



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:15 AM GMT

PDB ID : 2WC0  
Title : CRYSTAL STRUCTURE OF HUMAN INSULIN DEGRADING ENZYME  
IN COMPLEX WITH IODINATED INSULIN  
Authors : Manolopoulou, M.; Guo, Q.; Malito, E.; Schilling, A.B.; Tang, W.J.  
Deposited on : 2009-03-06  
Resolution : 2.80 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

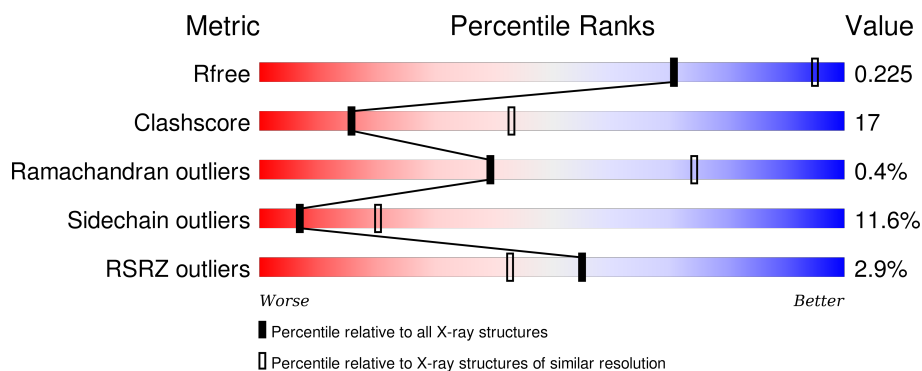
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	990	 61% 30% 5% . .
1	B	990	 59% 30% 6% . .
2	C	21	 29% 52% 14% 5%
2	E	21	 29% 43% 24% 5%
3	D	30	 33% 20% 10% 33%

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Mol	Chain	Length	Quality of chain
3	F	30	

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
5	DIO	A	3015	-	-	-	X
5	DIO	B	3015	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16597 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	953	Total	C	N	O	S	0	0	1
			7781	5013	1307	1439	22			
1	B	955	Total	C	N	O	S	0	0	1
			7790	5019	1308	1441	22			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
A	974	ALA	CYS	ENGINEERED MUTATION	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 INSULIN A CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	21	Total 155	C 95	N 24	O 32	S 4	0	0	1
2	E	21	Total 155	C 95	N 24	O 32	S 4	0	0	1

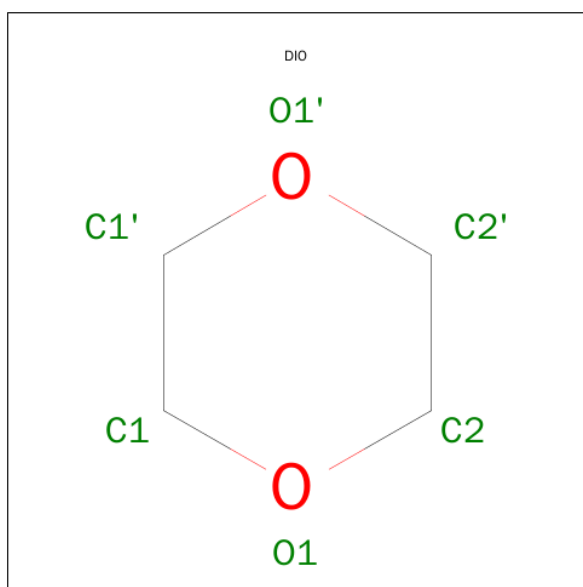
- Molecule 3 is a protein called INSULIN B CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	20	Total 153	C 99	N 26	O 26	S 2	0	0	0
3	F	20	Total 153	C 99	N 26	O 26	S 2	0	0	0

- 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	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 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
5	A	1	Total	C	O	0	0
			6	4	2		
5	A	1	Total	C	O	0	0
			6	4	2		
5	A	1	Total	C	O	0	0
			6	4	2		
5	A	1	Total	C	O	0	0
			6	4	2		
5	B	1	Total	C	O	0	0
			6	4	2		
5	B	1	Total	C	O	0	0
			6	4	2		
5	B	1	Total	C	O	0	0
			6	4	2		
5	B	1	Total	C	O	0	0
			6	4	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	189	Total	O	0	0
			189	189		
6	B	163	Total	O	0	0
			163	163		
6	C	3	Total	O	0	0
			3	3		
6	D	2	Total	O	0	0
			2	2		

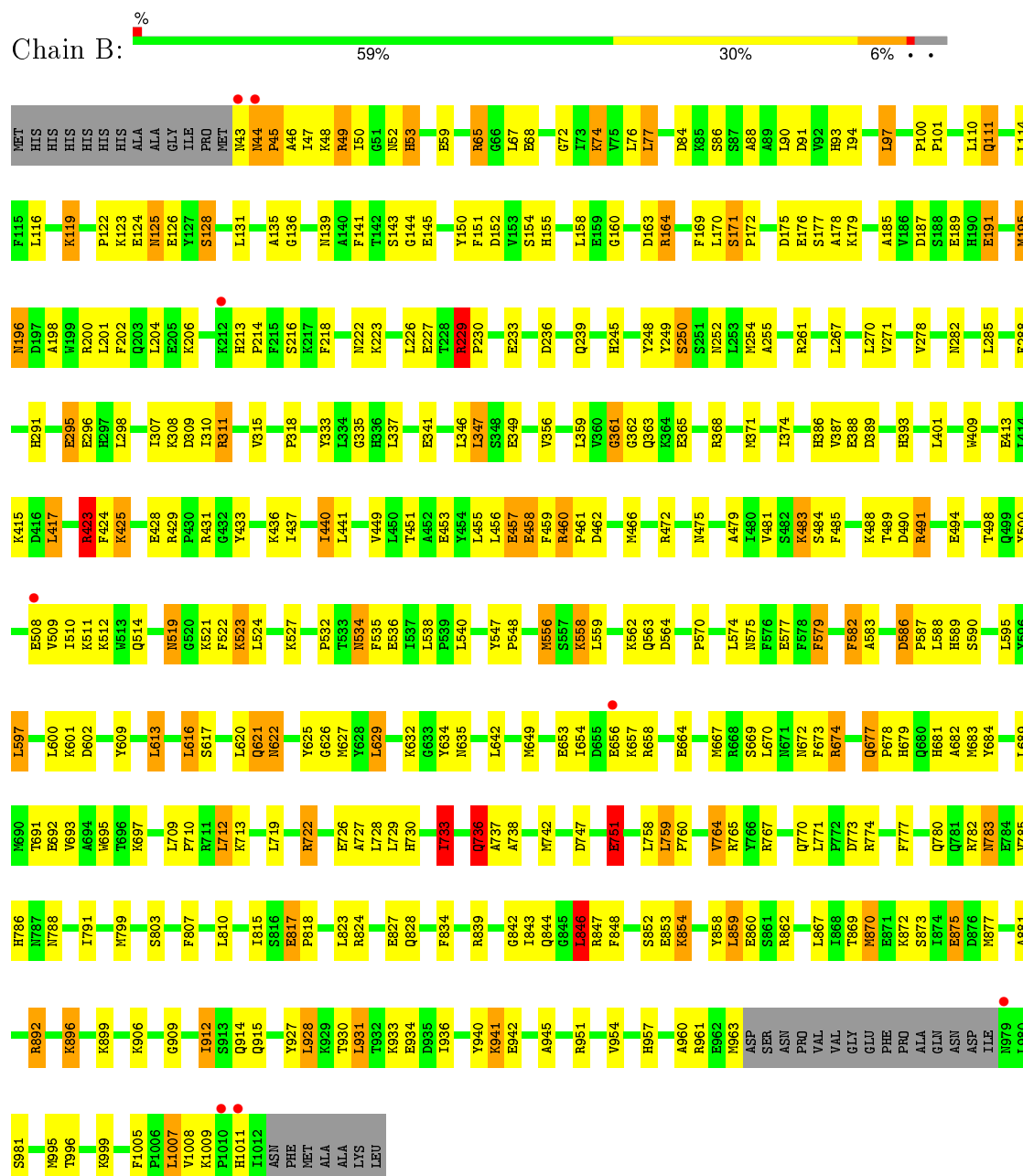
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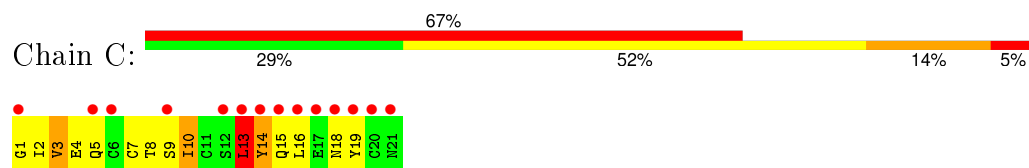
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	1	Total	O	0	0
			1	1		
6	F	2	Total	O	0	0
			2	2		



