH:O	2.18	0.43
1:D:896:LEU:O	1:D:897:ASP:CB	2.66	0.43
1:A:617:ARG:HH22	1:C:893:THR:HG22	1.83	0.43
1:C:975:LEU:HA	1:C:975:LEU:HD23	1.77	0.43
1:A:619:ALA:HB1	1:C:899:THR:HG21	2.00	0.43
1:A:944:PRO:HG2	1:A:945:ASP:OD1	2.18	0.43
1:C:833:HIS:CD2	1:C:835:ASP:H	2.32	0.43
1:D:958:ILE:O	1:D:962:ILE:HG12	2.19	0.43
1:C:836:LEU:HG	1:C:914:ILE:CD1	2.49	0.43
1:D:652:HIS:CE1	1:D:654:TYR:H	2.37	0.43
1:A:944:PRO:HG2	1:A:945:ASP:H	1.83	0.43
1:A:932:LEU:O	1:A:936:ARG:HG2	2.18	0.43
1:A:926:MET:O	1:A:927:GLU:C	2.56	0.43
1:C:768:ARG:HH21	1:D:646:LEU:HD11	1.83	0.43
1:A:621:ASP:OD1	1:A:621:ASP:N	2.49	0.43
1:D:926:MET:SD	1:D:926:MET:N	2.92	0.43
1:C:650:LEU:O	1:C:657:ARG:NH1	2.51	0.43
1:A:955:LYS:O	1:A:959:ARG:HB2	2.18	0.43
1:C:617:ARG:HH12	1:C:622:SER:C	2.23	0.43
1:C:908:MET:HE2	1:C:971:GLY:C	2.38	0.43
1:A:908:MET:HE1	1:A:972:ALA:HA	2.01	0.43
1:A:833:HIS:HA	1:A:854:PHE:CD2	2.54	0.42
1:D:631:ARG:HH12	1:D:769:ARG:HG3	1.83	0.42
1:C:621:ASP:OD1	1:C:623:ARG:CB	2.67	0.42
1:B:784:LEU:CD2	1:B:786:ILE:HG13	2.48	0.42
1:D:885:ILE:HG23	1:D:885:ILE:O	2.18	0.42
1:A:613:VAL:HG22	1:A:628:LYS:HG2	2.01	0.42
1:D:656:VAL:HG21	1:D:852:GLY:HA3	2.01	0.42
1:C:833:HIS:O	1:C:834:ARG:HB2	2.19	0.42
1:D:631:ARG:HD2	1:D:783:THR:CG2	2.48	0.42
1:B:922:PHE:CE2	1:B:928:ARG:HG3	2.54	0.42
1:C:595:TYR:CE1	1:C:627:ILE:HD13	2.54	0.42
1:D:885:ILE:HD11	1:D:887:THR:HB	2.01	0.42
1:C:650:LEU:HD21	1:C:829:GLN:HG3	2.01	0.42
1:C:972:ALA:O	1:C:975:LEU:HB2	2.19	0.42
1:A:642:SER:O	1:A:646:LEU:HD12	2.18	0.42
1:C:905:LYS:HG2	1:C:966:PRO:O	2.20	0.42
1:C:637:LEU:HD11	1:C:782:SER:O	2.19	0.42
1:D:887:THR:HG22	1:D:887:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:656:VAL:CG2	1:C:850:LYS:HG2	2.50	0.42
1:C:664:GLU:O	1:C:782:SER:HB2	2.20	0.42
1:C:928:ARG:NH1	1:C:932:LEU:CD1	2.77	0.42
1:A:838:PRO:HB2	1:A:839:MET:HE2	2.01	0.42
1:C:646:LEU:HA	1:C:646:LEU:HD23	1.76	0.42
1:A:947:ASP:OD1	1:A:950:LYS:HB2	2.20	0.42
1:A:663:LEU:HB2	1:B:645:MET:HB3	2.01	0.42
1:A:613:VAL:HG22	1:A:628:LYS:CG	2.48	0.42
1:D:598:ASP:CG	1:D:620:LEU:HD11	2.40	0.42
1:C:808:GLN:N	1:C:808:GLN:OE1	2.53	0.42
1:C:771:PHE:HE2	1:D:830:GLY:CA	2.32	0.42
1:B:653:GLN:HE21	1:B:653:GLN:HB3	1.55	0.42
1:D:819:ILE:HG21	1:D:911:LEU:HD21	2.01	0.42
