



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 08:03 PM EDT

PDB ID : 2G56  
Title : crystal structure of human insulin-degrading enzyme in complex with insulin B chain  
Authors : Shen, Y.; Tang, W.-J.  
Deposited on : 2006-02-22  
Resolution : 2.20 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
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) : 2.23.2

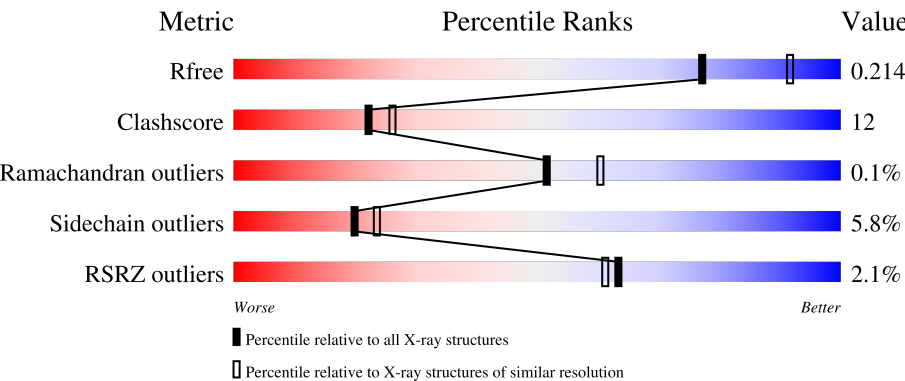
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


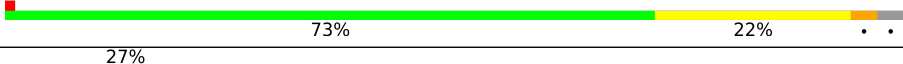
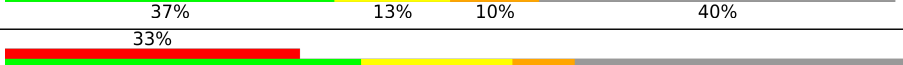

The reported resolution of this entry is 2.20 Å.

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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 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	990	
1	B	990	
2	C	30	
2	D	30	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16964 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 Insulin-degrading enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	964	Total	C	N	O	S	0	0	0
			7853	5053	1319	1447	34			
1	B	964	Total	C	N	O	S	0	0	0
			7850	5052	1318	1446	34			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	initiating methionine	UNP Q5T5N2
A	31	HIS	-	expression tag	UNP Q5T5N2
A	32	HIS	-	expression tag	UNP Q5T5N2
A	33	HIS	-	expression tag	UNP Q5T5N2
A	34	HIS	-	expression tag	UNP Q5T5N2
A	35	HIS	-	expression tag	UNP Q5T5N2
A	36	HIS	-	expression tag	UNP Q5T5N2
A	37	ALA	-	cloning artifact	UNP Q5T5N2
A	38	ALA	-	cloning artifact	UNP Q5T5N2
A	39	GLY	-	cloning artifact	UNP Q5T5N2
A	40	ILE	-	cloning artifact	UNP Q5T5N2
A	41	PRO	-	cloning artifact	UNP Q5T5N2
A	111	GLN	GLU	engineered mutation	UNP Q5T5N2
B	30	MET	-	initiating methionine	UNP Q5T5N2
B	31	HIS	-	expression tag	UNP Q5T5N2
B	32	HIS	-	expression tag	UNP Q5T5N2
B	33	HIS	-	expression tag	UNP Q5T5N2
B	34	HIS	-	expression tag	UNP Q5T5N2
B	35	HIS	-	expression tag	UNP Q5T5N2
B	36	HIS	-	expression tag	UNP Q5T5N2
B	37	ALA	-	cloning artifact	UNP Q5T5N2
B	38	ALA	-	cloning artifact	UNP Q5T5N2
B	39	GLY	-	cloning artifact	UNP Q5T5N2
B	40	ILE	-	cloning artifact	UNP Q5T5N2
B	41	PRO	-	cloning artifact	UNP Q5T5N2

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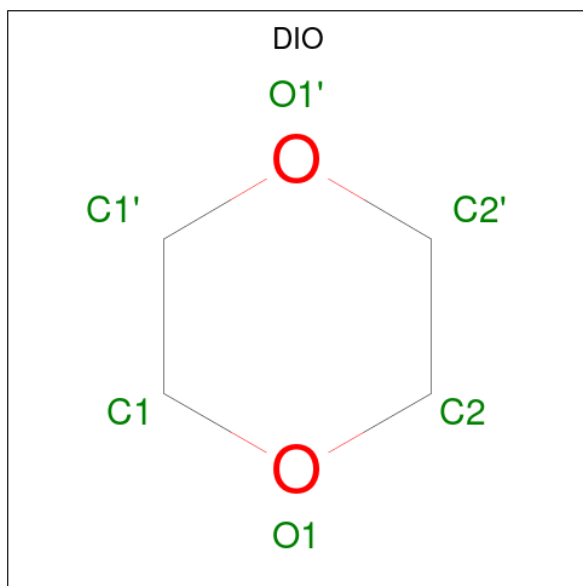
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Chain	Residue	Modelled	Actual	Comment	Reference
B	111	GLN	GLU	engineered mutation	UNP Q5T5N2

- Molecule 2 is a protein called Insulin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	18	Total	C	N	O	0	0	0
			103	63	20	20			
2	D	19	Total	C	N	O	0	0	0
			108	66	21	21			

- Molecule 3 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	4	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	541	Total	O	0	0
			541	541		
4	B	500	Total	O	0	0
			500	500		
4	C	2	Total	O	0	0
			2	2		