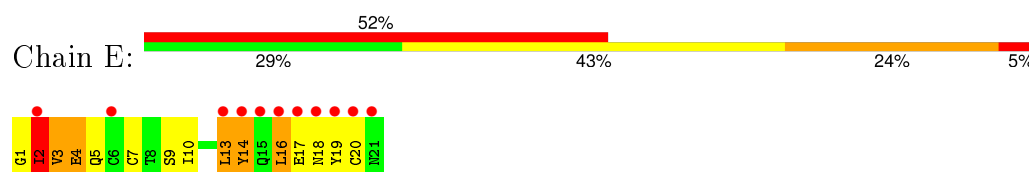




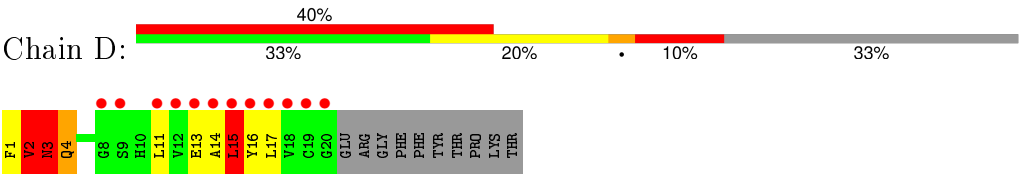
• Molecule 2: INSULIN A CHAIN



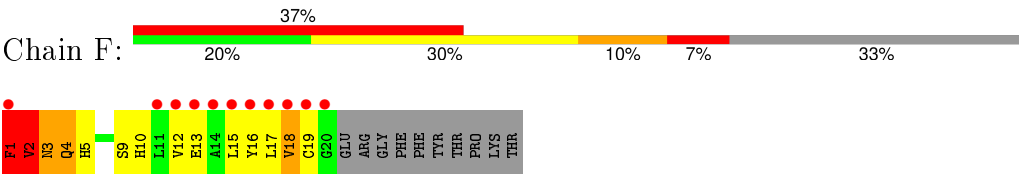
• Molecule 2: INSULIN A CHAIN



● Molecule 3: INSULIN B CHAIN



● Molecule 3: INSULIN B CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	263.17Å 263.17Å 90.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.85 – 2.80 29.85 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.85-2.80) 99.7 (29.85-2.80)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.36 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.170 , 0.220 0.181 , 0.225	Depositor DCC
$R_{free}$ test set	4422 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.1	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 60.3	EDS
Estimated twinning fraction	0.026 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 88359 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16597	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% 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

### 5.1 Standard geometry

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	1.48	53/7973 (0.7%)	1.27	51/10784 (0.5%)
1	B	1.37	27/7985 (0.3%)	1.24	42/10805 (0.4%)
2	C	1.33	0/156	1.41	2/211 (0.9%)
2	E	1.10	1/156 (0.6%)	1.41	2/211 (0.9%)
3	D	1.66	0/156	1.68	5/211 (2.4%)
3	F	1.38	1/156 (0.6%)	2.00	8/211 (3.8%)
All	All	1.42	82/16582 (0.5%)	1.27	110/22433 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
3	D	1	2
All	All	1	3

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	367	ALA	CA-CB	-9.07	1.33	1.52
1	A	871	GLU	CG-CD	9.06	1.65	1.51
1	A	189	GLU	CD-OE1	8.43	1.34	1.25
1	B	189	GLU	CG-CD	8.25	1.64	1.51
1	A	458	GLU	CB-CG	-8.25	1.36	1.52
1	A	189	GLU	CG-CD	8.08	1.64	1.51
1	A	287	GLU	CG-CD	7.92	1.63	1.51
1	A	536	GLU	CG-CD	7.91	1.63	1.51
1	A	673	PHE	CE1-CZ	7.85	1.52	1.37
1	B	458	GLU	CG-CD	7.49	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	508	GLU	CG-CD	7.42	1.63	1.51
1	A	447	GLU	CG-CD	7.29	1.62	1.51
1	B	632	LYS	CD-CE	7.17	1.69	1.51
1	A	784	GLU	CG-CD	7.14	1.62	1.51
1	A	768	GLU	CD-OE1	7.08	1.33	1.25
1	A	577	GLU	CG-CD	7.03	1.62	1.51
1	B	764	VAL	CA-CB	7.00	1.69	1.54
1	A	150	TYR	CE1-CZ	6.96	1.47	1.38
1	A	880	GLU	CG-CD	6.78	1.62	1.51
1	B	349	GLU	CG-CD	6.71	1.62	1.51
1	B	494	GLU	CG-CD	6.64	1.61	1.51
1	A	243	LYS	CD-CE	6.57	1.67	1.51
1	B	361	GLY	C-O	6.52	1.34	1.23
1	A	582	PHE	CB-CG	-6.46	1.40	1.51
3	F	16	TYR	CE1-CZ	6.46	1.47	1.38
1	B	218	PHE	CE2-CZ	6.31	1.49	1.37
1	B	853	GLU	CG-CD	6.30	1.61	1.51
1	A	141	PHE	CD1-CE1	6.13	1.51	1.39
1	A	854	LYS	CB-CG	6.09	1.69	1.52
1	A	243	LYS	CB-CG	6.05	1.68	1.52
1	B	511	LYS	CD-CE	6.03	1.66	1.51
1	A	582	PHE	CE2-CZ	6.00	1.48	1.37
1	B	673	PHE	CE2-CZ	5.98	1.48	1.37
1	A	669	SER	CA-CB	-5.95	1.44	1.52
1	B	189	GLU	CD-OE2	5.93	1.32	1.25
1	A	1005	PHE	CE1-CZ	5.84	1.48	1.37
1	A	243	LYS	CG-CD	5.83	1.72	1.52
1	A	676	GLU	CG-CD	5.83	1.60	1.51
1	A	517	ASP	CB-CG	5.79	1.64	1.51
1	B	834	PHE	CD2-CE2	5.79	1.50	1.39
1	A	168	PHE	CE2-CZ	5.71	1.48	1.37
1	B	494	GLU	CB-CG	5.69	1.62	1.52
1	B	621	GLN	CG-CD	5.68	1.64	1.51
1	A	934	GLU	CD-OE1	5.66	1.31	1.25
1	A	150	TYR	CD1-CE1	5.66	1.47	1.39
1	A	854	LYS	CD-CE	5.63	1.65	1.51
1	A	287	GLU	CD-OE2	5.59	1.31	1.25
1	A	295	GLU	CG-CD	5.59	1.60	1.51
1	A	632	LYS	CD-CE	5.54	1.65	1.51
1	A	453	GLU	CD-OE2	5.53	1.31	1.25
1	A	854	LYS	CE-NZ	5.51	1.62	1.49
1	A	523	LYS	CD-CE	5.50	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	239	GLN	CG-CD	5.49	1.63	1.51
1	B	736	GLN	CG-CD	5.47	1.63	1.51
1	A	713	LYS	CD-CE	5.39	1.64	1.51
1	A	522	PHE	CE1-CZ	5.34	1.47	1.37
1	B	834	PHE	CD1-CE1	5.32	1.49	1.39
1	A	191	GLU	CD-OE1	5.25	1.31	1.25
1	A	277	GLU	CG-CD	5.25	1.59	1.51
1	A	503	GLU	CB-CG	-5.22	1.42	1.52
1	A	159	GLU	CD-OE1	5.21	1.31	1.25
1	B	582	PHE	CE1-CZ	5.20	1.47	1.37
1	A	703	ALA	CA-CB	-5.19	1.41	1.52
1	B	191	GLU	CG-CD	5.19	1.59	1.51
1	A	188	SER	CB-OG	-5.17	1.35	1.42
1	A	511	LYS	CG-CD	5.17	1.70	1.52
1	A	59	GLU	CD-OE2	5.16	1.31	1.25
1	B	315	VAL	CB-CG2	-5.15	1.42	1.52
1	B	494	GLU	CD-OE2	5.13	1.31	1.25
1	A	614	ALA	CA-CB	-5.13	1.41	1.52
1	B	579	PHE	CE2-CZ	5.11	1.47	1.37
1	A	130	PHE	CE1-CZ	5.10	1.47	1.37
1	B	669	SER	CB-OG	-5.08	1.35	1.42
1	A	854	LYS	CG-CD	5.07	1.69	1.52
1	A	365	GLU	CG-CD	5.06	1.59	1.51
1	A	577	GLU	CD-OE1	5.04	1.31	1.25
1	B	632	LYS	CG-CD	5.04	1.69	1.52
1	A	511	LYS	CD-CE	5.03	1.63	1.51
1	A	527	LYS	CD-CE	5.03	1.63	1.51
1	B	481	VAL	CB-CG2	-5.03	1.42	1.52
2	E	14	TYR	CG-CD1	5.03	1.45	1.39
1	A	349	GLU	CG-CD	5.00	1.59	1.51