1:C:899:THR:HG22	1:C:900:GLY:H	1.85	0.42
1:D:843:ILE:HA	1:D:848:ASN:O	2.20	0.42
1:D:768:ARG:HA	1:D:782:SER:CB	2.50	0.42
1:A:610:PHE:CD1	1:A:610:PHE:N	2.88	0.42
1:D:929:VAL:O	1:D:933:LYS:HG2	2.20	0.41
1:C:804:ASN:C	1:C:806:ASN:H	2.22	0.41
1:C:804:ASN:O	1:C:808:GLN:OE1	2.38	0.41
1:A:926:MET:HA	1:A:929:VAL:CG2	2.46	0.41
1:B:966:PRO:HA	1:B:969:ARG:HE	1.85	0.41
1:A:645:MET:HG3	1:B:641:LEU:HD13	2.01	0.41
1:A:805:LEU:HD12	1:A:805:LEU:HA	1.80	0.41
1:D:605:LEU:HD13	1:D:613:VAL:HG12	2.02	0.41
1:C:957:ILE:O	1:C:958:ILE:C	2.58	0.41
1:C:610:PHE:HB3	1:C:631:ARG:O	2.20	0.41
1:A:924:THR:OG1	1:A:927:GLU:HB2	2.21	0.41
1:A:640:ILE:HA	1:A:643:GLU:HG3	2.01	0.41
1:D:632:HIS:CE1	1:D:636:LYS:HD3	2.55	0.41
1:C:851:ILE:H	1:C:851:ILE:HD12	1.84	0.41
1:B:940:ILE:HD13	1:B:959:ARG:HH11	1.81	0.41
1:C:804:ASN:C	1:C:806:ASN:N	2.73	0.41
1:B:806:ASN:HD21	1:B:921:PRO:HB3	1.83	0.41
1:D:784:LEU:HD12	1:D:785:PHE:N	2.36	0.41
1:A:930:ASN:O	1:A:931:ILE:C	2.57	0.41
1:B:949:ASN:O	1:B:952:LYS:HB2	2.21	0.41
1:B:894:GLU:HG2	1:B:969:ARG:HH22	1.86	0.41
1:B:812:TYR:C	1:B:812:TYR:CD1	2.94	0.41
1:C:809:ARG:CZ	1:C:809:ARG:HB3	2.51	0.41
1:A:890:TYR:O	1:A:910:SER:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:973:ARG:HH11	1:B:976:LEU:HD12	1.85	0.41
1:A:855:GLY:O	1:A:856:LEU:C	2.58	0.41
1:A:829:GLN:NE2	1:A:829:GLN:CA	2.84	0.41
1:C:664:GLU:HG3	1:C:785:PHE:CE1	2.56	0.41
1:C:804:ASN:N	1:C:804:ASN:HD22	2.19	0.41
1:C:798:ASP:O	1:C:799:LEU:C	2.60	0.41
1:D:828:SER:C	1:D:830:GLY:H	2.24	0.41
1:C:654:TYR:HD1	1:C:821:GLU:HB2	1.85	0.41
1:B:632:HIS:NE2	1:B:636:LYS:NZ	2.68	0.41
1:C:887:THR:O	1:C:887:THR:HG22	2.21	0.41
1:D:821:GLU:O	1:D:822:ALA:C	2.58	0.41
1:D:621:ASP:OD2	1:D:623:ARG:HG3	2.21	0.41
1:D:846:SER:O	1:D:847:ARG:HB2	2.20	0.41
1:C:806:ASN:OD1	1:C:807:GLN:HG3	2.21	0.41
1:A:656:VAL:HG23	1:A:851:ILE:O	2.21	0.41
1:A:959:ARG:HH11	1:A:963:ASP:HA	1.85	0.40
1:A:964:HIS:O	1:A:966:PRO:HD3	2.21	0.40
1:A:960:LEU:HB3	1:A:970:PRO:HD3	2.02	0.40
1:D:854:PHE:O	1:D:856:LEU:HD12	2.22	0.40
1:A:904:GLU:HG2	1:A:905:LYS:N	2.36	0.40
1:A:647:LEU:HD13	1:A:831:ILE:HG21	2.03	0.40
1:D:859:ASN:OD1	1:D:860:VAL:N	2.54	0.40
1:C:940:ILE:HG21	1:C:959:ARG:NH2	2.36	0.40
