



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2021 – 08:30 PM EDT

PDB ID : 3H44
Title : Crystal Structure of Insulin Degrading Enzyme in Complex with macrophage inflammatory protein 1 alpha
Authors : Ren, M.; Guo, Q.; Tang, W.J.
Deposited on : 2009-04-17
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

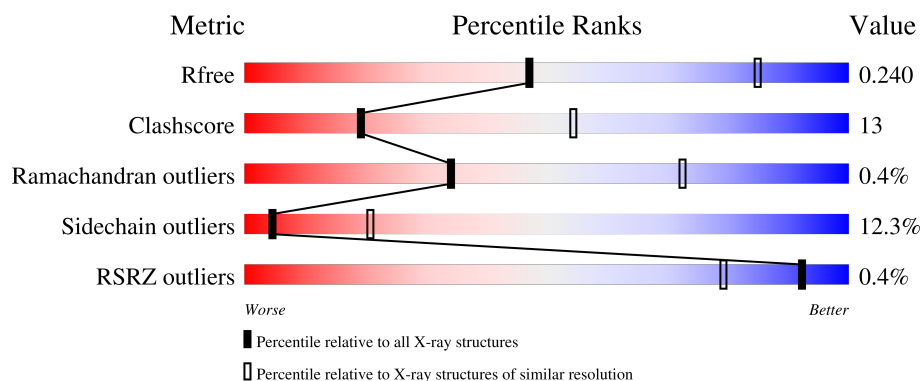
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 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	990	
1	B	990	
2	C	70	
2	D	70	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DIO	A	2001	-	-	-	X
3	DIO	B	2001	-	-	X	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15937 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	956	Total	C	N	O	S	0	0	0
			7821	5036	1314	1449	22			
1	B	955	Total	C	N	O	S	0	0	0
			7815	5033	1313	1447	22			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	expression tag	UNP P14735
A	31	HIS	-	expression tag	UNP P14735
A	32	HIS	-	expression tag	UNP P14735
A	33	HIS	-	expression tag	UNP P14735
A	34	HIS	-	expression tag	UNP P14735
A	35	HIS	-	expression tag	UNP P14735
A	36	HIS	-	expression tag	UNP P14735
A	37	ALA	-	expression tag	UNP P14735
A	38	ALA	-	expression tag	UNP P14735
A	39	GLY	-	expression tag	UNP P14735
A	40	ILE	-	expression tag	UNP P14735
A	41	PRO	-	expression tag	UNP P14735
A	110	LEU	CYS	engineered mutation	UNP P14735
A	111	GLN	GLU	engineered mutation	UNP P14735
A	171	SER	CYS	engineered mutation	UNP P14735
A	178	ALA	CYS	engineered mutation	UNP P14735
A	257	VAL	CYS	engineered mutation	UNP P14735
A	414	LEU	CYS	engineered mutation	UNP P14735
A	573	ASN	CYS	engineered mutation	UNP P14735
A	590	SER	CYS	engineered mutation	UNP P14735
A	789	SER	CYS	engineered mutation	UNP P14735
A	812	ALA	CYS	engineered mutation	UNP P14735
A	819	ALA	CYS	engineered mutation	UNP P14735
A	904	SER	CYS	engineered mutation	UNP P14735
A	966	ASN	CYS	engineered mutation	UNP P14735

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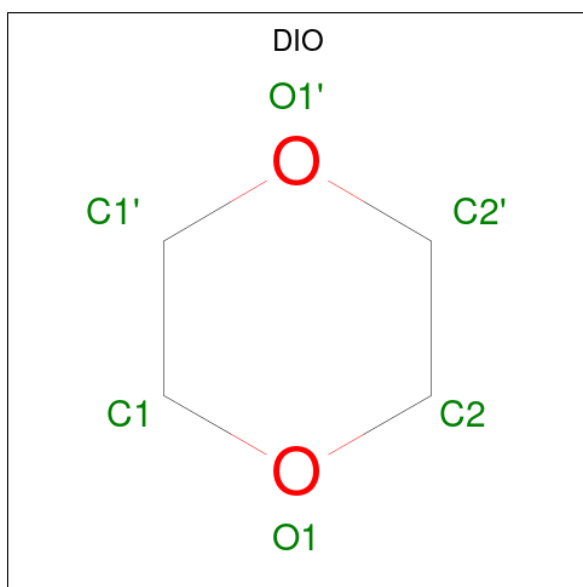
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Chain	Residue	Modelled	Actual	Comment	Reference
A	974	ALA	CYS	engineered mutation	UNP P14735
B	30	MET	-	expression tag	UNP P14735
B	31	HIS	-	expression tag	UNP P14735
B	32	HIS	-	expression tag	UNP P14735
B	33	HIS	-	expression tag	UNP P14735
B	34	HIS	-	expression tag	UNP P14735
B	35	HIS	-	expression tag	UNP P14735
B	36	HIS	-	expression tag	UNP P14735
B	37	ALA	-	expression tag	UNP P14735
B	38	ALA	-	expression tag	UNP P14735
B	39	GLY	-	expression tag	UNP P14735
B	40	ILE	-	expression tag	UNP P14735
B	41	PRO	-	expression tag	UNP P14735
B	110	LEU	CYS	engineered mutation	UNP P14735
B	111	GLN	GLU	engineered mutation	UNP P14735
B	171	SER	CYS	engineered mutation	UNP P14735
B	178	ALA	CYS	engineered mutation	UNP P14735
B	257	VAL	CYS	engineered mutation	UNP P14735
B	414	LEU	CYS	engineered mutation	UNP P14735
B	573	ASN	CYS	engineered mutation	UNP P14735
B	590	SER	CYS	engineered mutation	UNP P14735
B	789	SER	CYS	engineered mutation	UNP P14735
B	812	ALA	CYS	engineered mutation	UNP P14735
B	819	ALA	CYS	engineered mutation	UNP P14735
B	904	SER	CYS	engineered mutation	UNP P14735
B	966	ASN	CYS	engineered mutation	UNP P14735
B	974	ALA	CYS	engineered mutation	UNP P14735

- Molecule 2 is a protein called C-C motif chemokine 3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	0	0	0
			75	44	18	13			
2	D	8	Total	C	N	O	0	0	0
			55	32	12	11			

- Molecule 3 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: C₄H₈O₂).