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	674	ARG	NE-CZ-NH1	16.35	128.47	120.30
3	F	1	PHE	N-CA-C	-14.93	70.69	111.00
1	A	586	ASP	CB-CG-OD1	13.06	130.05	118.30
1	B	460	ARG	NE-CZ-NH1	-11.26	114.67	120.30
3	F	2	VAL	N-CA-CB	-11.24	86.78	111.50
1	A	460	ARG	NE-CZ-NH2	-11.11	114.75	120.30
1	B	667	MET	CG-SD-CE	10.93	117.69	100.20
1	B	49	ARG	CB-CA-C	10.56	131.52	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	431	ARG	NE-CZ-NH2	-10.06	115.27	120.30
1	B	295	GLU	CB-CA-C	-9.75	90.90	110.40
1	A	65	ARG	NE-CZ-NH1	-9.66	115.47	120.30
1	A	674	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	A	181	ARG	NE-CZ-NH2	-9.43	115.58	120.30
1	A	460	ARG	NE-CZ-NH1	9.32	124.96	120.30
1	B	839	ARG	NE-CZ-NH1	-9.14	115.73	120.30
3	F	2	VAL	CB-CA-C	-9.00	94.30	111.40
1	B	892	ARG	NE-CZ-NH2	8.68	124.64	120.30
1	A	586	ASP	CB-CG-OD2	-8.64	110.52	118.30
1	B	295	GLU	N-CA-C	8.20	133.14	111.00
3	D	14	ALA	CB-CA-C	8.19	122.39	110.10
1	B	674	ARG	NE-CZ-NH2	-7.97	116.32	120.30
1	A	65	ARG	NE-CZ-NH2	7.92	124.26	120.30
1	B	189	GLU	CG-CD-OE2	7.89	134.09	118.30
3	D	3	ASN	C-N-CA	7.71	140.98	121.70
1	A	347	LEU	CA-CB-CG	7.59	132.77	115.30
1	A	431	ARG	NE-CZ-NH1	-7.59	116.51	120.30
1	A	49	ARG	CB-CA-C	7.50	125.41	110.40
1	B	423	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	A	181	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	B	847	ARG	NE-CZ-NH2	-7.09	116.76	120.30
1	B	195	MET	CG-SD-CE	7.03	111.45	100.20
1	A	862	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	A	824	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	A	667	MET	CG-SD-CE	6.92	111.28	100.20
1	A	510	ILE	CG1-CB-CG2	-6.84	96.35	111.40
1	A	402	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	B	116	LEU	CB-CG-CD2	6.73	122.45	111.00
3	D	3	ASN	CB-CA-C	-6.54	97.32	110.40
1	B	846	LEU	CA-CB-CG	6.53	130.32	115.30
3	F	17	LEU	CA-CB-CG	6.44	130.11	115.30
1	B	229	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	B	67	LEU	CA-CB-CG	6.29	129.76	115.30
1	B	425	LYS	CD-CE-NZ	6.25	126.07	111.70
1	A	681	HIS	CB-CA-C	-6.23	97.94	110.40
1	A	565	ASP	CB-CG-OD2	6.22	123.90	118.30
1	A	681	HIS	N-CA-CB	6.21	121.78	110.60
3	F	19	CYS	N-CA-C	6.21	127.76	111.00
1	A	60	ASP	CB-CG-OD1	6.20	123.88	118.30
1	A	713	LYS	CD-CE-NZ	6.19	125.95	111.70
1	B	423	ARG	NE-CZ-NH2	-6.17	117.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	ILE	CB-CA-C	6.16	123.92	111.60
1	B	52	ASN	N-CA-C	6.14	127.57	111.00
1	B	53	HIS	N-CA-C	-6.08	94.57	111.00
2	C	13	LEU	CA-CB-CG	6.04	129.19	115.30
1	A	462	ASP	CB-CG-OD2	6.02	123.72	118.30
1	B	401	LEU	CB-CG-CD2	5.98	121.17	111.00
1	B	311	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	A	886	ILE	CG1-CB-CG2	-5.93	98.35	111.40
1	B	65	ARG	NE-CZ-NH1	-5.91	117.34	120.30
1	A	674	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	B	564	ASP	CB-CG-OD1	5.88	123.59	118.30
1	B	597	LEU	CB-CG-CD1	5.88	120.99	111.00
1	A	226	LEU	CB-CG-CD2	-5.87	101.01	111.00
1	A	705	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	B	669	SER	N-CA-CB	-5.79	101.81	110.50
3	F	3	ASN	CB-CA-C	5.76	121.93	110.40
2	C	14	TYR	CB-CA-C	-5.73	98.93	110.40
1	A	189	GLU	CG-CD-OE1	5.67	129.65	118.30
1	A	930	THR	CA-CB-CG2	5.67	120.33	112.40
3	F	17	LEU	CB-CG-CD2	5.66	120.63	111.00
1	A	601	LYS	CD-CE-NZ	-5.66	98.69	111.70
3	F	1	PHE	CB-CA-C	5.64	121.69	110.40
1	A	711	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	B	854	LYS	CB-CG-CD	5.59	126.14	111.60
1	A	67	LEU	CB-CG-CD2	-5.58	101.51	111.00
1	A	309	ASP	CB-CG-OD1	5.55	123.30	118.30
1	B	261	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	A	824	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	A	667	MET	CA-CB-CG	5.53	122.69	113.30
1	A	175	ASP	CB-CG-OD1	-5.51	113.34	118.30
1	A	490	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	767	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	321	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	B	751	GLU	N-CA-C	5.41	125.61	111.00
1	A	92	VAL	CB-CA-C	-5.40	101.14	111.40
1	A	483	LYS	CD-CE-NZ	-5.39	99.30	111.70
3	D	15	LEU	CA-CB-CG	5.37	127.64	115.30
1	A	429	ARG	CG-CD-NE	-5.26	100.76	111.80
1	B	632	LYS	CD-CE-NZ	5.25	123.77	111.70
1	B	77	LEU	CB-CG-CD1	-5.24	102.08	111.00
1	A	229	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	327	LYS	CD-CE-NZ	-5.21	99.71	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	LEU	CB-CA-C	-5.19	100.33	110.20
1	B	613	LEU	CB-CG-CD2	5.16	119.77	111.00
1	A	838	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	668	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	670	LEU	CB-CG-CD2	5.12	119.71	111.00
1	B	954	VAL	CB-CA-C	-5.11	101.70	111.40
1	B	337	LEU	CB-CG-CD1	-5.10	102.33	111.00
1	A	313	LEU	CB-CG-CD2	-5.09	102.34	111.00
1	A	229	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	B	854	LYS	CA-CB-CG	5.08	124.57	113.40