1:B:633:THR:HB	1:B:634:GLU:H	1.24	0.40
1:B:804:ASN:HB3	1:B:807:GLN:HB2	2.03	0.40
1:A:976:LEU:HA	1:A:981:LEU:HD22	2.03	0.40
1:B:654:TYR:O	1:B:850:LYS:HA	2.21	0.40
1:B:647:LEU:HD23	1:B:647:LEU:HA	1.95	0.40
1:C:899:THR:C	1:C:901:HIS:H	2.23	0.40
1:A:641:LEU:HA	1:A:644:VAL:CG1	2.49	0.40
1:D:813:TRP:O	1:D:816:PHE:HB3	2.21	0.40
1:C:845:GLU:C	1:C:847:ARG:H	2.25	0.40
1:B:792:GLU:HA	1:B:792:GLU:OE1	2.22	0.40
1:A:809:ARG:HA	1:A:812:TYR:CZ	2.56	0.40
1:B:935:LEU:C	1:B:937:SER:H	2.24	0.40
1:C:922:PHE:CG	1:C:928:ARG:HG3	2.57	0.40
1:D:931:ILE:O	1:D:935:LEU:HB2	2.21	0.40
1:A:659:TYR:HE1	1:A:789:GLU:HA	1.87	0.40
1:A:820:LEU:HD23	1:A:820:LEU:HA	1.85	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	255/303 (84%)	201 (79%)	42 (16%)	12 (5%)	3	17
1	B	246/303 (81%)	191 (78%)	46 (19%)	9 (4%)	4	23
1	C	265/303 (88%)	200 (76%)	51 (19%)	14 (5%)	2	14
1	D	250/303 (82%)	202 (81%)	34 (14%)	14 (6%)	2	13
All	All	1016/1212 (84%)	794 (78%)	173 (17%)	49 (5%)	3	17

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	858	LYS
1	C	770	ASN
1	D	904	GLU
1	A	639	THR
1	A	937	SER
1	A	947	ASP
1	B	622	SER
1	B	638	SER
1	C	594	ARG
1	C	808	GLN
1	C	947	ASP
1	C	948	ASP
1	D	620	LEU
1	D	894	GLU
1	D	895	VAL
1	D	948	ASP
1	A	802	SER
1	B	632	HIS
1	C	803	GLU
1	C	858	LYS
1	C	954	GLU
1	D	793	ASN

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Mol	Chain	Res	Type
1	D	824	SER
1	D	845	GLU
1	D	897	ASP
1	A	636	LYS
1	A	897	ASP
1	A	905	LYS
1	A	929	VAL
1	B	804	ASN
1	B	897	ASP
1	C	622	SER
1	B	896	LEU
1	C	846	SER
1	C	966	PRO
1	C	994	LEU
1	D	802	SER
1	D	823	LEU
1	D	859	ASN
1	D	940	ILE
1	A	831	ILE
1	B	859	ASN
1	C	632	HIS
1	C	940	ILE
1	A	940	ILE
1	B	983	VAL
1	D	602	ILE
1	A	640	ILE
1	B	940	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	234/272 (86%)	216 (92%)	18 (8%)	16	50
1	B	227/272 (84%)	201 (88%)	26 (12%)	7	28
1	C	243/272 (89%)	220 (90%)	23 (10%)	11	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	229/272 (84%)	212 (93%)	17 (7%)	17	52
All	All	933/1088 (86%)	849 (91%)	84 (9%)	12	41

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	593	LEU
1	A	610	PHE
1	A	614	VAL
1	A	637	LEU
1	A	639	THR
1	A	663	LEU
1	A	769	ARG
1	A	770	ASN
1	A	810	ASP
1	A	812	TYR
1	A	829	GLN
1	A	839	MET