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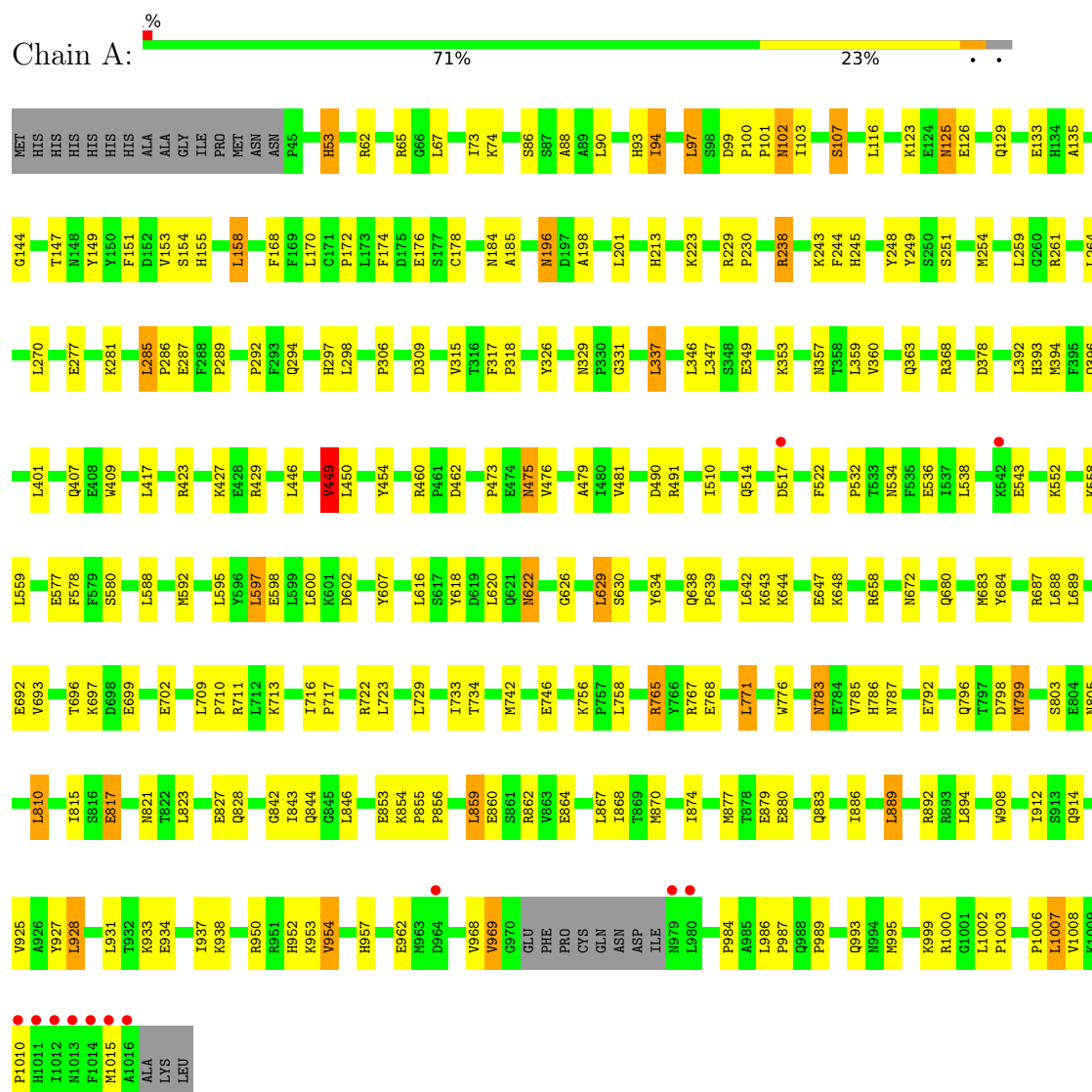
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	O	0	0
			1	1		

### 3 Residue-property plots

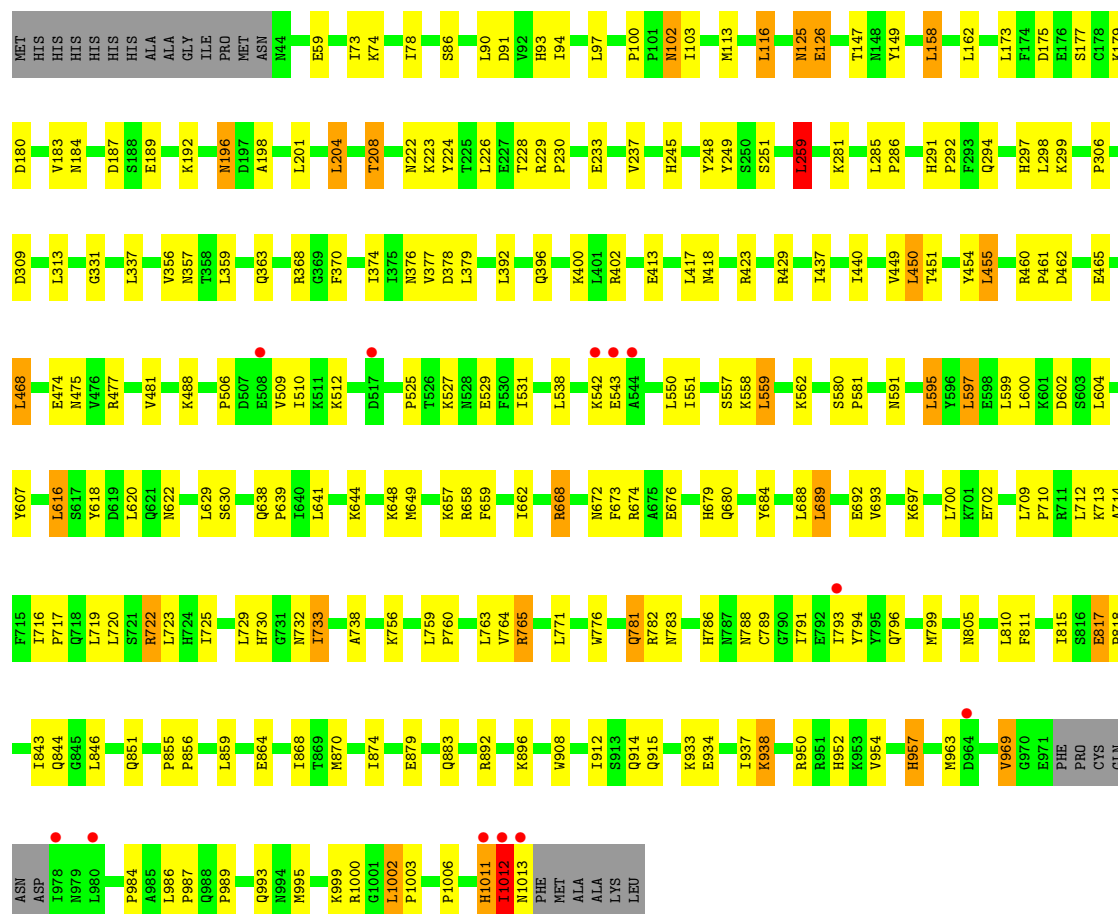
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

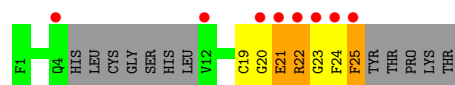
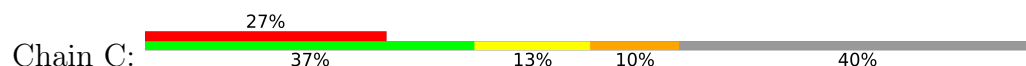


#### • Molecule 1: Insulin-degrading enzyme

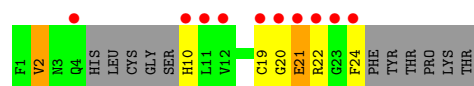




● Molecule 2: Insulin



● Molecule 2: Insulin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	262.25Å 262.25Å 90.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.75 – 2.20 29.75 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.1 (29.75-2.20) 95.0 (29.75-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.25 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.205 , 0.225 0.195 , 0.214	Depositor DCC
$R_{free}$ test set	17390 reflections (9.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.5	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 46.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16964	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DIO