1	A	450	LEU	CB-CG-CD1	5.07	119.62	111.00
3	D	14	ALA	N-CA-C	5.07	124.70	111.00
1	B	751	GLU	CB-CA-C	-5.07	100.26	110.40
1	A	366	GLY	N-CA-C	-5.05	100.46	113.10
1	A	97	LEU	CB-CG-CD1	5.03	119.55	111.00
1	B	733	ILE	CB-CA-C	-5.02	101.56	111.60
2	E	16	LEU	CB-CA-C	-5.00	100.69	110.20
1	B	163	ASP	CB-CG-OD2	-5.00	113.80	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	14	ALA	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1010	PRO	Peptide
3	D	2	VAL	Peptide
3	D	3	ASN	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	7781	0	7719	242	0
1	B	7790	0	7719	272	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	155	0	143	29	0
2	E	155	0	143	39	0
3	D	153	0	149	8	0
3	F	153	0	149	20	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	24	0	32	1	0
5	B	24	0	32	6	0
6	A	189	0	0	43	0
6	B	163	0	0	27	0
6	C	3	0	0	1	0
6	D	2	0	0	0	0
6	E	1	0	0	0	0
6	F	2	0	0	1	0
All	All	16597	0	16086	551	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (551) 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:597:LEU:HA	6:B:2095:HOH:O	1.17	1.33
1:B:361:GLY:O	2:E:2:ILE:HA	1.29	1.24
6:A:2116:HOH:O	2:C:2:ILE:HG22	1.24	1.24
1:B:736:GLN:HB2	6:B:2123:HOH:O	1.07	1.23
1:A:243:LYS:HG3	6:A:2041:HOH:O	1.38	1.21
1:A:195:MET:HA	6:A:2034:HOH:O	1.39	1.18
1:A:782:ARG:HD3	6:A:2145:HOH:O	1.47	1.14
1:A:856:PRO:O	1:A:858:TYR:N	1.85	1.10
1:A:359:LEU:O	2:C:1:GLY:HA2	1.52	1.10
6:A:2116:HOH:O	2:C:2:ILE:CG2	1.81	1.08
1:A:577:GLU:HG3	6:A:2141:HOH:O	1.55	1.07
2:E:3:VAL:HG12	2:E:7:CYS:SG	1.94	1.06
1:A:431:ARG:HD2	6:A:2022:HOH:O	1.55	1.05
1:B:597:LEU:HD12	6:B:2095:HOH:O	1.53	1.05
1:B:335:GLY:HA3	2:E:2:ILE:CG2	1.86	1.04
1:B:577:GLU:OE2	6:B:2091:HOH:O	1.74	1.03
1:B:44:ASN:O	6:B:2001:HOH:O	1.77	1.01
1:A:361:GLY:N	2:C:1:GLY:O	1.93	1.00
1:A:429:ARG:NH2	2:C:14:TYR:HE1	1.62	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:898:LYS:HE2	6:A:2010:HOH:O	1.63	0.97
1:A:365:GLU:OE2	2:C:9:SER:HB3	1.65	0.96
1:B:335:GLY:CA	2:E:2:ILE:CG2	2.44	0.95
1:B:368:ARG:HD2	6:B:2036:HOH:O	1.65	0.94
1:B:335:GLY:HA3	2:E:2:ILE:HG21	1.45	0.93
1:A:274:LEU:HG	6:A:2046:HOH:O	1.68	0.93
2:C:16:LEU:HG	6:C:2002:HOH:O	1.70	0.90
1:B:456:LEU:C	6:B:2070:HOH:O	2.07	0.90
1:A:782:ARG:CD	6:A:2145:HOH:O	2.08	0.90
1:B:363:GLN:O	2:E:3:VAL:HG21	1.72	0.89
1:A:622:ASN:H	1:A:622:ASN:HD22	1.13	0.89
1:B:622:ASN:H	1:B:622:ASN:HD22	1.16	0.89
1:A:243:LYS:CG	6:A:2041:HOH:O	2.04	0.88
1:B:68:GLU:HG2	6:B:2003:HOH:O	1.74	0.87
2:E:13:LEU:HD13	2:E:17:GLU:CD	1.96	0.86
1:B:196:ASN:ND2	1:B:198:ALA:H	1.74	0.85
2:E:13:LEU:HD11	2:E:17:GLU:OE2	1.76	0.85
2:E:17:GLU:HG2	3:F:18:VAL:HG13	1.57	0.85
1:B:995:MET:SD	6:B:2129:HOH:O	2.33	0.85
1:B:48:LYS:O	1:B:49:ARG:HB2	1.78	0.82
1:A:622:ASN:H	1:A:622:ASN:ND2	1.78	0.81
1:A:429:ARG:NH2	2:C:14:TYR:CE1	2.48	0.81
3:D:11:LEU:O	3:D:15:LEU:HB2	1.80	0.80
2:E:16:LEU:O	2:E:19:TYR:CD2	2.35	0.79
1:A:99:ASP:O	1:A:217:LYS:NZ	2.16	0.79
1:B:656:GLU:HG3	1:B:709:LEU:HD22	1.62	0.79
1:B:77:LEU:HD21	1:B:271:VAL:HG11	1.63	0.79
1:B:291:HIS:NE2	6:B:2053:HOH:O	2.14	0.78
1:A:486:GLU:HB2	6:A:2088:HOH:O	1.83	0.78
1:A:309:ASP:H	1:A:672:ASN:HD21	1.31	0.78
1:B:456:LEU:O	6:B:2070:HOH:O	2.01	0.78
2:E:16:LEU:O	2:E:19:TYR:HD2	1.64	0.78
1:B:782:ARG:HH21	1:B:963:MET:H	1.29	0.78
1:A:93:HIS:HE1	1:A:368:ARG:HH21	1.32	0.77
1:B:579:PHE:HE2	1:B:765:ARG:HH12	1.30	0.77
1:B:335:GLY:CA	2:E:2:ILE:HG21	2.12	0.77
1:A:199:TRP:HH2	3:D:3:ASN:HA	1.51	0.76
1:A:927:TYR:O	1:A:930:THR:HB	1.84	0.76
1:B:371:MET:O	6:B:2053:HOH:O	2.04	0.76
1:A:722:ARG:HB2	1:A:758:LEU:HD12	1.68	0.76
1:A:827:GLU:OE1	1:A:862:ARG:HD3	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:GLY:CA	2:E:2:ILE:HG23	2.15	0.75
1:B:361:GLY:N	2:E:1:GLY:O	2.20	0.75
1:B:296:GLU:OE2	1:B:296:GLU:N	2.18	0.75
1:A:875:GLU:HG2	1:B:53:HIS:CE1	2.23	0.74
1:A:423:ARG:CG	1:A:423:ARG:HH11	2.01	0.74
2:E:13:LEU:CD1	2:E:17:GLU:OE2	2.34	0.74
1:A:783:ASN:ND2	1:A:786:HIS:H	1.85	0.74
1:B:341:GLU:HG2	1:B:347:LEU:HD12	1.71	0.73
1:A:102:ASN:HD22	1:A:102:ASN:H	1.35	0.73
1:A:709:LEU:HB3	1:A:710:PRO:HD3	1.71	0.73
1:B:810:LEU:HD22	1:B:936:ILE:HG13	1.71	0.73
1:A:200:ARG:NH1	6:A:2034:HOH:O	2.21	0.72
1:A:294:GLN:H	1:A:297:HIS:HD2	1.37	0.72
1:B:49:ARG:O	1:B:50:ILE:HG13	1.89	0.72
1:A:934:GLU:OE1	1:B:53:HIS:HB2	1.90	0.72
1:B:691:THR:O	1:B:999:LYS:HE3	1.90	0.71
1:B:196:ASN:HD22	1:B:196:ASN:C	1.92	0.71
1:A:277:GLU:HG2	6:A:2047:HOH:O	1.89	0.71
1:A:671:ASN:OD1	1:A:701:LYS:HE2	1.91	0.71
1:A:431:ARG:CD	6:A:2022:HOH:O	2.23	0.71
1:B:747:ASP:O	1:B:751:GLU:HB2	1.90	0.71
1:A:199:TRP:CH2	3:D:3:ASN:HA	2.26	0.70
1:A:196:ASN:HD22	1:A:199:TRP:H	1.39	0.70
1:B:852:SER:HB3	1:B:859:LEU:HD21	1.72	0.70
1:B:574:LEU:HD22	1:B:729:LEU:HD22	1.75	0.69
1:A:229:ARG:HD2	1:A:233:GLU:OE2	1.93	0.69
1:A:783:ASN:HD22	1:A:786:HIS:H	1.40	0.69
1:A:382:GLU:HB2	6:A:2068:HOH:O	1.93	0.69
1:B:843:ILE:HG22	1:B:844:GLN:H	1.56	0.68