1	A	889	MET
1	A	897	ASP
1	A	926	MET
1	A	942	PHE
1	A	959	ARG
1	A	981	LEU
1	B	598	ASP
1	B	601	GLU
1	B	617	ARG
1	B	633	THR
1	B	636	LYS
1	B	653	GLN
1	B	793	ASN
1	B	794	ARG
1	B	795	THR
1	B	798	ASP
1	B	805	LEU
1	B	808	GLN
1	B	810	ASP
1	B	812	TYR
1	B	813	TRP
1	B	840	ASN
1	B	845	GLU
1	B	849	VAL

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Mol	Chain	Res	Type
1	B	894	GLU
1	B	906	ILE
1	B	927	GLU
1	B	942	PHE
1	B	950	LYS
1	B	959	ARG
1	B	973	ARG
1	B	984	LYS
1	C	593	LEU
1	C	598	ASP
1	C	617	ARG
1	C	621	ASP
1	C	622	SER
1	C	635	GLU
1	C	663	LEU
1	C	769	ARG
1	C	794	ARG
1	C	795	THR
1	C	803	GLU
1	C	812	TYR
1	C	813	TRP
1	C	849	VAL
1	C	859	ASN
1	C	860	VAL
1	C	896	LEU
1	C	905	LYS
1	C	911	LEU
1	C	923	SER
1	C	948	ASP
1	C	951	MET
1	C	959	ARG
1	D	605	LEU
1	D	610	PHE
1	D	639	THR
1	D	647	LEU
1	D	663	LEU
1	D	794	ARG
1	D	812	TYR
1	D	821	GLU
1	D	849	VAL
1	D	858	LYS
1	D	905	LYS

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Mol	Chain	Res	Type
1	D	906	ILE
1	D	926	MET
1	D	948	ASP
1	D	951	MET
1	D	959	ARG
1	D	984	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	632	HIS
1	A	652	HIS
1	A	787	GLN
1	A	807	GLN
1	A	829	GLN
1	A	967	ASN
1	B	607	GLN
1	B	612	GLN
1	B	652	HIS
1	B	653	GLN
1	B	787	GLN
1	B	793	ASN
1	B	804	ASN
1	B	807	GLN
1	B	808	GLN
1	B	840	ASN
1	B	964	HIS
1	B	967	ASN
1	C	652	HIS
1	C	770	ASN
1	C	801	HIS
1	C	804	ASN
1	C	833	HIS
1	C	859	ASN
1	C	930	ASN
1	C	985	HIS
1	D	607	GLN
1	D	612	GLN
1	D	653	GLN
1	D	770	ASN
1	D	787	GLN
1	D	808	GLN

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Mol	Chain	Res	Type
1	D	833	HIS
1	D	840	ASN
1	D	930	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	261/303 (86%)	-0.17	1 (0%) 93 80	41, 71, 112, 125	2 (0%)
1	B	254/303 (83%)	-0.20	3 (1%) 81 55	40, 78, 116, 132	0
1	C	271/303 (89%)	-0.17	0 100 100	41, 76, 110, 117	0
1	D	256/303 (84%)	-0.26	6 (2%) 64 33	37, 67, 106, 118	0
All	All	1042/1212 (85%)	-0.20	10 (0%) 84 60	37, 73, 111, 132	2 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	899	THR	4.3
1	B	886	GLY	3.1
1	D	897	ASP	3.0
1	D	859	ASN	2.7
1	B	897	ASP	2.6
1	A	931	ILE	2.4
1	D	781	LYS	2.2
1	D	896	LEU	2.2
1	D	900	GLY	2.1
1	B	895	VAL	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.