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	0.37	0/8049	0.58	1/10887 (0.0%)
1	B	0.39	0/8046	0.61	3/10884 (0.0%)
2	C	1.32	2/102 (2.0%)	2.51	10/137 (7.3%)
2	D	0.96	1/107 (0.9%)	1.48	4/144 (2.8%)
All	All	0.40	3/16304 (0.0%)	0.63	18/22052 (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
2	C	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	23	GLY	N-CA	-6.96	1.35	1.46
2	D	10	HIS	CA-CB	-5.59	1.41	1.53
2	C	25	PHE	CA-CB	-5.15	1.42	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	25	PHE	N-CA-C	12.78	145.49	111.00
2	C	24	PHE	CA-C-N	-10.05	95.09	117.20
1	B	1011	HIS	N-CA-C	-9.20	86.17	111.00
2	D	22	ARG	N-CA-C	8.49	133.93	111.00
2	C	22	ARG	CA-C-N	-8.29	99.62	116.20
1	A	449	VAL	CB-CA-C	-7.17	97.77	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	24	PHE	C-N-CA	7.02	139.24	121.70
2	C	24	PHE	CA-C-O	7.00	134.80	120.10
2	C	25	PHE	CA-C-O	-6.93	105.56	120.10
2	C	20	GLY	C-N-CA	-6.62	105.14	121.70
2	D	20	GLY	N-CA-C	-6.33	97.28	113.10
2	D	21	GLU	C-N-CA	5.94	136.55	121.70
2	C	23	GLY	C-N-CA	-5.91	106.93	121.70
2	D	21	GLU	N-CA-C	5.90	126.94	111.00
2	C	21	GLU	CA-C-N	-5.46	105.18	117.20
2	C	19	CYS	N-CA-C	-5.40	96.43	111.00
1	B	259	LEU	CA-CB-CG	5.32	127.53	115.30
1	B	1012	ILE	N-CA-C	5.14	124.87	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	21	GLU	Mainchain
2	C	22	ARG	Peptide

## 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	7853	0	7773	199	0
1	B	7850	0	7765	174	0
2	C	103	0	66	1	0
2	D	108	0	68	3	0
3	A	6	0	8	1	0
4	A	541	0	0	19	0
4	B	500	0	0	18	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
All	All	16964	0	15680	369	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 12.