1:B:335:GLY:C	2:E:2:ILE:HG23	2.14	0.68
1:B:860:GLU:OE2	1:B:957:HIS:HE1	1.76	0.68
1:B:309:ASP:H	1:B:672:ASN:HD21	1.39	0.68
1:B:843:ILE:HD13	1:B:843:ILE:N	2.08	0.68
1:B:47:ILE:HG22	1:B:49:ARG:O	1.92	0.67
1:A:47:ILE:CG2	1:A:49:ARG:O	2.43	0.67
1:B:441:LEU:HD23	1:B:449:VAL:HG11	1.76	0.67
1:B:335:GLY:C	2:E:2:ILE:CG2	2.62	0.67
1:A:303:LYS:HD3	1:A:485:PHE:CE2	2.30	0.67
1:A:491:ARG:HG2	1:A:491:ARG:HH11	1.59	0.67
2:E:13:LEU:CD1	2:E:17:GLU:CD	2.63	0.66
1:B:622:ASN:N	1:B:622:ASN:HD22	1.89	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:783:ASN:HD22	1:B:785:VAL:H	1.42	0.66
1:B:621:GLN:HB3	6:B:2102:HOH:O	1.96	0.66
2:C:3:VAL:HG12	2:C:7:CYS:SG	2.35	0.66
1:A:674:ARG:NH1	6:A:2133:HOH:O	2.29	0.66
3:F:2:VAL:HG13	3:F:3:ASN:N	2.10	0.66
3:F:1:PHE:H3	3:F:1:PHE:HD2	1.44	0.66
1:A:431:ARG:NH1	2:C:14:TYR:HE2	1.94	0.66
1:A:125:ASN:HD22	1:A:125:ASN:H	1.41	0.65
1:B:196:ASN:ND2	1:B:198:ALA:N	2.44	0.65
1:B:93:HIS:HD2	1:B:145:GLU:O	1.80	0.65
1:B:709:LEU:HB3	1:B:710:PRO:HD3	1.78	0.65
1:A:491:ARG:HG2	1:A:491:ARG:NH1	2.12	0.65
1:A:422:PHE:O	6:A:2078:HOH:O	2.15	0.65
3:F:2:VAL:CG1	3:F:3:ASN:N	2.56	0.65
1:B:68:GLU:CG	6:B:2003:HOH:O	2.38	0.65
1:A:724:HIS:HA	6:A:2139:HOH:O	1.95	0.65
1:A:795:TYR:CE2	1:A:953:LYS:HD2	2.31	0.65
1:B:47:ILE:CG2	1:B:49:ARG:O	2.44	0.65
1:A:722:ARG:HB2	1:A:758:LEU:CD1	2.27	0.65
1:A:360:VAL:HA	2:C:1:GLY:HA2	1.79	0.64
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.33	0.64
1:B:713:LYS:HE2	6:B:2107:HOH:O	1.97	0.64
1:A:108:HIS:NE2	1:A:189:GLU:OE1	2.30	0.64
1:A:189:GLU:HG3	1:A:831:TYR:CE1	2.32	0.64
1:B:436:LYS:HE2	6:B:2065:HOH:O	1.96	0.64
1:A:184:ASN:HD21	1:A:223:LYS:HE2	1.62	0.64
1:B:191:GLU:HG3	1:B:788:ASN:HD21	1.63	0.63
1:A:880:GLU:CG	1:B:457:GLU:HG2	2.29	0.63
1:B:141:PHE:HA	3:F:1:PHE:N	2.14	0.63
1:B:510:ILE:O	1:B:514:GLN:HG3	1.98	0.63
1:B:125:ASN:H	1:B:125:ASN:HD22	1.46	0.63
2:E:3:VAL:CG1	2:E:7:CYS:SG	2.79	0.62
1:B:523:LYS:HD3	1:B:523:LYS:N	2.14	0.62
1:A:188:SER:HB3	1:A:831:TYR:HB2	1.80	0.62
1:B:843:ILE:HG22	1:B:844:GLN:N	2.13	0.62
1:A:486:GLU:CB	6:A:2088:HOH:O	2.43	0.62
1:B:309:ASP:H	1:B:672:ASN:ND2	1.97	0.62
1:A:771:LEU:HD21	1:A:954:VAL:CG2	2.30	0.61
1:A:108:HIS:CE1	1:A:189:GLU:OE1	2.53	0.61
1:B:722:ARG:CZ	6:B:2120:HOH:O	2.48	0.61
1:A:360:VAL:HA	2:C:1:GLY:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:PRO:HG2	1:B:475:ASN:HD21	1.65	0.61
1:A:423:ARG:HG2	1:A:423:ARG:HH11	1.65	0.61
1:A:431:ARG:NH1	2:C:14:TYR:CE2	2.68	0.61
1:B:429:ARG:CG	1:B:429:ARG:HH11	2.13	0.61
1:B:722:ARG:HB3	1:B:758:LEU:CD1	2.31	0.60
1:A:616:LEU:HD21	1:A:638:GLN:HG3	1.84	0.60
1:A:852:SER:HB3	1:A:859:LEU:HD21	1.83	0.60
1:B:451:THR:HB	1:B:455:LEU:HD12	1.83	0.60
1:A:577:GLU:CG	6:A:2141:HOH:O	2.28	0.59
1:B:93:HIS:HE1	1:B:368:ARG:HH21	1.51	0.59
1:A:730:HIS:HD2	1:A:904:SER:OG	1.86	0.59
1:B:48:LYS:CG	1:B:48:LYS:O	2.51	0.58
1:B:656:GLU:HG3	1:B:709:LEU:CD2	2.31	0.58
1:A:724:HIS:CA	6:A:2139:HOH:O	2.49	0.58
1:B:783:ASN:ND2	1:B:786:HIS:H	2.01	0.58
1:B:111:GLN:HE22	3:F:1:PHE:N	2.02	0.58
1:B:602:ASP:OD1	1:B:658:ARG:HD2	2.03	0.58
1:A:309:ASP:H	1:A:672:ASN:ND2	1.97	0.58
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.86	0.58
1:B:196:ASN:ND2	1:B:196:ASN:C	2.57	0.58
1:B:361:GLY:O	2:E:2:ILE:CA	2.25	0.57
1:A:874:ILE:HG22	1:A:937:ILE:HD11	1.85	0.57
1:B:817:GLU:HG3	1:B:818:PRO:HD3	1.86	0.57
1:A:677:GLN:HG3	1:A:678:PRO:HD2	1.87	0.57
1:B:783:ASN:ND2	1:B:785:VAL:H	2.02	0.57
1:A:460:ARG:HD2	1:A:462:ASP:OD2	2.04	0.57
1:B:362:GLY:HA3	2:E:2:ILE:HG22	1.87	0.57
5:B:3013:DIO:H22	6:B:2040:HOH:O	2.05	0.57
3:F:10:HIS:ND1	6:F:2001:HOH:O	2.33	0.57
1:A:162:LEU:HD23	1:A:270:LEU:CD1	2.35	0.57
1:B:692:GLU:HG2	1:B:693:VAL:HG23	1.87	0.57
1:A:423:ARG:NH1	1:A:423:ARG:CG	2.67	0.56
1:A:824:ARG:O	1:A:828:GLN:HA	2.04	0.56
1:B:583:ALA:CB	1:B:626:GLY:HA2	2.35	0.56
1:B:842:GLY:C	1:B:843:ILE:HD13	2.26	0.56
1:A:184:ASN:ND2	1:A:223:LYS:HE2	2.20	0.56
2:E:17:GLU:HG2	3:F:18:VAL:CG1	2.34	0.56
1:A:687:ARG:HD2	6:A:2136:HOH:O	2.04	0.56
1:B:782:ARG:NH2	1:B:963:MET:H	2.03	0.56
1:A:294:GLN:H	1:A:297:HIS:CD2	2.22	0.56
1:B:491:ARG:CG	1:B:491:ARG:HH11	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:LEU:HD22	1:A:729:LEU:HD22	1.87	0.55
1:B:872:LYS:O	1:B:875:GLU:HB2	2.06	0.55
1:B:722:ARG:HB3	1:B:758:LEU:HD13	1.87	0.55
1:B:479:ALA:HB2	5:B:3013:DIO:H21	1.88	0.55
1:B:875:GLU:HA	1:B:875:GLU:OE1	2.06	0.55
1:B:679:HIS:O	1:B:683:MET:HG3	2.06	0.55
1:A:722:ARG:CB	1:A:758:LEU:HD12	2.35	0.55
1:B:459:PHE:CE2	1:B:461:PRO:HG3	2.42	0.55
6:A:2116:HOH:O	2:C:2:ILE:HG21	1.75	0.55
1:B:810:LEU:HD12	1:B:928:LEU:CD2	2.37	0.55
1:A:136:GLY:HA3	1:A:152:ASP:O	2.06	0.55
1:B:361:GLY:O	2:E:2:ILE:CG2	2.55	0.55
1:A:815:ILE:HG22	1:A:870:MET:HG3	1.88	0.55
1:A:423:ARG:HG2	1:A:423:ARG:NH1	2.20	0.54
1:B:45:PRO:HG2	1:B:46:ALA:H	1.72	0.54
1:B:810:LEU:HD23	1:B:810:LEU:C	2.28	0.54
1:A:529:GLU:HA	1:A:529:GLU:OE2	2.08	0.54