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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	66	Total	O	0	0
			66	66		

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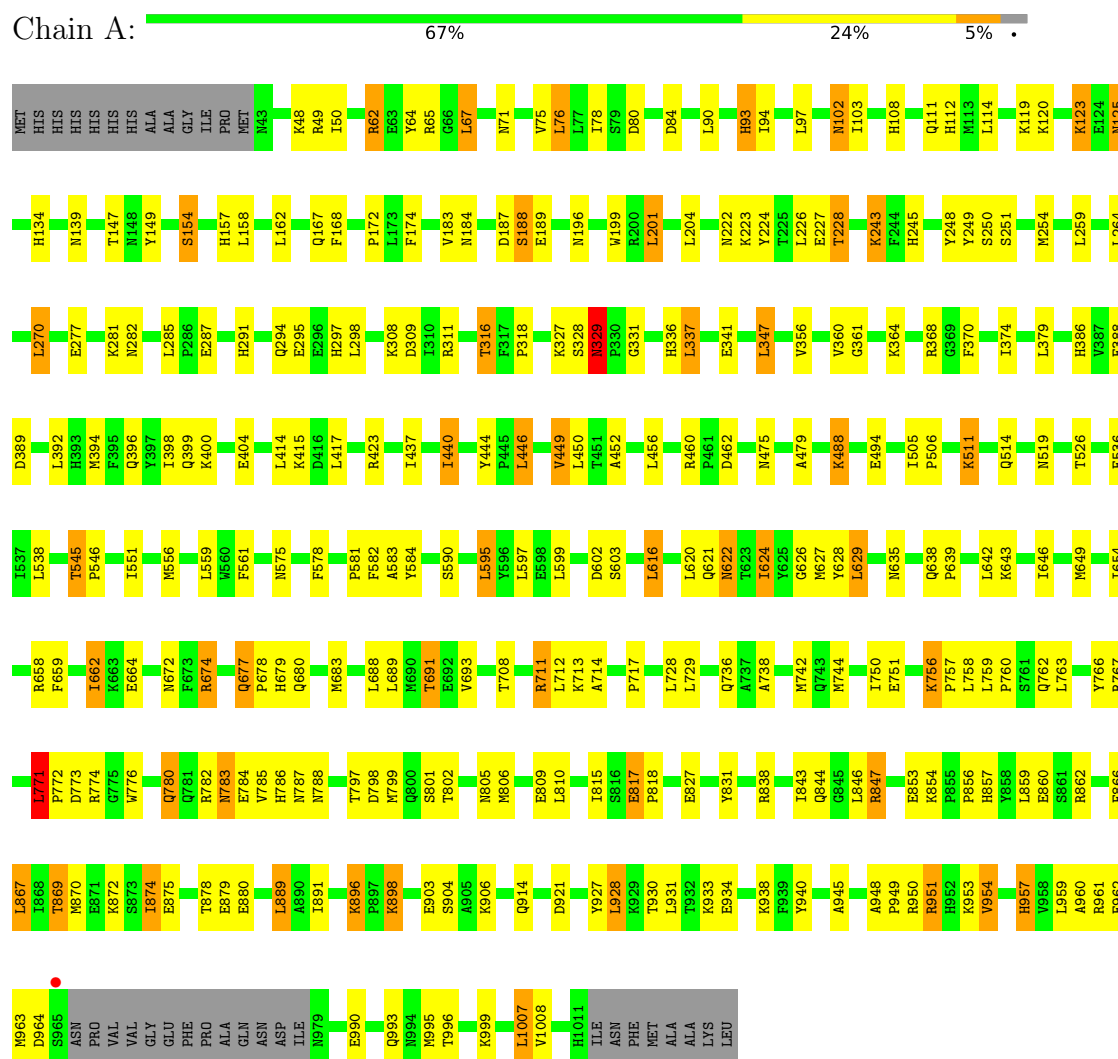
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	61	Total 61	O 61	0	0
5	C	1	Total 1	O 1	0	0
5	D	5	Total 5	O 5	0	0

3 Residue-property plots

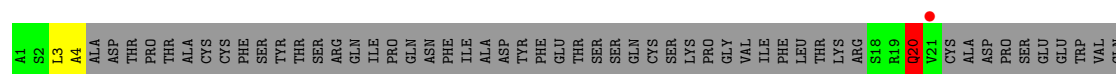
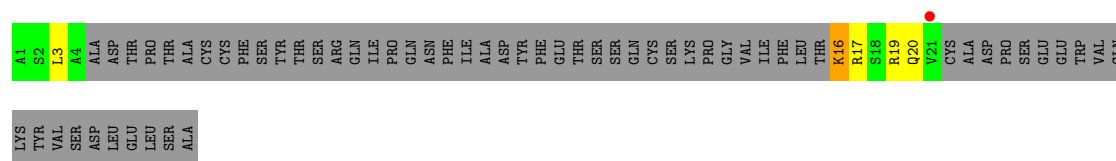
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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





LYS
TYR
VAL
SER
ASP
LEU
GLU
LEU
SER
ALA

4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	262.74Å 262.74Å 90.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.00 49.65 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.00-3.00) 99.7 (49.65-3.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0044	Depositor
R, R_{free}	0.183 , 0.237 0.192 , 0.240	Depositor DCC
R_{free} test set	3612 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15937	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.68	0/8016	0.79	8/10843 (0.1%)
1	B	0.66	2/8010 (0.0%)	0.78	7/10835 (0.1%)
2	C	1.06	0/73	1.10	0/93
2	D	0.88	0/53	1.90	1/68 (1.5%)
All	All	0.67	2/16152 (0.0%)	0.79	16/21839 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	229	ARG	CG-CD	5.87	1.66	1.51
1	B	189	GLU	CG-CD	5.63	1.60	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	20	GLN	CB-CA-C	12.67	135.74	110.40
1	B	52	ASN	CB-CA-C	-7.28	95.84	110.40
1	B	53	HIS	N-CA-C	-7.28	91.35	111.00
1	B	52	ASN	N-CA-C	7.05	130.03	111.00
1	A	328	SER	CB-CA-C	-6.54	97.68	110.10
1	B	667	MET	CG-SD-CE	5.99	109.79	100.20
1	B	797	THR	N-CA-C	5.90	126.92	111.00
1	A	226	LEU	CA-CB-CG	5.75	128.54	115.30
1	B	406	PRO	CB-CA-C	-5.73	97.67	112.00
1	A	798	ASP	N-CA-CB	5.71	120.87	110.60
1	A	771	LEU	CA-CB-CG	5.67	128.33	115.30
1	A	329	ASN	N-CA-C	5.60	126.13	111.00
1	A	62	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	228	THR	CB-CA-C	-5.29	97.30	111.60
1	A	797	THR	N-CA-C	5.13	124.85	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	847	ARG	NE-CZ-NH1	5.08	122.84	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7821	0	7760	197	0
1	B	7815	0	7755	209	0
2	C	75	0	81	6	0
2	D	55	0	55	6	0
3	A	18	0	24	7	0
3	B	18	0	24	6	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	66	0	0	4	0
5	B	61	0	0	3	0
5	C	1	0	0	0	0
5	D	5	0	0	0	0
All	All	15937	0	15699	406	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 13.