All (369) 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:B:208:THR:HG23	1:B:477:ARG:HH22	1.11	1.08
1:B:892:ARG:HD2	4:B:1459:HOH:O	1.57	1.02
1:B:208:THR:CG2	1:B:477:ARG:HH22	1.77	0.97
1:B:817:GLU:HG3	1:B:818:PRO:HD3	1.47	0.97
1:B:765:ARG:NH1	1:B:914:GLN:OE1	2.02	0.93
1:A:815:ILE:HA	1:A:870:MET:HE2	1.51	0.93
1:B:864:GLU:HG2	1:B:986:LEU:HD21	1.49	0.92
1:A:94:ILE:HD11	1:A:244:PHE:CZ	2.05	0.91
1:A:309:ASP:H	1:A:672:ASN:HD21	1.17	0.89
1:A:680:GLN:OE1	2:C:25:PHE:CB	2.20	0.88
1:A:102:ASN:H	1:A:102:ASN:HD22	1.22	0.88
1:A:93:HIS:HE1	1:A:368:ARG:HH21	1.23	0.87
1:A:879:GLU:HG2	4:A:1330:HOH:O	1.74	0.86
1:B:102:ASN:HD22	1:B:102:ASN:H	1.22	0.85
1:A:765:ARG:NH1	1:A:914:GLN:OE1	2.10	0.85
1:B:309:ASP:H	1:B:672:ASN:HD21	1.24	0.83
1:A:864:GLU:HG2	1:A:986:LEU:HD21	1.58	0.83
1:A:886:ILE:HG23	1:A:928:LEU:HD22	1.58	0.83
1:A:534:ASN:OD1	1:A:536:GLU:HG2	1.79	0.83
1:B:294:GLN:H	1:B:297:HIS:HD2	1.25	0.82
1:B:429:ARG:HD2	4:B:1352:HOH:O	1.80	0.81
1:A:287:GLU:HG2	1:A:289:PRO:HD3	1.63	0.80
1:B:950:ARG:HD2	4:B:1252:HOH:O	1.83	0.79
1:B:599:LEU:HD23	1:B:662:ILE:HD12	1.64	0.79
1:B:93:HIS:HE1	1:B:368:ARG:HH21	1.31	0.78
1:B:208:THR:HG23	1:B:477:ARG:NH2	1.96	0.77
1:A:309:ASP:H	1:A:672:ASN:ND2	1.83	0.77
1:B:805:ASN:HD22	1:B:844:GLN:HE22	1.33	0.76
1:A:294:GLN:H	1:A:297:HIS:HD2	1.31	0.76
1:B:604:LEU:HD13	1:B:648:LYS:HG2	1.65	0.76
1:A:1000:ARG:HD2	4:B:1297:HOH:O	1.85	0.76
1:B:783:ASN:ND2	1:B:786:HIS:H	1.83	0.76
1:B:59:GLU:OE2	4:B:1464:HOH:O	2.02	0.76
1:A:827:GLU:OE1	1:A:862:ARG:HD3	1.85	0.75
1:B:791:ILE:HD11	1:B:793:ILE:HD11	1.69	0.75
1:A:538:LEU:HD23	1:A:734:THR:HG23	1.69	0.74
1:A:184:ASN:HD21	1:A:223:LYS:NZ	1.85	0.74
1:B:674:ARG:HD3	4:B:1239:HOH:O	1.88	0.73
1:A:783:ASN:HD22	1:A:785:VAL:H	1.36	0.72
1:A:783:ASN:ND2	1:A:785:VAL:H	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:ASP:H	1:B:672:ASN:ND2	1.86	0.72
1:A:711:ARG:O	1:A:711:ARG:NH2	2.24	0.71
1:B:817:GLU:HG3	1:B:818:PRO:CD	2.19	0.71
1:B:451:THR:HB	1:B:455:LEU:HD22	1.72	0.70
1:A:805:ASN:HD22	1:A:844:GLN:HE22	1.39	0.70
1:A:135:ALA:HA	1:A:892:ARG:NH2	2.08	0.69
1:A:102:ASN:HD22	1:A:102:ASN:N	1.90	0.69
1:B:538:LEU:H	1:B:732:ASN:HD21	1.38	0.69
1:A:491:ARG:HD2	4:A:1220:HOH:O	1.93	0.68
1:B:709:LEU:HG	1:B:713:LYS:HE3	1.75	0.68
1:A:174:PHE:O	1:A:238:ARG:HD3	1.94	0.68
1:A:88:ALA:HB3	1:A:151:PHE:CE2	2.29	0.67
1:A:716:ILE:HB	1:A:717:PRO:HD3	1.76	0.67
1:A:517:ASP:HB2	4:A:1230:HOH:O	1.93	0.67
1:B:102:ASN:HD22	1:B:102:ASN:N	1.88	0.67
1:B:527:LYS:HD2	1:B:529:GLU:OE2	1.95	0.67
1:A:298:LEU:HD21	1:A:318:PRO:HG2	1.77	0.67
1:A:100:PRO:HG2	1:A:103:ILE:HB	1.76	0.66
1:B:868:ILE:HD12	1:B:984:PRO:HD3	1.76	0.66
1:A:368:ARG:HD2	4:A:1195:HOH:O	1.96	0.66
1:B:1012:ILE:O	1:B:1013:ASN:CB	2.43	0.66
1:A:294:GLN:H	1:A:297:HIS:CD2	2.13	0.65
1:A:722:ARG:HB3	1:A:758:LEU:HD13	1.78	0.65
1:B:543:GLU:N	1:B:543:GLU:OE2	2.30	0.64
1:B:658:ARG:NH2	4:B:1480:HOH:O	2.30	0.64
1:B:102:ASN:H	1:B:102:ASN:ND2	1.95	0.64
1:B:294:GLN:H	1:B:297:HIS:CD2	2.12	0.64
1:A:883:GLN:NE2	4:A:1094:HOH:O	2.30	0.64
1:B:883:GLN:NE2	4:B:1458:HOH:O	2.30	0.64
1:B:125:ASN:HD22	1:B:125:ASN:H	1.46	0.64
1:B:229:ARG:HB3	1:B:230:PRO:HD3	1.80	0.63
1:A:771:LEU:HD21	1:A:954:VAL:HG12	1.80	0.63
1:B:781:GLN:HE21	1:B:782:ARG:H	1.45	0.63
1:A:309:ASP:N	1:A:672:ASN:HD21	1.95	0.63
1:A:317:PHE:HD2	1:A:475:ASN:HD21	1.47	0.63
1:A:934:GLU:HG2	1:A:938:LYS:HE3	1.80	0.62
1:A:969:VAL:HG21	1:A:989:PRO:HD2	1.81	0.62
1:A:709:LEU:HG	1:A:713:LYS:HE3	1.81	0.62
1:A:889:LEU:HB3	1:A:928:LEU:HD11	1.82	0.62
1:B:93:HIS:CE1	1:B:368:ARG:HH21	2.16	0.62
1:B:716:ILE:HB	1:B:717:PRO:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:908:TRP:CZ2	1:A:912:ILE:HD11	2.34	0.61
1:A:93:HIS:CE1	1:A:368:ARG:HH21	2.13	0.61
1:B:100:PRO:HG2	1:B:103:ILE:HB	1.82	0.61
1:A:125:ASN:H	1:A:125:ASN:HD22	1.47	0.61
1:A:767:ARG:NH1	1:A:1006:PRO:HA	2.16	0.61
1:B:357:ASN:HB2	1:B:378:ASP:OD1	2.01	0.61
1:B:874:ILE:O	1:B:933:LYS:HD2	2.02	0.60
1:A:643:LYS:HE3	1:A:647:GLU:OE2	2.00	0.60
1:A:950:ARG:HD2	4:A:1303:HOH:O	2.01	0.60
1:A:168:PHE:O	1:A:172:PRO:HG3	2.01	0.60
1:A:315:VAL:HG21	1:A:394:MET:CE	2.32	0.59
1:B:423:ARG:NH2	4:B:1464:HOH:O	2.28	0.59
1:B:331:GLY:HA3	1:B:363:GLN:HE21	1.67	0.59
1:A:99:ASP:OD2	1:A:107:SER:HB3	2.02	0.59
1:A:184:ASN:HD21	1:A:223:LYS:HZ2	1.48	0.58
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.84	0.58
1:A:803:SER:HA	1:A:927:TYR:CE2	2.37	0.58
1:B:423:ARG:NE	4:B:1464:HOH:O	2.27	0.58
1:A:102:ASN:H	1:A:102:ASN:ND2	1.96	0.58
1:B:94:ILE:HG13	1:B:248:TYR:HB3	1.85	0.58
1:B:285:LEU:HD13	1:B:286:PRO:O	2.03	0.58
1:A:129:GLN:O	1:A:133:GLU:HG3	2.04	0.58
1:A:957:HIS:HD2	4:A:1306:HOH:O	1.86	0.58
1:B:285:LEU:HD22	1:B:286:PRO:HD2	1.86	0.58
1:B:679:HIS:HD2	1:B:851:GLN:OE1	1.86	0.57
1:A:580:SER:HB2	1:A:723:LEU:HD23	1.85	0.57
1:B:208:THR:CG2	1:B:477:ARG:NH2	2.60	0.57
1:A:317:PHE:HD2	1:A:475:ASN:ND2	2.02	0.57
1:A:97:LEU:HB2	1:A:144:GLY:O	2.04	0.57
1:B:597:LEU:HG	1:B:620:LEU:HG	1.87	0.57
1:B:760:PRO:HA	1:B:763:LEU:HD23	1.85	0.57
1:B:402:ARG:HG2	1:B:468:LEU:HD13	1.85	0.57
1:B:331:GLY:HA3	1:B:363:GLN:NE2	2.20	0.57
1:A:490:ASP:OD1	1:A:491:ARG:HG3	2.04	0.57
1:A:597:LEU:HG	1:A:620:LEU:HG	1.87	0.57
1:A:407:GLN:HG3	1:A:409:TRP:CD1	2.39	0.56
1:A:185:ALA:HB2	1:A:828:GLN:HE22	1.70	0.56
1:B:449:VAL:HG13	1:B:450:LEU:HD13	1.86	0.56
1:A:74:LYS:HE2	4:A:1462:HOH:O	2.04	0.56
1:A:709:LEU:HB3	1:A:710:PRO:HD3	1.86	0.56
1:A:815:ILE:CA	1:A:870:MET:HE2	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:THR:HG22	1:B:149:TYR:CE1	2.41	0.56
1:A:125:ASN:HB3	1:A:821:ASN:ND2	2.20	0.55