2:E:19:TYR:CD2	3:F:15:LEU:HD21	2.42	0.54
1:B:457:GLU:N	6:B:2070:HOH:O	2.33	0.54
1:B:196:ASN:HD21	1:B:198:ALA:H	1.52	0.54
1:B:335:GLY:C	2:E:2:ILE:HG21	2.27	0.54
1:B:298:LEU:HD13	1:B:475:ASN:HD22	1.73	0.54
1:A:807:PHE:HE1	1:A:935:ASP:HB3	1.72	0.54
1:B:440:ILE:HD11	1:B:449:VAL:O	2.08	0.54
1:A:874:ILE:O	1:A:933:LYS:HE3	2.08	0.54
1:A:114:LEU:HD13	1:A:168:PHE:HB3	1.89	0.53
1:A:227:GLU:C	1:A:230:PRO:HD2	2.28	0.53
1:B:425:LYS:HD2	1:B:428:GLU:OE2	2.08	0.53
1:B:423:ARG:HD3	1:B:424:PHE:CZ	2.44	0.53
1:B:927:TYR:CE2	1:B:931:LEU:HD11	2.43	0.53
1:B:227:GLU:C	1:B:230:PRO:HD2	2.29	0.53
1:A:359:LEU:O	2:C:1:GLY:CA	2.43	0.53
1:A:559:LEU:HD22	1:A:742:MET:HB2	1.90	0.53
1:A:43:ASN:ND2	1:A:43:ASN:C	2.62	0.53
1:B:563:GLN:HG3	1:B:733:ILE:O	2.08	0.53
1:A:676:GLU:HA	1:A:676:GLU:OE1	2.09	0.53
1:B:774:ARG:HG2	1:B:774:ARG:NH1	2.24	0.53
1:B:860:GLU:OE2	1:B:957:HIS:CE1	2.59	0.52
1:A:112:HIS:NE2	1:A:189:GLU:OE1	2.42	0.52
1:A:360:VAL:HA	2:C:1:GLY:CA	2.38	0.52
1:B:310:ILE:HG13	1:B:310:ILE:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:GLU:OE2	2:E:9:SER:HA	2.09	0.52
1:B:196:ASN:HD22	1:B:198:ALA:N	2.07	0.52
1:A:880:GLU:HG3	1:B:457:GLU:HG2	1.90	0.52
1:A:689:LEU:CD2	1:A:995:MET:HG2	2.40	0.52
1:A:222:ASN:O	1:A:226:LEU:HB2	2.09	0.52
1:B:620:LEU:HD13	1:B:629:LEU:HG	1.92	0.52
1:A:360:VAL:HA	2:C:1:GLY:C	2.29	0.52
1:A:346:LEU:HD21	1:A:394:MET:HG2	1.92	0.51
1:B:48:LYS:O	1:B:48:LYS:HG2	2.09	0.51
1:A:147:THR:HG22	1:A:149:TYR:CE1	2.46	0.51
1:B:229:ARG:HD2	1:B:233:GLU:OE2	2.10	0.51
1:B:141:PHE:HA	3:F:1:PHE:O	2.10	0.51
1:A:824:ARG:O	1:A:828:GLN:N	2.42	0.51
1:B:213:HIS:ND1	1:B:214:PRO:HD2	2.25	0.51
1:B:770:GLN:HA	1:B:1005:PHE:CE1	2.46	0.51
1:B:622:ASN:H	1:B:622:ASN:ND2	1.97	0.51
1:A:93:HIS:HE1	1:A:368:ARG:NH2	2.06	0.51
1:B:59:GLU:OE1	1:B:423:ARG:NH1	2.44	0.51
1:B:388:GLU:HB2	5:B:3015:DIO:H11	1.93	0.51
1:B:84:ASP:OD2	1:B:896:LYS:HD3	2.11	0.51
1:B:941:LYS:HD3	1:B:942:GLU:N	2.26	0.50
3:D:17:LEU:HD12	3:D:17:LEU:O	2.11	0.50
1:B:47:ILE:HG22	1:B:49:ARG:H	1.75	0.50
1:A:805:ASN:HD22	1:A:844:GLN:HE22	1.59	0.50
1:A:963:MET:C	6:A:2184:HOH:O	2.49	0.50
1:B:72:GLY:HA2	6:B:2003:HOH:O	2.10	0.50
1:B:429:ARG:HH11	1:B:429:ARG:HG2	1.75	0.50
1:B:961:ARG:HD2	6:B:2157:HOH:O	2.10	0.50
1:B:110:LEU:C	1:B:110:LEU:HD23	2.32	0.50
1:B:815:ILE:HA	1:B:870:MET:HE2	1.94	0.50
1:B:453:GLU:O	5:B:3014:DIO:H2'1	2.12	0.50
1:A:93:HIS:CE1	1:A:368:ARG:HH21	2.21	0.50
1:A:187:ASP:OD1	1:A:222:ASN:HB2	2.12	0.50
1:B:575:ASN:O	1:B:727:ALA:HA	2.12	0.50
2:E:16:LEU:HA	2:E:19:TYR:CE2	2.47	0.50
1:A:651:THR:HG22	1:A:752:HIS:HB3	1.93	0.50
1:B:187:ASP:OD1	1:B:222:ASN:HB2	2.11	0.50
1:B:359:LEU:O	2:E:1:GLY:N	2.45	0.49
1:B:429:ARG:HD2	2:E:14:TYR:OH	2.12	0.49
1:A:929:LYS:HE2	6:A:2172:HOH:O	2.11	0.49
1:A:431:ARG:NE	6:A:2022:HOH:O	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:GLU:CG	1:B:788:ASN:HD21	2.26	0.49
1:A:521:LYS:HE3	6:A:2063:HOH:O	2.12	0.49
3:D:3:ASN:OD1	3:D:3:ASN:C	2.50	0.49
1:B:311:ARG:HH22	1:B:664:GLU:CD	2.16	0.49
1:A:429:ARG:CZ	2:C:14:TYR:CE1	2.96	0.49
1:B:534:ASN:HD22	1:B:536:GLU:H	1.59	0.49
1:A:475:ASN:OD1	1:A:475:ASN:N	2.44	0.49
1:B:389:ASP:O	1:B:393:HIS:HD2	1.95	0.49
1:A:784:GLU:O	1:A:961:ARG:HG3	2.12	0.49
1:B:534:ASN:ND2	1:B:536:GLU:H	2.10	0.49
1:A:511:LYS:N	1:A:511:LYS:HD2	2.27	0.49
1:A:140:ALA:HA	1:A:148:ASN:O	2.12	0.49
1:B:43:ASN:O	1:B:45:PRO:O	2.30	0.49
1:B:597:LEU:HD23	1:B:621:GLN:C	2.33	0.49
1:B:810:LEU:HD22	1:B:936:ILE:CG1	2.42	0.49
1:A:162:LEU:HD23	1:A:270:LEU:HD11	1.93	0.49
1:A:771:LEU:HD21	1:A:954:VAL:HG23	1.94	0.49
1:A:824:ARG:O	1:A:828:GLN:CA	2.61	0.48
1:A:455:LEU:HA	6:A:2084:HOH:O	2.13	0.48
1:B:767:ARG:HG2	1:B:1007:LEU:HD13	1.95	0.48
1:A:587:PRO:HD3	1:A:695:TRP:CE2	2.48	0.48
1:B:587:PRO:HD3	1:B:695:TRP:CE2	2.48	0.48
1:A:153:VAL:HG22	1:A:154:SER:N	2.28	0.48
1:A:795:TYR:HE2	1:A:953:LYS:HD2	1.75	0.48
1:B:940:TYR:CE1	1:B:945:ALA:HB2	2.47	0.48
1:B:135:ALA:HA	1:B:892:ARG:NH2	2.28	0.48
1:A:431:ARG:HH11	2:C:14:TYR:HE2	1.58	0.48
1:B:415:LYS:HG3	6:B:2070:HOH:O	2.12	0.48
1:A:257:VAL:HG21	1:A:437:ILE:HB	1.94	0.48
1:B:335:GLY:O	2:E:2:ILE:HG23	2.14	0.48
1:B:196:ASN:HD22	1:B:198:ALA:H	1.59	0.48
2:E:13:LEU:HD13	2:E:17:GLU:OE1	2.13	0.48
3:F:1:PHE:CD2	3:F:1:PHE:C	2.86	0.48
1:B:111:GLN:HE22	3:F:1:PHE:H1	1.61	0.48
1:A:324:LYS:HE3	1:A:325:TYR:CZ	2.48	0.48
1:A:657:LYS:O	1:A:661:ILE:HG12	2.14	0.48
1:A:259:LEU:C	1:A:259:LEU:HD23	2.34	0.48
1:B:597:LEU:CA	6:B:2095:HOH:O	2.05	0.48
1:B:49:ARG:O	1:B:50:ILE:CG1	2.60	0.48
1:B:625:TYR:CZ	1:B:765:ARG:HD3	2.48	0.48
1:B:729:LEU:HD12	1:B:738:ALA:HB1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ILE:HG22	1:A:49:ARG:O	2.14	0.48
1:A:429:ARG:CZ	2:C:14:TYR:HE1	2.24	0.47
1:B:388:GLU:OE1	1:B:509:VAL:HG22	2.13	0.47
1:B:114:LEU:HD22	1:B:172:PRO:HB3	1.96	0.47
1:A:243:LYS:CB	6:A:2041:HOH:O	2.56	0.47
1:B:97:LEU:HB2	1:B:144:GLY:O	2.14	0.47