All (406) 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:855:PRO:HB2	1:B:857:HIS:CD2	1.69	1.25
1:A:329:ASN:O	1:A:329:ASN:ND2	1.82	1.10
1:B:427:LYS:NZ	3:B:2001:DIO:H22	1.78	0.98
1:B:855:PRO:CG	1:B:857:HIS:NE2	2.28	0.97
1:B:427:LYS:HZ1	3:B:2001:DIO:H22	1.28	0.95
1:B:855:PRO:CB	1:B:857:HIS:CD2	2.49	0.94
1:B:309:ASP:H	1:B:672:ASN:HD21	1.16	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:855:PRO:HB2	1:B:857:HIS:HD2	1.11	0.91
1:A:622:ASN:H	1:A:622:ASN:ND2	1.68	0.90
1:A:309:ASP:H	1:A:672:ASN:HD21	1.20	0.90
1:B:58:PRO:HG2	1:B:423:ARG:HD2	1.51	0.89
1:B:855:PRO:HG3	1:B:857:HIS:NE2	1.90	0.87
1:A:622:ASN:H	1:A:622:ASN:HD22	0.90	0.87
1:A:329:ASN:HD22	1:A:329:ASN:C	1.78	0.86
1:B:341:GLU:HG2	1:B:347:LEU:HD12	1.58	0.85
1:B:188:SER:HB3	1:B:831:TYR:HB2	1.57	0.85
1:B:622:ASN:HD22	1:B:622:ASN:H	1.23	0.85
1:A:84:ASP:H	3:A:2001:DIO:H12	1.42	0.83
1:A:139:ASN:OD1	2:C:20:GLN:HG3	1.77	0.83
1:B:602:ASP:OD1	1:B:658:ARG:HD3	1.79	0.83
1:B:896:LYS:HB2	3:B:2001:DIO:H1'1	1.60	0.83
1:B:776:TRP:CD1	1:B:953:LYS:HG2	2.15	0.82
1:A:783:ASN:ND2	1:A:786:HIS:H	1.78	0.82
1:A:693:VAL:HB	1:A:766:TYR:CE2	2.14	0.81
1:B:783:ASN:HD22	1:B:785:VAL:H	1.26	0.81
1:A:688:LEU:HB3	1:A:995:MET:HE1	1.63	0.80
1:A:189:GLU:HG3	1:A:831:TYR:CE1	2.15	0.80
1:B:693:VAL:HB	1:B:766:TYR:CE2	2.17	0.80
1:A:817:GLU:HG3	1:A:818:PRO:HD3	1.63	0.79
1:A:759:LEU:HB2	1:A:762:GLN:HG3	1.65	0.79
1:A:964:ASP:HA	5:A:1058:HOH:O	1.82	0.79
1:B:771:LEU:HD21	1:B:954:VAL:HG22	1.65	0.79
1:B:771:LEU:HD21	1:B:954:VAL:CG2	2.14	0.78
1:B:87:SER:HB2	1:B:151:PHE:O	1.84	0.77
1:B:817:GLU:HG3	1:B:818:PRO:HD3	1.67	0.76
1:B:384:LEU:HD12	1:B:384:LEU:O	1.86	0.76
1:B:309:ASP:H	1:B:672:ASN:ND2	1.83	0.75
1:A:870:MET:O	1:A:874:ILE:HG12	1.87	0.74
1:B:774:ARG:NH1	1:B:948:ALA:O	2.21	0.74
2:C:19:ARG:HG2	2:C:20:GLN:H	1.52	0.73
1:A:646:ILE:HA	1:A:649:MET:CE	2.19	0.72
1:A:622:ASN:HD22	1:A:622:ASN:N	1.74	0.72
1:A:396:GLN:OE1	1:A:519:ASN:HB2	1.88	0.72
1:A:581:PRO:HG2	1:A:582:PHE:HD1	1.56	0.71
1:B:600:LEU:HD21	1:B:649:MET:HB2	1.72	0.71
2:C:16:LYS:HB2	2:C:17:ARG:HG2	1.72	0.71
1:A:708:THR:OG1	1:A:711:ARG:HD3	1.90	0.71
1:A:584:TYR:CE2	1:A:624:ILE:HG22	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:ILE:HD13	1:A:649:MET:HE3	1.74	0.70
1:B:831:TYR:CZ	2:D:20:GLN:O	2.44	0.70
1:B:908:TRP:CE2	1:B:912:ILE:CG2	2.75	0.70
1:A:294:GLN:H	1:A:297:HIS:HD2	1.40	0.70
1:B:294:GLN:H	1:B:297:HIS:HD2	1.39	0.70
1:B:460:ARG:NH1	1:B:462:ASP:OD1	2.25	0.70
1:A:646:ILE:HD13	1:A:649:MET:CE	2.22	0.69
1:B:855:PRO:CB	1:B:857:HIS:NE2	2.53	0.69
1:A:896:LYS:O	1:A:898:LYS:HE3	1.93	0.69
1:B:962:GLU:OE2	1:B:962:GLU:HA	1.93	0.69
1:A:780:GLN:HE22	1:A:959:LEU:HD11	1.58	0.68
1:B:93:HIS:HE1	1:B:368:ARG:HH21	1.41	0.68
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.29	0.68
1:A:783:ASN:HD21	1:A:786:HIS:H	1.40	0.67
1:A:805:ASN:HD22	1:A:844:GLN:HE22	1.43	0.67
1:B:433:TYR:O	1:B:437:ILE:HG12	1.93	0.67
1:B:908:TRP:NE1	1:B:912:ILE:HG21	2.09	0.67
1:A:309:ASP:H	1:A:672:ASN:ND2	1.90	0.67
1:A:162:LEU:HD23	1:A:270:LEU:HD11	1.77	0.66
1:B:119:LYS:NZ	1:B:171:SER:HB2	2.11	0.66
2:C:16:LYS:HZ2	2:C:16:LYS:N	1.93	0.66
1:A:93:HIS:HE1	1:A:368:ARG:HH21	1.43	0.65
1:A:880:GLU:HB3	1:B:457:GLU:HG2	1.78	0.65
1:A:196:ASN:ND2	1:A:199:TRP:HD1	1.93	0.65
1:A:654:ILE:HD12	1:A:713:LYS:HD2	1.78	0.65
1:B:416:ASP:O	1:B:420:VAL:HG23	1.95	0.65
1:B:556:MET:O	1:B:556:MET:HG3	1.96	0.65
1:A:112:HIS:CE1	1:A:189:GLU:OE1	2.48	0.65
1:B:551:ILE:HG12	1:B:561:PHE:HB3	1.79	0.65
1:A:646:ILE:HA	1:A:649:MET:HE3	1.78	0.65
1:B:76:LEU:HD12	1:B:437:ILE:HG21	1.77	0.65
1:B:622:ASN:H	1:B:622:ASN:ND2	1.94	0.65
1:B:346:LEU:HA	1:B:522:PHE:HE2	1.62	0.64
1:B:906:LYS:NZ	1:B:921:ASP:OD2	2.31	0.64
1:A:616:LEU:HD21	1:A:638:GLN:HG3	1.79	0.64
1:B:346:LEU:HA	1:B:522:PHE:CE2	2.34	0.63
1:A:880:GLU:CB	1:B:457:GLU:HG2	2.28	0.63
1:B:783:ASN:ND2	1:B:785:VAL:H	1.95	0.62
1:A:479:ALA:HB2	3:A:2002:DIO:H2*1	1.82	0.62
1:B:303:LYS:HD2	1:B:485:PHE:CE2	2.34	0.62
1:A:341:GLU:HG2	1:A:347:LEU:HD12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:PRO:HG2	1:A:582:PHE:CD1	2.34	0.62
1:A:674:ARG:HD2	1:A:784:GLU:OE2	2.00	0.62
1:B:831:TYR:OH	2:D:20:GLN:O	2.16	0.62
1:B:308:LYS:HD3	1:B:672:ASN:HB3	1.81	0.62
1:B:349:GLU:OE2	1:B:521:LYS:HD2	2.00	0.61
1:B:285:LEU:HD22	1:B:286:PRO:HD2	1.83	0.61
1:A:147:THR:HG22	1:A:149:TYR:CE1	2.35	0.61
1:B:767:ARG:HG2	1:B:1007:LEU:HD13	1.83	0.61
1:A:184:ASN:HD21	1:A:223:LYS:HE2	1.66	0.61
1:A:114:LEU:HD13	1:A:168:PHE:HB3	1.82	0.61
1:A:392:LEU:HG	1:A:396:GLN:HE21	1.65	0.61
1:A:311:ARG:HH22	1:A:664:GLU:CD	2.04	0.61
1:B:309:ASP:N	1:B:672:ASN:HD21	1.93	0.60
1:A:806:MET:CE	1:A:928:LEU:HG	2.30	0.60
1:A:125:ASN:H	1:A:125:ASN:HD22	1.50	0.60
1:B:446:LEU:HD22	1:B:446:LEU:H	1.66	0.60
1:B:388:GLU:OE2	1:B:509:VAL:HG22	2.02	0.59
1:B:855:PRO:CG	1:B:857:HIS:CD2	2.82	0.59
1:B:932:THR:OG1	1:B:934:GLU:HB2	2.03	0.59
1:A:787:ASN:HB2	1:A:961:ARG:NH1	2.17	0.59
1:B:427:LYS:HZ3	3:B:2001:DIO:H22	1.66	0.59
1:A:102:ASN:H	1:A:102:ASN:HD22	1.51	0.59
1:B:404:GLU:O	1:B:405:GLY:O	2.21	0.58
1:B:638:GLN:HB3	1:B:639:PRO:HD3	1.85	0.58
1:A:831:TYR:OH	2:C:20:GLN:HA	2.04	0.58
1:B:860:GLU:OE2	1:B:957:HIS:HE1	1.86	0.58
1:A:847:ARG:NH1	5:A:1025:HOH:O	2.36	0.58
1:B:250:SER:HB3	1:B:283:VAL:HG23	1.86	0.58
1:B:552:LYS:HB3	1:B:559:LEU:HB3	1.86	0.58
1:A:84:ASP:N	3:A:2001:DIO:H12	2.17	0.58
1:A:948:ALA:HB3	1:A:951:ARG:HB2	1.85	0.57
1:A:316:THR:HB	1:A:374:ILE:HG22	1.87	0.57
1:B:123:LYS:HB3	1:B:126:GLU:HB2	1.85	0.57
1:A:646:ILE:HA	1:A:649:MET:HE2	1.87	0.57
1:B:520:GLY:O	1:B:523:LYS:HE2	2.04	0.57
2:C:17:ARG:HE	2:C:19:ARG:HH22	1.52	0.57
1:A:446:LEU:O	1:A:449:VAL:HG22	2.04	0.56
1:B:236:ASP:OD1	1:B:236:ASP:C	2.43	0.56
1:B:538:LEU:HD23	1:B:734:THR:HG23	1.87	0.56
1:B:597:LEU:HD21	1:B:627:MET:HG2	1.87	0.56
1:A:188:SER:HB3	1:A:831:TYR:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:636:ASP:OD1	1:B:637:LYS:HE2	2.06	0.56
1:B:73:ILE:HG13	1:B:251:SER:HB2	1.87	0.56
1:A:162:LEU:HD23	1:A:270:LEU:CD1	2.36	0.55
1:A:771:LEU:HD21	1:A:954:VAL:CG2	2.36	0.55
1:A:196:ASN:ND2	1:A:199:TRP:CD1	2.73	0.55