1:A:783:ASN:ND2	1:A:786:HIS:H	2.04	0.55
1:A:196:ASN:ND2	1:A:198:ALA:H	2.03	0.55
1:B:461:PRO:O	1:B:465:GLU:HG3	2.07	0.55
1:B:184:ASN:HD21	1:B:223:LYS:NZ	2.04	0.55
1:A:349:GLU:O	1:A:353:LYS:HG3	2.06	0.55
1:A:684:TYR:OH	1:A:697:LYS:HG2	2.06	0.55
1:B:356:VAL:CG1	1:B:377:VAL:HB	2.36	0.55
1:B:474:GLU:C	1:B:475:ASN:HD22	2.11	0.55
1:A:874:ILE:HG22	1:A:937:ILE:HD11	1.90	0.54
1:B:474:GLU:HG2	1:B:475:ASN:ND2	2.23	0.54
1:B:733:ILE:HD13	1:B:733:ILE:N	2.23	0.54
1:B:673:PHE:CD1	1:B:697:LYS:HE3	2.42	0.54
1:A:460:ARG:NH1	1:A:462:ASP:OD2	2.41	0.54
1:B:392:LEU:O	1:B:396:GLN:HG3	2.08	0.54
1:A:196:ASN:C	1:A:196:ASN:HD22	2.11	0.54
1:A:823:LEU:N	1:A:823:LEU:HD12	2.21	0.54
1:A:229:ARG:HB3	1:A:230:PRO:HD3	1.90	0.53
1:A:73:ILE:HG13	1:A:251:SER:HB2	1.90	0.53
1:A:123:LYS:HB3	1:A:126:GLU:HB2	1.89	0.53
1:B:709:LEU:N	1:B:710:PRO:HD2	2.23	0.53
1:A:94:ILE:HD11	1:A:244:PHE:HZ	1.71	0.53
1:A:598:GLU:OE2	4:A:1455:HOH:O	2.18	0.53
1:A:622:ASN:HD22	1:A:622:ASN:H	1.54	0.53
1:A:475:ASN:ND2	1:A:475:ASN:C	2.63	0.53
1:B:591:ASN:O	1:B:595:LEU:HD22	2.07	0.53
1:A:658:ARG:NH2	4:A:1192:HOH:O	2.41	0.53
1:A:1002:LEU:C	1:B:1006:PRO:HB3	2.29	0.52
1:B:460:ARG:NH1	1:B:462:ASP:OD1	2.42	0.52
1:B:180:ASP:O	1:B:183:VAL:HG12	2.10	0.52
1:B:374:ILE:HD12	1:B:376:ASN:ND2	2.24	0.52
1:B:879:GLU:HB2	4:B:1510:HOH:O	2.08	0.52
1:A:696:THR:OG1	1:A:699:GLU:HG3	2.08	0.52
1:A:315:VAL:HG21	1:A:394:MET:HE3	1.91	0.52
1:A:331:GLY:HA3	1:A:363:GLN:OE1	2.09	0.52
1:B:602:ASP:OD1	1:B:658:ARG:HD3	2.09	0.52
1:A:783:ASN:HD22	1:A:783:ASN:C	2.14	0.52
1:A:821:ASN:HB2	4:A:1063:HOH:O	2.10	0.52
1:A:53:HIS:HB3	4:A:1384:HOH:O	2.09	0.52
1:A:155:HIS:ND1	1:A:261:ARG:HD2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:MET:O	1:A:746:GLU:HG3	2.09	0.51
1:B:580:SER:HB2	1:B:723:LEU:HD23	1.91	0.51
1:A:1015:MET:CB	4:A:1250:HOH:O	2.58	0.51
1:B:418:ASN:HB3	1:B:454:TYR:O	2.10	0.51
1:B:999:LYS:NZ	4:B:1442:HOH:O	2.38	0.51
1:B:599:LEU:HD21	1:B:659:PHE:HA	1.92	0.51
1:B:413:GLU:HG2	1:B:531:ILE:HD11	1.93	0.51
1:A:532:PRO:HG3	1:A:634:TYR:CD2	2.46	0.51
1:A:600:LEU:HD11	1:A:648:LYS:HB3	1.91	0.51
1:A:688:LEU:O	1:A:999:LYS:HE2	2.11	0.50
1:A:810:LEU:HA	1:A:889:LEU:HD12	1.92	0.50
1:A:170:LEU:HD21	1:A:277:GLU:HG3	1.93	0.50
1:B:551:ILE:HD11	1:B:559:LEU:HD13	1.93	0.50
1:A:969:VAL:HG21	1:A:989:PRO:CD	2.42	0.50
1:A:184:ASN:ND2	1:A:223:LYS:NZ	2.58	0.50
1:A:393:HIS:HE1	4:A:1189:HOH:O	1.95	0.50
1:A:689:LEU:HG	1:A:995:MET:HE1	1.94	0.50
1:A:479:ALA:HB2	3:A:1020:DIO:H12	1.93	0.50
1:A:1006:PRO:HB3	1:B:1002:LEU:C	2.31	0.50
1:B:298:LEU:HD13	1:B:475:ASN:HA	1.93	0.50
1:A:285:LEU:HD23	1:A:286:PRO:HD2	1.93	0.49
1:A:908:TRP:CE2	1:A:912:ILE:HD11	2.47	0.49
1:B:259:LEU:HD12	1:B:259:LEU:C	2.33	0.49
1:B:600:LEU:CD2	1:B:649:MET:HG2	2.41	0.49
1:B:789:CYS:SG	1:B:963:MET:SD	3.10	0.49
1:A:392:LEU:O	1:A:396:GLN:HG3	2.12	0.49
1:A:692:GLU:HG2	1:A:693:VAL:HG23	1.95	0.49
1:B:229:ARG:O	1:B:233:GLU:HG3	2.13	0.49
1:B:680:GLN:HE22	2:D:24:PHE:HA	1.76	0.49
1:B:776:TRP:CE3	1:B:989:PRO:HB3	2.47	0.49
1:B:229:ARG:HG3	1:B:229:ARG:HH11	1.77	0.49
1:B:559:LEU:HD21	1:B:729:LEU:HD22	1.93	0.49
1:B:805:ASN:ND2	1:B:844:GLN:HE22	2.05	0.49
1:A:1006:PRO:HD3	1:B:1003:PRO:HB3	1.95	0.48
1:B:102:ASN:N	1:B:102:ASN:ND2	2.59	0.48
1:B:506:PRO:HG2	1:B:509:VAL:CG2	2.43	0.48
1:A:65:ARG:HB3	1:A:264:LEU:HD22	1.94	0.48
1:A:473:PRO:O	1:A:476:VAL:HG12	2.14	0.48
1:B:969:VAL:HG21	1:B:989:PRO:CD	2.43	0.48
1:A:618:TYR:HA	1:A:630:SER:O	2.13	0.48
1:A:602:ASP:OD1	1:A:658:ARG:HD3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:776:TRP:HA	1:A:953:LYS:O	2.14	0.48
1:B:356:VAL:HG13	1:B:377:VAL:HB	1.96	0.48
1:B:843:ILE:HG22	1:B:844:GLN:N	2.28	0.48
1:A:196:ASN:HD22	1:A:198:ALA:N	2.12	0.47
1:B:224:TYR:CE2	1:B:229:ARG:HD2	2.48	0.47
1:B:313:LEU:HB2	1:B:379:LEU:HD11	1.96	0.47
1:A:429:ARG:CZ	4:A:1086:HOH:O	2.62	0.47
1:A:933:LYS:O	1:A:937:ILE:HG12	2.15	0.47
1:A:346:LEU:HA	1:A:522:PHE:CE2	2.49	0.47
1:A:607:TYR:CE2	1:A:644:LYS:HG2	2.50	0.47
1:B:638:GLN:HB2	1:B:639:PRO:HD3	1.96	0.47
1:B:196:ASN:ND2	1:B:198:ALA:H	2.13	0.47
1:B:915:GLN:O	1:B:1011:HIS:HB3	2.14	0.47
1:A:702:GLU:OE2	1:B:759:LEU:HD11	2.14	0.47
1:B:113:MET:HA	1:B:116:LEU:HD22	1.96	0.47
1:B:616:LEU:HD22	1:B:641:LEU:HD23	1.97	0.47
1:A:600:LEU:HD23	1:A:620:LEU:HD21	1.96	0.46
1:A:877:MET:O	1:A:933:LYS:NZ	2.41	0.46
1:A:86:SER:HB3	1:A:158:LEU:HG	1.97	0.46
1:B:622:ASN:HD22	1:B:622:ASN:H	1.62	0.46
1:A:538:LEU:HD23	1:A:734:THR:CG2	2.43	0.46
1:A:796:GLN:HB3	1:A:952:HIS:HB2	1.98	0.46
1:A:842:GLY:HA3	1:A:1008:VAL:HG23	1.97	0.46
1:A:1010:PRO:HG2	4:A:1525:HOH:O	2.15	0.46
1:B:684:TYR:CZ	1:B:688:LEU:HD11	2.50	0.46
1:A:196:ASN:HD22	1:A:198:ALA:H	1.62	0.46
1:B:562:LYS:HD3	1:B:730:HIS:CE1	2.50	0.46
1:A:357:ASN:HB2	1:A:378:ASP:OD1	2.15	0.46
1:A:683:MET:HA	1:A:792:GLU:OE2	2.16	0.46
1:B:600:LEU:HD21	1:B:649:MET:HG2	1.97	0.46
1:A:934:GLU:CG	1:A:938:LYS:HE3	2.46	0.46
1:A:968:VAL:HG23	1:A:969:VAL:HG23	1.97	0.46
1:A:1003:PRO:HB3	1:B:1006:PRO:HD3	1.98	0.46
1:B:618:TYR:HA	1:B:630:SER:O	2.16	0.46
1:B:783:ASN:HD22	1:B:786:HIS:H	1.58	0.46
1:B:874:ILE:HG22	1:B:937:ILE:HD11	1.97	0.46
1:B:934:GLU:HG2	1:B:938:LYS:HE3	1.97	0.46
1:A:245:HIS:O	1:A:249:TYR:HB2	2.16	0.46
1:B:245:HIS:O	1:B:249:TYR:HB2	2.15	0.46
1:A:93:HIS:HE1	1:A:368:ARG:NH2	2.02	0.46
1:A:259:LEU:C	1:A:259:LEU:HD23	2.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:LEU:O	1:A:449:VAL:HG22	2.15	0.46
1:B:796:GLN:HB3	1:B:952:HIS:HB2	1.97	0.46
1:B:908:TRP:CZ2	1:B:912:ILE:HD11	2.51	0.46
1:A:147:THR:HG22	1:A:149:TYR:CE1	2.51	0.45
1:A:868:ILE:HD12	1:A:984:PRO:HD3	1.99	0.45