1:B:386:HIS:HD2	1:B:389:ASP:OD2	1.96	0.47
1:B:170:LEU:HD21	1:B:278:VAL:HG22	1.97	0.47
1:B:202:PHE:CE2	3:F:4:GLN:HB3	2.50	0.47
2:C:10:ILE:HG22	3:D:4:GLN:C	2.35	0.47
1:A:855:PRO:O	1:A:858:TYR:HB3	2.15	0.47
1:A:389:ASP:O	1:A:393:HIS:HD2	1.97	0.47
1:A:540:LEU:HD12	1:A:540:LEU:HA	1.59	0.47
1:B:433:TYR:CE1	1:B:437:ILE:HD11	2.50	0.47
1:B:267:LEU:O	1:B:271:VAL:HG12	2.14	0.47
1:A:803:SER:HB2	1:A:927:TYR:OH	2.14	0.47
1:B:90:LEU:HD23	1:B:90:LEU:C	2.35	0.47
1:A:425:LYS:HE3	6:A:2078:HOH:O	2.13	0.47
2:E:17:GLU:C	2:E:19:TYR:H	2.18	0.47
1:A:402:ARG:NH1	1:A:468:LEU:O	2.48	0.47
1:A:156:GLU:HB2	1:A:157:HIS:CD2	2.50	0.47
1:A:400:LYS:HE3	1:A:404:GLU:HG2	1.97	0.46
1:B:128:SER:HB2	6:B:2010:HOH:O	2.14	0.46
1:A:868:ILE:HD12	1:A:984:PRO:HD3	1.97	0.46
1:A:856:PRO:HB2	1:A:957:HIS:CD2	2.51	0.46
1:B:961:ARG:NH1	6:B:2157:HOH:O	2.48	0.46
1:A:691:THR:HG23	1:A:841:ASN:HD21	1.81	0.46
1:B:622:ASN:N	1:B:622:ASN:ND2	2.58	0.46
1:B:491:ARG:HH11	1:B:491:ARG:HG3	1.80	0.46
1:B:588:LEU:HD23	1:B:589:HIS:CD2	2.51	0.46
1:A:671:ASN:O	1:A:674:ARG:HB3	2.16	0.46
1:A:815:ILE:CG2	1:A:870:MET:HG3	2.45	0.46
1:B:586:ASP:HA	1:B:695:TRP:CZ2	2.50	0.46
1:B:587:PRO:HD3	1:B:695:TRP:CD2	2.51	0.46
1:B:556:MET:O	1:B:556:MET:HG3	2.16	0.46
1:A:488:LYS:HE3	1:A:488:LYS:HB3	1.56	0.46
1:A:715:PHE:CZ	1:A:719:LEU:HD22	2.50	0.46
2:C:10:ILE:H	2:C:10:ILE:HG12	1.65	0.46
1:A:706:ASP:OD1	1:A:706:ASP:N	2.48	0.46
1:A:677:GLN:HE21	1:A:786:HIS:CE1	2.33	0.46
1:B:175:ASP:HB3	1:B:178:ALA:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:LEU:HA	1:B:417:LEU:HD12	1.83	0.46
2:E:19:TYR:CD2	3:F:15:LEU:CD2	2.99	0.46
2:C:5:GLN:OE1	2:C:5:GLN:HA	2.15	0.46
1:B:195:MET:HE3	1:B:307:ILE:HG13	1.97	0.46
1:A:360:VAL:CA	2:C:1:GLY:O	2.63	0.46
1:B:296:GLU:CD	1:B:296:GLU:H	2.16	0.46
1:A:48:LYS:O	1:A:49:ARG:HB3	2.14	0.46
1:A:689:LEU:HD23	1:A:995:MET:HG2	1.98	0.46
1:B:236:ASP:OD1	1:B:236:ASP:C	2.55	0.46
1:A:182:GLU:OE2	1:A:182:GLU:HA	2.16	0.45
1:B:119:LYS:O	1:B:122:PRO:HD3	2.15	0.45
3:F:2:VAL:HG12	3:F:2:VAL:O	2.03	0.45
1:B:684:TYR:OH	1:B:697:LYS:HG2	2.16	0.45
1:B:462:ASP:OD2	1:B:462:ASP:N	2.47	0.45
1:B:827:GLU:OE1	1:B:862:ARG:HD3	2.16	0.45
1:A:709:LEU:HB3	1:A:710:PRO:CD	2.44	0.45
1:A:49:ARG:C	1:A:50:ILE:HD12	2.37	0.45
1:B:136:GLY:HA3	1:B:152:ASP:O	2.17	0.45
1:A:490:ASP:OD1	1:A:491:ARG:HD2	2.17	0.45
1:A:933:LYS:O	1:A:937:ILE:HG12	2.17	0.45
1:B:387:VAL:HG12	5:B:3015:DIO:H12	1.98	0.45
1:B:484:SER:O	1:B:488:LYS:HE3	2.16	0.45
1:B:547:TYR:HB3	1:B:548:PRO:CD	2.47	0.45
1:A:53:HIS:HE1	6:A:2005:HOH:O	1.99	0.45
1:A:586:ASP:HA	1:A:695:TRP:CZ2	2.52	0.45
1:A:801:SER:O	1:A:802:THR:C	2.56	0.45
1:B:44:ASN:HA	1:B:45:PRO:HA	1.72	0.45
1:B:773:ASP:O	1:B:774:ARG:HB2	2.17	0.45
1:A:586:ASP:OD1	1:A:589:HIS:HD2	2.00	0.45
1:A:389:ASP:O	1:A:393:HIS:CD2	2.70	0.45
1:B:877:MET:HG2	1:B:881:ALA:HB3	1.98	0.45
1:A:262:GLU:OE2	1:A:262:GLU:N	2.49	0.45
1:B:558:LYS:HB3	1:B:726:GLU:HG3	1.99	0.45
1:B:657:LYS:HB3	1:B:657:LYS:HE2	1.60	0.45
1:B:202:PHE:CD2	3:F:4:GLN:HB3	2.52	0.44
1:A:552:LYS:NZ	1:A:746:GLU:OE1	2.34	0.44
1:A:67:LEU:N	1:A:67:LEU:HD23	2.33	0.44
1:B:311:ARG:NH2	1:B:664:GLU:OE2	2.50	0.44
1:B:160:GLY:O	1:B:164:ARG:HD2	2.17	0.44
1:A:425:LYS:HD3	1:A:454:TYR:OH	2.16	0.44
1:A:529:GLU:CB	5:A:3014:DIO:H12	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:ASN:HD22	1:B:534:ASN:C	2.20	0.44
1:B:877:MET:O	1:B:933:LYS:CE	2.66	0.44
1:A:94:ILE:HD12	1:A:94:ILE:HG23	1.55	0.44
1:B:88:ALA:HB3	1:B:151:PHE:CE2	2.53	0.44
1:B:736:GLN:CD	1:B:736:GLN:H	2.20	0.44
1:A:422:PHE:CZ	1:A:451:THR:HG22	2.52	0.44
1:A:798:ASP:HB3	1:A:804:GLU:HG2	2.00	0.44
1:A:131:LEU:CD1	1:A:138:SER:HB2	2.47	0.44
1:B:43:ASN:OD1	6:B:2001:HOH:O	2.21	0.44
1:A:131:LEU:HD23	1:A:131:LEU:HA	1.71	0.44
1:A:587:PRO:HD3	1:A:695:TRP:CD2	2.53	0.44
1:B:169:PHE:O	1:B:170:LEU:HD23	2.18	0.44
1:A:206:LYS:HB3	1:A:216:SER:HA	1.99	0.44
1:B:535:PHE:HB3	1:B:570:PRO:HG3	1.99	0.44
1:A:143:SER:HB2	2:C:10:ILE:HD12	2.00	0.44
1:B:74:LYS:O	1:B:255:ALA:HA	2.17	0.44
1:B:204:LEU:HD23	5:B:3013:DIO:H1'1	2.00	0.44
1:B:588:LEU:HD23	1:B:589:HIS:HD2	1.81	0.44
1:A:120:LYS:HE3	1:B:409:TRP:CD1	2.53	0.44
1:A:806:MET:CE	1:A:928:LEU:HG	2.48	0.43
1:B:562:LYS:HD3	1:B:730:HIS:CE1	2.53	0.43
1:B:559:LEU:HD22	1:B:742:MET:HB2	2.00	0.43
1:A:50:ILE:HD12	1:A:50:ILE:N	2.33	0.43
1:A:526:THR:O	1:A:527:LYS:C	2.57	0.43
2:E:10:ILE:HD11	3:F:5:HIS:CE1	2.53	0.43
1:B:200:ARG:NH2	1:B:498:THR:HA	2.33	0.43
1:A:722:ARG:NH1	6:A:2138:HOH:O	2.51	0.43
1:B:927:TYR:O	1:B:930:THR:HB	2.19	0.43
1:B:858:TYR:CZ	1:B:862:ARG:HD2	2.54	0.43
2:E:14:TYR:O	2:E:18:ASN:HB2	2.18	0.43
1:A:298:LEU:HD13	1:A:475:ASN:HB3	2.00	0.43
1:B:483:LYS:O	1:B:485:PHE:N	2.51	0.43
1:A:151:PHE:C	1:A:151:PHE:CD1	2.92	0.43
1:B:597:LEU:HD23	1:B:622:ASN:N	2.34	0.43
1:B:534:ASN:C	1:B:534:ASN:ND2	2.72	0.43
1:B:483:LYS:C	1:B:485:PHE:H	2.22	0.43