1:A:691:THR:O	1:A:999:LYS:HE3	2.07	0.55
1:A:583:ALA:CB	1:A:626:GLY:HA2	2.37	0.55
1:A:767:ARG:HG2	1:A:1007:LEU:CD1	2.37	0.55
1:A:67:LEU:HD23	1:A:75:VAL:HB	1.88	0.55
1:A:827:GLU:OE1	1:A:862:ARG:HD3	2.07	0.55
1:B:93:HIS:CE1	1:B:368:ARG:HH21	2.22	0.54
1:A:806:MET:HE3	1:A:928:LEU:HG	1.88	0.54
1:B:459:PHE:O	1:B:461:PRO:HD3	2.06	0.54
1:A:927:TYR:O	1:A:930:THR:HB	2.07	0.54
1:B:572:ALA:HB3	1:B:638:GLN:OE1	2.08	0.54
1:B:119:LYS:HB2	1:B:171:SER:OG	2.08	0.54
1:A:602:ASP:OD1	1:A:658:ARG:HD3	2.08	0.54
1:B:102:ASN:HD22	1:B:102:ASN:H	1.54	0.54
1:B:62:ARG:HG2	1:B:80:ASP:HB2	1.88	0.53
1:B:196:ASN:ND2	1:B:198:ALA:H	2.06	0.53
1:B:147:THR:HG22	1:B:149:TYR:CE1	2.44	0.53
1:B:154:SER:OG	1:B:891:ILE:HD13	2.07	0.53
1:A:311:ARG:HB3	1:A:379:LEU:HB2	1.89	0.53
1:A:879:GLU:O	1:A:879:GLU:HG3	2.07	0.53
1:B:914:GLN:HE21	1:B:914:GLN:HA	1.73	0.53
1:B:119:LYS:HZ2	1:B:171:SER:HB2	1.73	0.53
1:A:677:GLN:HG3	1:A:678:PRO:HD2	1.91	0.53
1:B:318:PRO:HG2	1:B:475:ASN:HD22	1.73	0.53
1:B:908:TRP:NE1	1:B:912:ILE:CG2	2.72	0.53
1:A:228:THR:O	1:A:228:THR:HG22	2.09	0.52
1:A:172:PRO:HG2	1:A:174:PHE:CE1	2.44	0.52
1:B:386:HIS:HD2	1:B:389:ASP:OD2	1.92	0.52
1:A:760:PRO:HA	1:A:763:LEU:HD12	1.92	0.52
1:A:906:LYS:NZ	1:A:921:ASP:OD2	2.34	0.52
1:A:295:GLU:OE2	1:A:295:GLU:HA	2.09	0.52
1:B:741:ILE:O	1:B:745:VAL:HG23	2.10	0.52
1:A:277:GLU:O	1:A:277:GLU:HG2	2.09	0.52
1:B:629:LEU:HD22	1:B:630:SER:N	2.24	0.52
1:A:94:ILE:HG13	1:A:248:TYR:HB3	1.92	0.52
1:A:400:LYS:HE3	1:A:404:GLU:CG	2.40	0.52
1:B:962:GLU:OE2	1:B:962:GLU:CA	2.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:GLU:C	1:B:230:PRO:HD2	2.30	0.52
1:B:155:HIS:ND1	1:B:261:ARG:HD2	2.25	0.52
1:B:908:TRP:CE2	1:B:912:ILE:HG21	2.45	0.52
1:A:65:ARG:HB2	1:A:264:LEU:HD13	1.92	0.51
1:B:351:LYS:HE3	1:B:602:ASP:OD2	2.10	0.51
1:A:620:LEU:HD12	1:A:628:TYR:O	2.10	0.51
1:A:184:ASN:HD21	1:A:223:LYS:CE	2.24	0.51
1:A:767:ARG:HG2	1:A:1007:LEU:HD13	1.91	0.51
1:B:674:ARG:HB3	1:B:674:ARG:NH1	2.25	0.51
1:B:843:ILE:HG22	1:B:844:GLN:N	2.26	0.51
1:A:776:TRP:CD1	1:A:953:LYS:HG2	2.44	0.51
1:B:827:GLU:OE1	1:B:862:ARG:HD3	2.11	0.51
1:B:311:ARG:HH22	1:B:664:GLU:CD	2.13	0.51
1:A:294:GLN:H	1:A:297:HIS:CD2	2.25	0.51
1:B:800:GLN:HG2	1:B:805:ASN:HD21	1.76	0.51
1:B:294:GLN:H	1:B:297:HIS:CD2	2.24	0.50
1:B:722:ARG:HD3	1:B:756:LYS:HG2	1.93	0.50
1:B:960:ALA:HB3	1:B:963:MET:HG3	1.93	0.50
1:A:940:TYR:CE1	1:A:945:ALA:HB2	2.47	0.50
1:B:90:LEU:HD23	1:B:91:ASP:N	2.26	0.50
1:A:677:GLN:H	1:A:680:GLN:HE21	1.60	0.50
1:B:427:LYS:HZ1	3:B:2001:DIO:C2	2.13	0.50
1:A:930:THR:O	1:A:930:THR:CG2	2.60	0.50
1:B:192:LYS:HD2	1:B:832:ILE:HD11	1.93	0.50
1:B:810:LEU:HG	1:B:928:LEU:HD21	1.94	0.50
1:A:120:LYS:HG2	1:A:167:GLN:HG3	1.94	0.50
1:A:336:HIS:HD2	1:A:337:LEU:HD13	1.76	0.49
1:B:795:TYR:CE2	1:B:953:LYS:HD2	2.47	0.49
1:B:136:GLY:CA	1:B:152:ASP:O	2.61	0.49
1:B:693:VAL:HB	1:B:766:TYR:HE2	1.73	0.49
1:B:603:SER:OG	1:B:648:LYS:HE3	2.12	0.49
1:B:111:GLN:NE2	1:B:142:THR:OG1	2.44	0.49
1:A:599:LEU:HD21	1:A:659:PHE:HA	1.94	0.49
1:A:783:ASN:ND2	1:A:785:VAL:H	2.11	0.49
1:B:1002:LEU:HB2	1:B:1003:PRO:HD2	1.93	0.49
1:A:756:LYS:HB3	1:A:756:LYS:HE3	1.52	0.49
1:B:807:PHE:HE1	1:B:935:ASP:HB3	1.78	0.49
1:A:187:ASP:OD1	1:A:222:ASN:HB2	2.12	0.49
1:A:298:LEU:HD13	1:A:475:ASN:HD22	1.77	0.49
1:A:827:GLU:OE2	1:A:862:ARG:NH1	2.45	0.49
1:B:843:ILE:HG22	1:B:844:GLN:H	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:TYR:HD2	1:A:76:LEU:HD11	1.78	0.48
1:A:386:HIS:HD2	1:A:389:ASP:OD2	1.95	0.48
1:A:714:ALA:O	1:A:717:PRO:HD2	2.13	0.48
1:B:299:LYS:HE3	5:B:1042:HOH:O	2.13	0.48
1:A:930:THR:HG22	1:A:931:LEU:HD12	1.94	0.48
1:B:108:HIS:CE1	1:B:189:GLU:CD	2.83	0.48
1:B:831:TYR:CE1	2:D:20:GLN:O	2.65	0.48
1:A:120:LYS:HE3	1:B:409:TRP:HB3	1.96	0.48
1:A:689:LEU:CD2	1:A:995:MET:HG2	2.43	0.48
1:B:783:ASN:ND2	1:B:786:HIS:H	2.11	0.48
1:A:866:PHE:O	1:A:869:THR:HB	2.13	0.48
1:A:196:ASN:HD22	1:A:199:TRP:H	1.62	0.48
1:A:806:MET:HE2	1:A:928:LEU:HG	1.95	0.48
1:B:711:ARG:HD2	5:B:1049:HOH:O	2.14	0.48
1:B:604:LEU:HD23	1:B:604:LEU:HA	1.73	0.47
1:A:184:ASN:ND2	1:A:223:LYS:CE	2.77	0.47
1:A:511:LYS:HD2	1:A:514:GLN:OE1	2.14	0.47
1:A:201:LEU:HB3	3:A:2000:DIO:O1	2.13	0.47
1:A:336:HIS:CD2	1:A:337:LEU:HD13	2.50	0.47
1:A:805:ASN:HD22	1:A:844:GLN:NE2	2.08	0.47
1:B:189:GLU:HG2	1:B:831:TYR:CE1	2.50	0.47
1:B:722:ARG:HB3	1:B:758:LEU:CD1	2.44	0.47
1:A:638:GLN:HB3	1:A:639:PRO:HD3	1.96	0.47
1:B:827:GLU:OE2	1:B:862:ARG:NH1	2.48	0.47
1:A:62:ARG:HG2	1:A:80:ASP:HB2	1.96	0.47
1:A:545:THR:HG22	1:A:546:PRO:HD2	1.96	0.47
1:A:93:HIS:CE1	1:A:368:ARG:HH21	2.28	0.47
1:A:843:ILE:HG22	1:A:844:GLN:N	2.29	0.47
1:B:314:TYR:HB2	1:B:479:ALA:HB3	1.97	0.47
1:B:879:GLU:O	1:B:882:PHE:HB3	2.15	0.47
1:A:196:ASN:ND2	1:A:199:TRP:H	2.12	0.47
1:A:291:HIS:CE1	1:A:318:PRO:HB3	2.50	0.47
1:B:65:ARG:HB3	1:B:264:LEU:HD22	1.97	0.47
1:B:250:SER:HB3	1:B:283:VAL:CG2	2.45	0.47
1:A:780:GLN:NE2	1:A:959:LEU:HD11	2.27	0.46
1:B:616:LEU:HD21	1:B:638:GLN:HG3	1.97	0.46
1:B:709:LEU:HB3	1:B:710:PRO:HD2	1.97	0.46
1:B:136:GLY:HA3	1:B:152:ASP:O	2.14	0.46
1:B:596:TYR:OH	1:B:649:MET:HG3	2.14	0.46
1:A:154:SER:HB2	1:A:891:ILE:HD13	1.97	0.46
1:A:224:TYR:HA	1:A:228:THR:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:799:MET:HE3	1:A:1008:VAL:HA	1.97	0.46
2:D:3:LEU:HG	2:D:4:ALA:N	2.30	0.46
1:B:512:LYS:HE3	1:B:512:LYS:HB3	1.56	0.46
1:B:632:LYS:NZ	5:B:1020:HOH:O	2.48	0.46
1:A:188:SER:HB3	1:A:831:TYR:CB	2.46	0.46
1:B:384:LEU:HD12	1:B:384:LEU:C	2.36	0.46
1:B:644:LYS:O	1:B:648:LYS:HB2	2.15	0.46
1:A:243:LYS:HD3	1:A:243:LYS:HA	1.87	0.46
1:A:400:LYS:HE3	1:A:404:GLU:HG2	1.96	0.46
1:A:308:LYS:HD3	1:A:672:ASN:HB3	1.97	0.46
1:B:946:VAL:HA	1:B:951:ARG:NE	2.30	0.46
1:B:205:GLU:HG2	1:B:293:PHE:HZ	1.79	0.46
1:B:833:VAL:HG22	1:B:850:ILE:HG12	1.97	0.46
1:B:65:ARG:NH2	1:B:264:LEU:HB3	2.30	0.46
1:B:196:ASN:C	1:B:196:ASN:HD22	2.19	0.46
1:B:311:ARG:HB3	1:B:379:LEU:HB2	1.98	0.46
1:A:559:LEU:HD22	1:A:742:MET:HB2	1.98	0.45
1:B:190:HIS:O	1:B:194:VAL:HG23	2.16	0.45
1:B:361:GLY:HA2	1:B:374:ILE:O	2.16	0.45
1:A:782:ARG:HH12	1:A:963:MET:H	1.63	0.45
1:B:299:LYS:HD2	1:B:510:ILE:HD13	1.98	0.45