1:B:356:VAL:HG11	1:B:377:VAL:HB	1.98	0.45
1:B:957:HIS:HD2	4:B:1503:HOH:O	1.98	0.45
1:B:799:MET:SD	1:B:1006:PRO:HG2	2.56	0.45
1:A:243:LYS:HB2	1:A:243:LYS:NZ	2.31	0.45
1:A:337:LEU:HD23	1:A:401:LEU:HD22	1.99	0.45
1:A:927:TYR:CE2	1:A:931:LEU:HD11	2.52	0.45
1:B:908:TRP:CE2	1:B:912:ILE:HD11	2.52	0.45
1:B:187:ASP:OD1	1:B:222:ASN:HB2	2.17	0.45
1:B:805:ASN:HD22	1:B:844:GLN:NE2	2.07	0.45
1:A:771:LEU:HD21	1:A:954:VAL:CG1	2.46	0.45
1:A:588:LEU:O	1:A:592:MET:HG3	2.17	0.45
1:B:74:LYS:HE2	4:B:1309:HOH:O	2.16	0.45
1:B:126:GLU:HG3	4:B:1370:HOH:O	2.17	0.45
1:B:460:ARG:HD2	1:B:462:ASP:OD2	2.17	0.45
1:B:969:VAL:HG21	1:B:989:PRO:HD3	1.98	0.45
1:A:407:GLN:HG3	1:A:409:TRP:NE1	2.31	0.45
1:A:823:LEU:N	1:A:823:LEU:CD1	2.80	0.45
1:A:67:LEU:HD12	1:A:67:LEU:C	2.37	0.44
1:A:135:ALA:HA	1:A:892:ARG:CZ	2.47	0.44
1:A:429:ARG:NH2	4:A:1086:HOH:O	2.49	0.44
2:D:19:CYS:O	2:D:21:GLU:N	2.50	0.44
1:B:437:ILE:HA	1:B:440:ILE:HG12	1.99	0.44
1:A:968:VAL:HG23	1:A:969:VAL:CG2	2.48	0.44
1:B:359:LEU:C	1:B:359:LEU:HD23	2.38	0.44
1:B:676:GLU:OE2	1:B:676:GLU:HA	2.17	0.44
1:B:811:PHE:CE1	1:B:815:ILE:HD13	2.52	0.44
1:A:558:LYS:HZ3	1:A:558:LYS:HB2	1.82	0.44
1:B:299:LYS:HD2	1:B:510:ILE:HD12	1.99	0.44
1:A:787:ASN:OD1	1:A:962:GLU:HG2	2.17	0.44
1:A:817:GLU:HB3	4:A:1319:HOH:O	2.16	0.44
1:B:175:ASP:OD2	1:B:177:SER:HB3	2.17	0.44
1:A:559:LEU:HD11	1:A:729:LEU:HG	2.00	0.44
1:B:600:LEU:HD23	1:B:620:LEU:CD2	2.48	0.44
1:A:306:PRO:HB3	1:A:481:VAL:CG1	2.48	0.43
1:A:359:LEU:C	1:A:359:LEU:HD23	2.38	0.43
1:B:692:GLU:HG2	1:B:693:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LEU:CD2	1:A:277:GLU:HG3	2.49	0.43
1:B:189:GLU:O	1:B:192:LYS:HG2	2.17	0.43
1:B:402:ARG:CG	1:B:468:LEU:HD13	2.48	0.43
1:A:815:ILE:HG22	1:A:870:MET:CE	2.48	0.43
1:B:506:PRO:HG2	1:B:509:VAL:HG23	2.00	0.43
1:B:100:PRO:HB2	1:B:102:ASN:ND2	2.34	0.43
1:A:90:LEU:HD11	1:A:254:MET:CE	2.48	0.43
1:A:776:TRP:CD2	1:A:989:PRO:HB3	2.53	0.43
1:A:176:GLU:OE2	1:A:238:ARG:HG3	2.19	0.43
1:A:684:TYR:CZ	1:A:688:LEU:HD11	2.53	0.43
1:A:213:HIS:CE1	1:A:292:PRO:HG3	2.54	0.43
1:A:805:ASN:ND2	1:A:844:GLN:HE22	2.11	0.43
1:A:843:ILE:HG22	1:A:844:GLN:N	2.33	0.43
1:B:309:ASP:O	1:B:668:ARG:HG2	2.19	0.43
1:B:622:ASN:H	1:B:622:ASN:ND2	2.17	0.43
1:B:794:TYR:HB3	1:B:954:VAL:HG13	1.99	0.43
1:A:638:GLN:N	1:A:639:PRO:CD	2.82	0.43
1:B:291:HIS:CD2	1:B:370:PHE:HB2	2.53	0.43
1:B:986:LEU:HA	1:B:987:PRO:HD3	1.89	0.43
1:A:359:LEU:HD23	1:A:360:VAL:N	2.33	0.42
1:B:78:ILE:O	1:B:259:LEU:HA	2.18	0.42
1:A:326:TYR:HA	1:A:329:ASN:OD1	2.19	0.42
1:A:629:LEU:HD22	1:A:630:SER:N	2.33	0.42
1:B:722:ARG:HD2	1:B:756:LYS:HB2	2.01	0.42
1:B:843:ILE:HG22	1:B:844:GLN:H	1.84	0.42
1:A:798:ASP:CG	1:A:799:MET:H	2.23	0.42
1:B:600:LEU:HD23	1:B:620:LEU:HD21	2.01	0.42
1:B:933:LYS:O	1:B:937:ILE:HG12	2.19	0.42
1:A:768:GLU:HB3	1:A:843:ILE:HG13	2.01	0.42
1:B:299:LYS:HD2	1:B:510:ILE:CD1	2.49	0.42
1:A:510:ILE:O	1:A:514:GLN:HG3	2.19	0.42
1:A:733:ILE:HG12	1:A:734:THR:N	2.34	0.42
1:A:53:HIS:ND1	1:A:53:HIS:N	2.62	0.42
1:A:475:ASN:C	1:A:475:ASN:HD22	2.22	0.42
1:B:557:SER:HA	1:B:725:ILE:O	2.19	0.42
1:B:729:LEU:HD23	1:B:738:ALA:HA	2.02	0.42
1:A:423:ARG:NE	4:A:1542:HOH:O	2.53	0.42
1:A:860:GLU:OE2	1:A:957:HIS:HE1	2.03	0.42
1:A:100:PRO:HA	1:A:101:PRO:HD3	1.95	0.42
1:B:306:PRO:HB3	1:B:481:VAL:CG1	2.49	0.42
1:B:810:LEU:HD23	1:B:810:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:689:LEU:HD13	1:B:995:MET:CE	2.50	0.42
1:B:714:ALA:O	1:B:717:PRO:HD2	2.20	0.42
1:A:116:LEU:CD1	1:A:178:CYS:HB3	2.49	0.42
1:B:179:LYS:HD2	1:B:237:VAL:HB	2.02	0.42
1:B:400:LYS:HD3	4:B:1189:HOH:O	2.19	0.42
1:B:815:ILE:HG22	1:B:870:MET:HE2	2.02	0.42
4:B:1433:HOH:O	2:D:2:VAL:HG13	2.20	0.42
1:A:767:ARG:HH12	1:A:1006:PRO:HA	1.82	0.41
1:A:62:ARG:HD3	1:A:427:LYS:HE3	2.02	0.41
1:A:125:ASN:HD22	1:A:125:ASN:N	2.10	0.41
1:A:153:VAL:HG22	1:A:154:SER:N	2.34	0.41
1:A:94:ILE:HD13	1:A:248:TYR:CG	2.55	0.41
1:A:184:ASN:HD21	1:A:223:LYS:HZ1	1.65	0.41
1:B:73:ILE:HG13	1:B:251:SER:HB2	2.03	0.41
1:B:184:ASN:HD21	1:B:223:LYS:HZ1	1.66	0.41
1:B:90:LEU:C	1:B:90:LEU:HD23	2.41	0.41
1:A:94:ILE:CD1	1:A:244:PHE:CZ	2.91	0.41
1:A:855:PRO:HA	1:A:856:PRO:HD3	1.89	0.41
1:B:204:LEU:O	1:B:208:THR:HB	2.21	0.41
1:B:525:PRO:HG3	4:B:1296:HOH:O	2.20	0.41
1:B:580:SER:HA	1:B:581:PRO:HD3	1.88	0.41
1:A:184:ASN:ND2	1:A:223:LYS:HZ2	2.18	0.41
1:A:622:ASN:H	1:A:622:ASN:ND2	2.17	0.41
1:A:689:LEU:HG	1:A:995:MET:CE	2.51	0.41
1:A:1007:LEU:HD23	1:B:1000:ARG:HG2	2.03	0.41
1:B:90:LEU:HD23	1:B:91:ASP:N	2.35	0.41
1:B:259:LEU:C	1:B:259:LEU:CD1	2.89	0.41
1:B:817:GLU:N	1:B:818:PRO:CD	2.84	0.41
1:A:578:PHE:O	1:A:626:GLY:HA3	2.21	0.41
1:A:986:LEU:HA	1:A:987:PRO:HD3	1.92	0.41
1:B:291:HIS:ND1	1:B:292:PRO:HD2	2.36	0.41
1:B:607:TYR:CE2	1:B:644:LYS:HG2	2.55	0.41
1:B:196:ASN:HD21	1:B:198:ALA:HB3	1.86	0.41
1:B:855:PRO:HA	1:B:856:PRO:HD3	1.94	0.41
1:A:894:LEU:HG	1:A:925:VAL:HG21	2.03	0.40
1:B:224:TYR:OH	1:B:229:ARG:NH1	2.53	0.40
1:A:151:PHE:CD1	1:A:151:PHE:C	2.94	0.40
1:A:254:MET:HB3	1:A:254:MET:HE2	1.98	0.40
1:B:550:LEU:HD11	1:B:558:LYS:HG2	2.03	0.40
1:A:854:LYS:HB2	1:A:859:LEU:CD1	2.51	0.40
1:A:577:GLU:OE2	1:A:577:GLU:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:SER:HB3	1:B:158:LEU:HG	2.04	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	960/990 (97%)	928 (97%)	32 (3%)	0	100	100
1	B	960/990 (97%)	931 (97%)	27 (3%)	2 (0%)	47	55
2	C	14/30 (47%)	14 (100%)	0	0	100	100
2	D	15/30 (50%)	12 (80%)	3 (20%)	0	100	100
All	All	1949/2040 (96%)	1885 (97%)	62 (3%)	2 (0%)	51	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	228	THR
1	B	1012	ILE