1:B:359:LEU:C	1:B:359:LEU:HD23	2.37	0.45
1:B:942:GLU:O	1:B:948:ALA:HB1	2.17	0.45
1:B:299:LYS:CD	1:B:510:ILE:HD13	2.47	0.45
1:B:364:LYS:HB3	1:B:372:PHE:HB2	1.99	0.45
1:B:119:LYS:HZ1	1:B:171:SER:HB2	1.82	0.45
1:B:425:LYS:NZ	1:B:425:LYS:HB3	2.31	0.45
1:B:559:LEU:HD22	1:B:742:MET:HB2	1.98	0.45
1:B:992:ILE:HG23	1:B:998:PHE:HB2	1.98	0.45
1:A:875:GLU:O	1:A:933:LYS:NZ	2.46	0.45
1:A:880:GLU:HB3	1:B:457:GLU:CG	2.45	0.45
1:A:248:TYR:O	1:A:250:SER:N	2.49	0.45
1:B:622:ASN:ND2	1:B:622:ASN:N	2.64	0.45
1:A:71:ASN:HB2	1:A:251:SER:OG	2.17	0.45
1:A:437:ILE:HA	1:A:440:ILE:HG12	1.99	0.45
1:A:815:ILE:HG22	1:A:870:MET:CE	2.47	0.45
1:A:843:ILE:CG2	1:A:844:GLN:N	2.79	0.45
1:B:417:LEU:HD12	1:B:417:LEU:HA	1.85	0.44
1:B:746:GLU:O	1:B:750:ILE:HG12	2.17	0.44
1:A:108:HIS:CE1	1:A:189:GLU:OE1	2.70	0.44
1:A:329:ASN:O	1:A:331:GLY:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:827:GLU:CD	1:A:862:ARG:HH11	2.20	0.44
1:A:799:MET:HE3	1:A:1008:VAL:HG22	1.99	0.44
1:A:84:ASP:H	3:A:2001:DIO:C1	2.19	0.44
1:B:946:VAL:HA	1:B:951:ARG:CZ	2.48	0.44
1:A:201:LEU:HB3	3:A:2000:DIO:C2	2.47	0.44
1:A:245:HIS:O	1:A:249:TYR:HB2	2.18	0.44
1:A:394:MET:O	1:A:398:ILE:HG13	2.17	0.44
1:B:878:THR:HG23	1:B:881:ALA:HB2	1.99	0.44
1:B:97:LEU:HB2	1:B:144:GLY:O	2.17	0.44
1:B:856:PRO:HB2	1:B:957:HIS:CD2	2.52	0.44
1:B:870:MET:O	1:B:874:ILE:HG13	2.18	0.44
1:A:799:MET:HB3	1:A:843:ILE:HG13	1.99	0.44
1:B:409:TRP:CE2	1:B:410:VAL:HG23	2.53	0.44
1:A:788:ASN:O	1:A:960:ALA:HA	2.18	0.43
1:B:756:LYS:HD2	1:B:756:LYS:N	2.33	0.43
1:B:896:LYS:HB2	3:B:2001:DIO:C1'	2.41	0.43
1:A:595:LEU:HD12	1:A:662:ILE:HG22	2.00	0.43
1:A:860:GLU:OE2	1:A:957:HIS:HE1	2.00	0.43
1:B:413:GLU:OE2	1:B:527:LYS:HD2	2.18	0.43
1:A:551:ILE:HG12	1:A:561:PHE:HB3	2.00	0.43
1:A:672:ASN:HD22	1:A:672:ASN:HA	1.62	0.43
1:A:677:GLN:HB2	1:A:680:GLN:HE21	1.84	0.43
1:B:75:VAL:HA	1:B:256:VAL:O	2.18	0.43
1:B:381:GLU:OE2	1:B:664:GLU:HG3	2.18	0.43
1:A:361:GLY:HA2	1:A:374:ILE:O	2.18	0.43
1:A:801:SER:O	1:A:802:THR:C	2.57	0.43
1:A:311:ARG:NH2	1:A:664:GLU:OE2	2.52	0.43
1:A:646:ILE:HD13	1:A:649:MET:HE1	1.99	0.43
1:A:787:ASN:HB2	1:A:961:ARG:HH12	1.84	0.43
1:A:867:LEU:HD12	1:A:867:LEU:HA	1.91	0.43
1:B:86:SER:OG	1:B:260:GLY:HA2	2.19	0.43
1:B:236:ASP:O	1:B:240:GLU:HG2	2.18	0.43
1:B:599:LEU:HD23	1:B:662:ILE:HD12	1.99	0.43
1:A:201:LEU:HB3	3:A:2000:DIO:H21	2.01	0.43
1:A:400:LYS:HE3	1:A:404:GLU:OE2	2.19	0.43
1:A:996:THR:HG23	5:A:1048:HOH:O	2.19	0.43
1:B:928:LEU:O	1:B:931:LEU:HB2	2.19	0.43
1:A:817:GLU:HG3	1:A:818:PRO:CD	2.42	0.43
1:A:578:PHE:HB2	1:A:627:MET:HB2	2.01	0.42
1:A:599:LEU:HD23	1:A:662:ILE:HD13	2.01	0.42
1:A:903:GLU:O	1:A:904:SER:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:600:LEU:CD2	1:B:649:MET:HB2	2.45	0.42
1:B:873:SER:O	1:B:877:MET:HB3	2.19	0.42
1:A:679:HIS:O	1:A:683:MET:HG3	2.18	0.42
1:A:689:LEU:HD23	1:A:995:MET:HG2	2.01	0.42
1:B:195:MET:HB2	1:B:786:HIS:CE1	2.54	0.42
1:B:519:ASN:O	1:B:521:LYS:N	2.53	0.42
1:A:948:ALA:HA	1:A:949:PRO:HD2	1.71	0.42
1:B:429:ARG:HB2	1:B:429:ARG:HH11	1.84	0.42
1:B:774:ARG:HH22	1:B:947:ASP:HA	1.84	0.42
1:B:782:ARG:NH1	1:B:963:MET:O	2.52	0.42
1:A:90:LEU:HD21	1:A:254:MET:HG2	2.00	0.42
1:A:559:LEU:HD11	1:A:729:LEU:HG	2.01	0.42
1:A:622:ASN:ND2	1:A:622:ASN:N	2.42	0.42
1:A:857:HIS:O	1:A:860:GLU:HB2	2.20	0.42
1:B:112:HIS:CE1	1:B:189:GLU:OE1	2.57	0.42
1:B:396:GLN:HG2	1:B:517:ASP:O	2.20	0.42
1:B:656:GLU:OE1	1:B:709:LEU:HD22	2.20	0.42
1:B:81:PRO:O	1:B:261:ARG:HG2	2.20	0.42
1:B:112:HIS:CE1	2:D:20:GLN:HB3	2.55	0.42
1:B:530:PHE:O	1:B:531:ILE:C	2.58	0.42
1:B:714:ALA:O	1:B:718:GLN:HB2	2.20	0.42
1:A:223:LYS:HD2	1:A:227:GLU:OE1	2.20	0.42
1:A:584:TYR:CZ	1:A:624:ILE:HG22	2.55	0.42
1:B:58:PRO:CG	1:B:423:ARG:HD2	2.37	0.42
1:B:189:GLU:HG2	1:B:831:TYR:CZ	2.55	0.42
1:B:457:GLU:HA	1:B:457:GLU:OE2	2.19	0.42
1:B:756:LYS:N	1:B:756:LYS:CD	2.83	0.42
1:A:415:LYS:HG3	1:A:456:LEU:HB2	2.01	0.42
1:A:444:TYR:CD1	1:A:452:ALA:HB1	2.55	0.42
1:B:425:LYS:HD3	1:B:454:TYR:CZ	2.55	0.42
1:B:1002:LEU:CB	1:B:1003:PRO:HD2	2.50	0.42
1:A:78:ILE:O	1:A:259:LEU:HA	2.20	0.41
1:A:184:ASN:ND2	1:A:223:LYS:HE3	2.35	0.41
1:B:246:SER:O	1:B:281:LYS:CD	2.68	0.41
1:B:600:LEU:HD23	1:B:620:LEU:HD21	2.02	0.41
1:B:673:PHE:CD1	1:B:676:GLU:HG3	2.55	0.41
1:B:948:ALA:HB3	1:B:951:ARG:HB2	2.02	0.41
1:A:583:ALA:HB2	1:A:626:GLY:HA2	2.02	0.41
1:A:938:LYS:HB2	1:A:938:LYS:NZ	2.35	0.41
1:B:528:ASN:HB3	1:B:531:ILE:HD11	2.02	0.41
1:A:184:ASN:ND2	1:A:223:LYS:HE2	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LEU:O	1:A:204:LEU:HG	2.20	0.41
1:B:108:HIS:HE1	1:B:189:GLU:CD	2.23	0.41
1:B:597:LEU:HD12	1:B:597:LEU:HA	1.90	0.41
1:A:460:ARG:NH1	1:A:462:ASP:OD1	2.54	0.41
1:A:805:ASN:ND2	1:A:844:GLN:HE22	2.13	0.41
1:B:800:GLN:CB	1:B:805:ASN:HD21	2.33	0.41
1:B:831:TYR:OH	2:D:20:GLN:C	2.58	0.41
1:B:960:ALA:O	1:B:962:GLU:N	2.54	0.41
1:A:48:LYS:HE3	1:A:48:LYS:HB2	1.77	0.41
1:B:869:THR:O	1:B:873:SER:HB2	2.21	0.41
1:B:887:GLN:HE21	1:B:891:ILE:HD11	1.85	0.41
1:A:134:HIS:HD2	1:A:157:HIS:CD2	2.38	0.41
1:A:505:ILE:HA	1:A:506:PRO:HD2	1.94	0.41
1:A:772:PRO:O	1:A:773:ASP:C	2.60	0.41
1:A:809:GLU:HB3	1:A:889:LEU:HD11	2.03	0.41
1:B:799:MET:HE3	1:B:799:MET:HB3	1.66	0.41
1:A:123:LYS:HE2	1:A:123:LYS:HB3	1.97	0.41
1:A:711:ARG:HH21	1:A:711:ARG:CG	2.34	0.41
1:A:620:LEU:HD13	1:A:629:LEU:HG	2.03	0.40
1:A:774:ARG:HD3	5:A:1059:HOH:O	2.21	0.40
1:A:878:THR:OG1	1:B:457:GLU:OE1	2.31	0.40
1:A:889:LEU:HA	1:A:889:LEU:HD23	1.81	0.40
1:B:556:MET:CE	1:B:750:ILE:HD11	2.51	0.40
1:B:979:ASN:HB2	1:B:980:LEU:HG	2.03	0.40
1:A:729:LEU:HD12	1:A:738:ALA:HB1	2.03	0.40
1:B:64:TYR:CE2	1:B:78:ILE:HG12	2.56	0.40
1:B:528:ASN:O	1:B:531:ILE:HG12	2.22	0.40
1:A:49:ARG:O	1:A:67:LEU:HB2	2.21	0.40
1:B:728:LEU:O	1:B:729:LEU:HD23	2.22	0.40
1:B:812:ALA:O	1:B:816:SER:HB2	2.21	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	952/990 (96%)	877 (92%)	69 (7%)	6 (1%)	25	64
1	B	951/990 (96%)	885 (93%)	64 (7%)	2 (0%)	47	82
2	C	6/70 (9%)	4 (67%)	2 (33%)	0	100	100
2	D	4/70 (6%)	2 (50%)	2 (50%)	0	100	100
All	All	1913/2120 (90%)	1768 (92%)	137 (7%)	8 (0%)	34	72

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	405	GLY
1	A	488	LYS
1	A	674	ARG
1	A	757	PRO
1	A	869	THR
1	B	961	ARG
1	A	329	ASN
1	A	750	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	852/879 (97%)	752 (88%)	100 (12%)	5	22
1	B	851/879 (97%)	743 (87%)	108 (13%)	4	19
2	C	7/62 (11%)	5 (71%)	2 (29%)	0	2
2	D	5/62 (8%)	4 (80%)	1 (20%)	1	7
All	All	1715/1882 (91%)	1504 (88%)	211 (12%)	4	21

All (211) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ILE
1	A	67	LEU
1	A	76	LEU
1	A	93	HIS
1	A	97	LEU
1	A	102	ASN
1	A	103	ILE
1	A	111	GLN
1	A	119	LYS
1	A	123	LYS
1	A	125	ASN
1	A	154	SER
1	A	158	LEU
1	A	183	VAL
1	A	188	SER
1	A	201	LEU
1	A	243	LYS
1	A	270	LEU
1	A	281	LYS
1	A	282	ASN
1	A	285	LEU
1	A	287	GLU
1	A	316	THR
1	A	327	LYS
1	A	329	ASN
1	A	337	LEU
1	A	347	LEU
1	A	356	VAL
1	A	360	VAL
1	A	364	LYS
1	A	388	GLU
1	A	399	GLN
1	A	414	LEU
1	A	417	LEU
1	A	423	ARG
1	A	440	ILE
1	A	446	LEU
1	A	449	VAL
1	A	450	LEU
1	A	488	LYS
1	A	494	GLU
1	A	511	LYS
1	A	526	THR