### 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	855/883 (97%)	809 (95%)	46 (5%)	22	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	854/883 (97%)	802 (94%)	52 (6%)	18	21
2	C	4/26 (15%)	4 (100%)	0	100	100
2	D	4/26 (15%)	3 (75%)	1 (25%)	0	0
All	All	1717/1818 (94%)	1618 (94%)	99 (6%)	20	23

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	94	ILE
1	A	97	LEU
1	A	102	ASN
1	A	107	SER
1	A	125	ASN
1	A	158	LEU
1	A	196	ASN
1	A	201	LEU
1	A	238	ARG
1	A	270	LEU
1	A	281	LYS
1	A	285	LEU
1	A	337	LEU
1	A	347	LEU
1	A	417	LEU
1	A	449	VAL
1	A	450	LEU
1	A	454	TYR
1	A	475	ASN
1	A	543	GLU
1	A	595	LEU
1	A	597	LEU
1	A	616	LEU
1	A	622	ASN
1	A	629	LEU
1	A	642	LEU
1	A	687	ARG
1	A	756	LYS
1	A	765	ARG
1	A	771	LEU
1	A	783	ASN
1	A	799	MET

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Mol	Chain	Res	Type
1	A	810	LEU
1	A	817	GLU
1	A	846	LEU
1	A	853	GLU
1	A	859	LEU
1	A	867	LEU
1	A	880	GLU
1	A	889	LEU
1	A	928	LEU
1	A	954	VAL
1	A	969	VAL
1	A	993	GLN
1	A	1007	LEU
1	B	97	LEU
1	B	102	ASN
1	B	116	LEU
1	B	125	ASN
1	B	126	GLU
1	B	158	LEU
1	B	162	LEU
1	B	173	LEU
1	B	196	ASN
1	B	201	LEU
1	B	204	LEU
1	B	208	THR
1	B	226	LEU
1	B	259	LEU
1	B	281	LYS
1	B	337	LEU
1	B	417	LEU
1	B	450	LEU
1	B	455	LEU
1	B	468	LEU
1	B	488	LYS
1	B	512	LYS
1	B	542	LYS
1	B	559	LEU
1	B	595	LEU
1	B	597	LEU
1	B	616	LEU
1	B	629	LEU
1	B	657	LYS