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Mol	Chain	Res	Type
1	A	536	GLU
1	A	538	LEU
1	A	545	THR
1	A	556	MET
1	A	575	ASN
1	A	590	SER
1	A	595	LEU
1	A	597	LEU
1	A	603	SER
1	A	616	LEU
1	A	621	GLN
1	A	622	ASN
1	A	624	ILE
1	A	629	LEU
1	A	635	ASN
1	A	642	LEU
1	A	643	LYS
1	A	662	ILE
1	A	677	GLN
1	A	691	THR
1	A	711	ARG
1	A	712	LEU
1	A	728	LEU
1	A	736	GLN
1	A	744	MET
1	A	751	GLU
1	A	756	LYS
1	A	758	LEU
1	A	771	LEU
1	A	780	GLN
1	A	783	ASN
1	A	810	LEU
1	A	817	GLU
1	A	838	ARG
1	A	846	LEU
1	A	847	ARG
1	A	853	GLU
1	A	854	LYS
1	A	856	PRO
1	A	859	LEU
1	A	867	LEU
1	A	872	LYS

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Mol	Chain	Res	Type
1	A	874	ILE
1	A	889	LEU
1	A	896	LYS
1	A	898	LYS
1	A	914	GLN
1	A	928	LEU
1	A	934	GLU
1	A	950	ARG
1	A	951	ARG
1	A	954	VAL
1	A	957	HIS
1	A	962	GLU
1	A	990	GLU
1	A	993	GLN
1	A	1007	LEU
1	B	43	ASN
1	B	56	LYS
1	B	61	LYS
1	B	63	GLU
1	B	67	LEU
1	B	76	LEU
1	B	84	ASP
1	B	97	LEU
1	B	102	ASN
1	B	103	ILE
1	B	111	GLN
1	B	119	LYS
1	B	125	ASN
1	B	148	ASN
1	B	177	SER
1	B	188	SER
1	B	196	ASN
1	B	201	LEU
1	B	212	LYS
1	B	226	LEU
1	B	243	LYS
1	B	252	ASN
1	B	282	ASN
1	B	285	LEU
1	B	316	THR
1	B	327	LYS
1	B	328	SER

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Mol	Chain	Res	Type
1	B	329	ASN
1	B	347	LEU
1	B	356	VAL
1	B	360	VAL
1	B	384	LEU
1	B	414	LEU
1	B	423	ARG
1	B	429	ARG
1	B	436	LYS
1	B	446	LEU
1	B	450	LEU
1	B	457	GLU
1	B	458	GLU
1	B	464	ILE
1	B	465	GLU
1	B	466	MET
1	B	472	ARG
1	B	511	LYS
1	B	512	LYS
1	B	517	ASP
1	B	521	LYS
1	B	523	LYS
1	B	524	LEU
1	B	529	GLU
1	B	533	THR
1	B	556	MET
1	B	590	SER
1	B	595	LEU
1	B	597	LEU
1	B	612	GLU
1	B	616	LEU
1	B	622	ASN
1	B	629	LEU
1	B	642	LEU
1	B	643	LYS
1	B	648	LYS
1	B	657	LYS
1	B	667	MET
1	B	705	ASP
1	B	711	ARG
1	B	712	LEU
1	B	718	GLN

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Mol	Chain	Res	Type
1	B	721	SER
1	B	722	ARG
1	B	728	LEU
1	B	733	ILE
1	B	756	LYS
1	B	758	LEU
1	B	759	LEU
1	B	771	LEU
1	B	780	GLN
1	B	783	ASN
1	B	788	ASN
1	B	791	ILE
1	B	810	LEU
1	B	817	GLU
1	B	823	LEU
1	B	825	THR
1	B	838	ARG
1	B	846	LEU
1	B	847	ARG
1	B	859	LEU
1	B	867	LEU
1	B	877	MET
1	B	878	THR
1	B	880	GLU
1	B	889	LEU
1	B	906	LYS
1	B	912	ILE
1	B	914	GLN
1	B	928	LEU
1	B	938	LYS
1	B	950	ARG
1	B	954	VAL
1	B	962	GLU
1	B	964	ASP
1	B	980	LEU
1	B	990	GLU
1	B	995	MET
1	B	1002	LEU
1	B	1007	LEU
2	C	3	LEU
2	C	16	LYS
2	D	20	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	102	ASN
1	A	125	ASN
1	A	148	ASN
1	A	184	ASN
1	A	196	ASN
1	A	231	ASN
1	A	232	GLN
1	A	294	GLN
1	A	297	HIS
1	A	300	GLN
1	A	329	ASN
1	A	336	HIS
1	A	386	HIS
1	A	393	HIS
1	A	475	ASN
1	A	502	GLN
1	A	575	ASN
1	A	605	ASN
1	A	622	ASN
1	A	672	ASN
1	A	677	GLN
1	A	680	GLN
1	A	730	HIS
1	A	770	GLN
1	A	780	GLN
1	A	783	ASN
1	A	805	ASN
1	A	828	GLN
1	A	841	ASN
1	A	957	HIS
1	B	43	ASN
1	B	93	HIS
1	B	102	ASN
1	B	111	GLN
1	B	125	ASN
1	B	148	ASN
1	B	184	ASN
1	B	196	ASN
1	B	231	ASN
1	B	297	HIS

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Mol	Chain	Res	Type
1	B	329	ASN
1	B	386	HIS
1	B	475	ASN
1	B	575	ASN
1	B	622	ASN
1	B	672	ASN
1	B	677	GLN
1	B	730	HIS
1	B	783	ASN
1	B	788	ASN
1	B	805	ASN
1	B	828	GLN
1	B	914	GLN
1	B	922	ASN
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](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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	B	2001	-	6,6,6	0.54	0	6,6,6	0.78	0
3	DIO	B	2000	-	6,6,6	0.52	0	6,6,6	0.99	0
3	DIO	A	2000	-	6,6,6	0.57	0	6,6,6	1.04	0
3	DIO	B	2002	-	6,6,6	0.52	0	6,6,6	0.96	0
3	DIO	A	2001	-	6,6,6	0.60	0	6,6,6	1.01	1 (16%)
3	DIO	A	2002	-	6,6,6	0.57	0	6,6,6	0.73	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	B	2001	-	-	-	0/1/1/1
3	DIO	B	2000	-	-	-	0/1/1/1
3	DIO	A	2000	-	-	-	0/1/1/1
3	DIO	B	2002	-	-	-	0/1/1/1
3	DIO	A	2001	-	-	-	0/1/1/1
3	DIO	A	2002	-	-	-	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	DIO	C2-O1-C1	2.04	116.71	109.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2001	DIO	6	0
3	A	2000	DIO	3	0
3	A	2001	DIO	3	0
3	A	2002	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 [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	956/990 (96%)	-0.51	1 (0%) 95 89	25, 45, 62, 80	0
1	B	955/990 (96%)	-0.42	4 (0%) 92 79	20, 54, 69, 85	0
2	C	10/70 (14%)	0.42	1 (10%) 7 2	40, 82, 86, 89	0
2	D	8/70 (11%)	0.54	1 (12%) 3 1	52, 59, 90, 92	0
All	All	1929/2120 (90%)	-0.45	7 (0%) 92 79	20, 49, 67, 92	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	857	HIS	3.2
2	D	21	VAL	2.6
1	A	965	SER	2.2
1	B	964	ASP	2.2
2	C	21	VAL	2.1
1	B	542	LYS	2.0
1	B	543	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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, 95th 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(\AA^2)	Q<0.9
3	DIO	A	2001	6/6	0.44	1.07	155,155,155,155	0
3	DIO	B	2001	6/6	0.50	1.22	158,158,158,159	0
3	DIO	A	2000	6/6	0.81	0.35	98,99,99,99	0
4	ZN	C	42	1/1	0.88	0.19	2,2,2,2	0
3	DIO	A	2002	6/6	0.93	0.24	52,54,56,58	0
3	DIO	B	2000	6/6	0.93	0.32	93,93,94,94	0
4	ZN	B	1	1/1	0.95	0.24	2,2,2,2	0
3	DIO	B	2002	6/6	0.97	0.25	55,56,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.