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Mol	Chain	Res	Type
1	B	668	ARG
1	B	689	LEU
1	B	700	LEU
1	B	702	GLU
1	B	712	LEU
1	B	719	LEU
1	B	720	LEU
1	B	722	ARG
1	B	733	ILE
1	B	764	VAL
1	B	765	ARG
1	B	771	LEU
1	B	781	GLN
1	B	788	ASN
1	B	817	GLU
1	B	846	LEU
1	B	859	LEU
1	B	896	LYS
1	B	938	LYS
1	B	957	HIS
1	B	969	VAL
1	B	993	GLN
1	B	1002	LEU
2	D	2	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	93	HIS
1	A	102	ASN
1	A	108	HIS
1	A	125	ASN
1	A	184	ASN
1	A	196	ASN
1	A	231	ASN
1	A	239	GLN
1	A	294	GLN
1	A	297	HIS
1	A	300	GLN
1	A	393	HIS
1	A	475	ASN

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Mol	Chain	Res	Type
1	A	575	ASN
1	A	622	ASN
1	A	672	ASN
1	A	783	ASN
1	A	805	ASN
1	A	821	ASN
1	A	828	GLN
1	A	841	ASN
1	A	922	ASN
1	A	957	HIS
1	A	993	GLN
1	B	93	HIS
1	B	102	ASN
1	B	125	ASN
1	B	129	GLN
1	B	184	ASN
1	B	196	ASN
1	B	232	GLN
1	B	294	GLN
1	B	297	HIS
1	B	300	GLN
1	B	332	HIS
1	B	363	GLN
1	B	376	ASN
1	B	475	ASN
1	B	499	GLN
1	B	502	GLN
1	B	515	ASN
1	B	622	ASN
1	B	672	ASN
1	B	679	HIS
1	B	680	GLN
1	B	730	HIS
1	B	732	ASN
1	B	743	GLN
1	B	770	GLN
1	B	780	GLN
1	B	781	GLN
1	B	783	ASN
1	B	788	ASN
1	B	805	ASN
1	B	828	GLN

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Mol	Chain	Res	Type
1	B	841	ASN
1	B	883	GLN
1	B	957	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	DIO	A	1020	-	6,6,6	0.76	0	6,6,6	0.25	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DIO	A	1020	-	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1020	DIO	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	964/990 (97%)	-0.30	12 (1%) 79 77	21, 31, 46, 62	0
1	B	964/990 (97%)	-0.35	12 (1%) 79 77	17, 28, 44, 59	0
2	C	18/30 (60%)	2.33	8 (44%) 0 0	25, 43, 60, 62	0
2	D	19/30 (63%)	1.76	10 (52%) 0 0	28, 41, 56, 56	0
All	All	1965/2040 (96%)	-0.28	42 (2%) 63 61	17, 30, 46, 62	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	25	PHE	7.6
2	C	23	GLY	7.4
1	A	1016	ALA	7.1
2	D	20	GLY	6.8
1	A	1015	MET	6.8
1	A	1014	PHE	6.6
2	D	11	LEU	6.2
2	C	24	PHE	5.7
1	A	964	ASP	4.8
2	C	21	GLU	4.6
1	B	978	ILE	4.5
1	A	1012	ILE	4.4
2	C	20	GLY	4.3
2	C	4	GLN	4.3
1	B	1012	ILE	4.1
2	D	24	PHE	3.8
1	A	1013	ASN	3.7
2	D	21	GLU	3.6
1	B	1011	HIS	3.5
1	B	517	ASP	3.4
2	C	12	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	543	GLU	3.3
1	A	1011	HIS	2.9
2	D	4	GLN	2.9
1	B	544	ALA	2.6
1	B	542	LYS	2.6
2	D	22	ARG	2.5
1	B	1013	ASN	2.5
2	D	23	GLY	2.5
1	A	980	LEU	2.4
1	A	542	LYS	2.3
1	B	980	LEU	2.3
1	A	1010	PRO	2.3
1	B	793	ILE	2.2
1	B	964	ASP	2.2
1	A	979	ASN	2.2
2	C	22	ARG	2.2
1	B	508	GLU	2.2
1	A	517	ASP	2.2
2	D	10	HIS	2.1
2	D	19	CYS	2.1
2	D	12	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	DIO	A	1020	6/6	0.93	0.16	36,38,39,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.