1:B:519:ASN:O	1:B:521:LYS:N	2.51	0.43
1:B:288:PHE:CD2	1:B:288:PHE:N	2.86	0.43
1:A:313:LEU:HD22	1:A:387:VAL:HG13	2.00	0.43
1:A:291:HIS:CE1	1:A:318:PRO:HB3	2.53	0.43
1:A:963:MET:CA	6:A:2184:HOH:O	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:SER:OG	1:B:155:HIS:HA	2.18	0.43
1:B:532:PRO:HG3	1:B:634:TYR:CD2	2.54	0.43
1:B:777:PHE:N	1:B:777:PHE:CD1	2.86	0.43
2:C:4:GLU:O	2:C:8:THR:HG22	2.19	0.43
1:A:898:LYS:CE	6:A:2010:HOH:O	2.41	0.43
1:B:176:GLU:OE1	1:B:179:LYS:NZ	2.51	0.43
1:A:381:GLU:OE2	1:A:664:GLU:HG3	2.19	0.43
1:A:672:ASN:HD22	1:A:672:ASN:HA	1.54	0.43
1:B:125:ASN:N	1:B:125:ASN:HD22	2.16	0.43
1:A:796:GLN:HB3	1:A:952:HIS:HB2	2.01	0.43
1:B:733:ILE:HG22	1:B:737:ALA:HB3	1.99	0.43
1:A:89:ALA:HA	1:A:149:TYR:O	2.19	0.43
1:B:94:ILE:HA	1:B:94:ILE:HD13	1.79	0.43
1:B:346:LEU:HA	1:B:522:PHE:CE2	2.53	0.43
1:A:47:ILE:HG22	1:A:49:ARG:H	1.83	0.42
1:B:90:LEU:HD23	1:B:91:ASP:N	2.34	0.42
1:B:307:ILE:O	1:B:483:LYS:NZ	2.51	0.42
1:A:622:ASN:N	1:A:622:ASN:ND2	2.54	0.42
1:A:422:PHE:O	1:A:423:ARG:C	2.55	0.42
1:A:296:GLU:OE1	6:A:2052:HOH:O	2.22	0.42
1:B:649:MET:HE3	1:B:649:MET:HB3	1.88	0.42
1:A:49:ARG:O	1:A:50:ILE:HD12	2.19	0.42
1:A:724:HIS:HB2	6:A:2139:HOH:O	2.19	0.42
1:B:123:LYS:HE2	1:B:125:ASN:HD21	1.85	0.42
1:B:94:ILE:HG13	1:B:248:TYR:HB3	2.02	0.42
1:B:824:ARG:O	1:B:828:GLN:HA	2.19	0.42
1:B:490:ASP:OD2	1:B:490:ASP:N	2.52	0.42
1:B:872:LYS:O	1:B:875:GLU:CB	2.67	0.42
1:A:66:GLY:O	1:A:67:LEU:HB3	2.19	0.42
3:D:2:VAL:O	3:D:2:VAL:HG12	2.20	0.42
1:A:110:LEU:C	1:A:110:LEU:HD23	2.40	0.42
1:A:880:GLU:HG2	1:B:457:GLU:HG2	2.00	0.42
1:A:108:HIS:CE1	1:A:189:GLU:CD	2.93	0.42
1:B:601:LYS:O	1:B:602:ASP:C	2.55	0.42
1:B:229:ARG:HD3	1:B:233:GLU:HG3	2.01	0.42
1:A:842:GLY:C	1:A:843:ILE:HD13	2.40	0.42
1:A:842:GLY:O	1:A:843:ILE:HD13	2.20	0.42
1:B:361:GLY:HA2	1:B:374:ILE:O	2.20	0.42
1:A:782:ARG:HD2	6:A:2145:HOH:O	1.94	0.42
1:B:267:LEU:HD23	1:B:267:LEU:HA	1.76	0.42
1:A:722:ARG:HA	1:A:756:LYS:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:774:ARG:HG2	1:B:774:ARG:HH11	1.84	0.42
1:A:311:ARG:NH2	1:A:664:GLU:OE2	2.53	0.42
1:B:909:GLY:HA2	1:B:912:ILE:HD13	2.01	0.42
1:A:760:PRO:HA	1:A:763:LEU:HD12	2.00	0.42
1:A:499:GLN:OE1	1:A:499:GLN:HA	2.20	0.42
1:B:206:LYS:HB3	1:B:216:SER:HA	2.01	0.42
1:B:654:ILE:HD13	1:B:712:LEU:HD13	2.01	0.42
1:A:60:ASP:OD1	1:A:62:ARG:HB2	2.19	0.42
1:B:124:GLU:OE2	1:B:178:ALA:HB2	2.20	0.41
1:B:139:ASN:HB3	1:B:150:TYR:CE1	2.55	0.41
1:A:643:LYS:NZ	6:A:2127:HOH:O	2.54	0.41
1:A:236:ASP:OD2	1:A:239:GLN:HG2	2.21	0.41
1:B:457:GLU:HA	6:B:2070:HOH:O	2.19	0.41
1:B:672:ASN:HD22	1:B:672:ASN:HA	1.55	0.41
1:B:185:ALA:HB2	1:B:828:GLN:HE22	1.85	0.41
1:B:250:SER:OG	1:B:252:ASN:OD1	2.37	0.41
1:A:940:TYR:CE1	1:A:945:ALA:HB2	2.54	0.41
1:B:616:LEU:HD23	1:B:616:LEU:HA	1.80	0.41
1:B:689:LEU:CD2	1:B:995:MET:HG2	2.50	0.41
1:B:817:GLU:N	1:B:818:PRO:CD	2.84	0.41
3:F:9:SER:HA	3:F:12:VAL:HG23	2.03	0.41
1:B:803:SER:O	1:B:807:PHE:CD1	2.73	0.41
1:B:677:GLN:HG3	1:B:678:PRO:HD2	2.03	0.41
1:B:846:LEU:HD13	1:B:848:PHE:CE1	2.55	0.41
1:B:817:GLU:N	1:B:818:PRO:HD2	2.35	0.41
1:A:711:ARG:HH21	1:A:711:ARG:CG	2.34	0.41
1:A:765:ARG:HD2	1:A:765:ARG:HA	1.68	0.41
1:B:308:LYS:NZ	3:F:13:GLU:HG3	2.36	0.41
1:A:413:GLU:HG2	1:A:531:ILE:CD1	2.50	0.41
1:B:361:GLY:O	2:E:2:ILE:HG22	2.21	0.41
1:B:489:THR:HB	1:B:500:TYR:C	2.41	0.41
1:A:237:VAL:O	1:A:238:ARG:C	2.58	0.41
1:A:793:ILE:O	1:A:847:ARG:HA	2.21	0.41
1:A:262:GLU:HB3	1:A:266:ASP:HB2	2.03	0.41
1:A:920:ARG:O	1:A:924:GLU:HG3	2.21	0.41
1:B:540:LEU:HA	1:B:540:LEU:HD12	1.78	0.41
1:A:102:ASN:ND2	1:A:102:ASN:H	2.11	0.41
1:B:123:LYS:HB3	1:B:126:GLU:HB2	2.01	0.41
1:B:250:SER:O	1:B:254:MET:HG3	2.21	0.41
1:A:780:GLN:NE2	1:A:959:LEU:HD11	2.35	0.41
1:A:193:ASN:O	1:A:194:VAL:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:13:LEU:O	2:E:17:GLU:HG3	2.20	0.41
1:A:616:LEU:HD23	1:A:616:LEU:HA	1.81	0.41
1:B:960:ALA:O	1:B:961:ARG:C	2.59	0.41
1:A:313:LEU:HD12	1:A:314:TYR:N	2.36	0.41
1:A:840:ALA:O	1:A:842:GLY:N	2.54	0.41
1:B:413:GLU:OE2	1:B:527:LYS:HD2	2.21	0.41
1:A:736:GLN:HG3	1:A:736:GLN:H	1.69	0.41
1:B:609:TYR:CE2	1:B:613:LEU:HD11	2.55	0.41
1:B:1008:VAL:HG13	1:B:1009:LYS:N	2.36	0.41
2:E:19:TYR:HD2	3:F:15:LEU:CD2	2.34	0.41
1:A:840:ALA:C	1:A:842:GLY:N	2.74	0.41
1:A:575:ASN:O	1:A:727:ALA:HA	2.21	0.41
2:C:15:GLN:O	2:C:18:ASN:HB3	2.20	0.41
1:A:429:ARG:HH21	2:C:14:TYR:HE1	1.56	0.40
1:B:171:SER:N	1:B:172:PRO:CD	2.83	0.40
1:A:592:MET:HB3	1:A:715:PHE:CD2	2.56	0.40
1:B:460:ARG:NH1	1:B:462:ASP:OD2	2.55	0.40
1:B:472:ARG:HH11	1:B:472:ARG:HG2	1.86	0.40
1:A:173:LEU:O	1:A:174:PHE:C	2.60	0.40
1:A:417:LEU:HD12	1:A:417:LEU:HA	1.84	0.40
1:A:896:LYS:HE2	1:A:896:LYS:HB2	1.90	0.40
2:E:4:GLU:O	2:E:7:CYS:HB3	2.21	0.40
1:A:862:ARG:NH2	1:A:981:SER:O	2.54	0.40
1:A:49:ARG:NH1	6:A:2001:HOH:O	2.54	0.40
1:A:924:GLU:OE2	6:A:2179:HOH:O	2.22	0.40
1:B:759:LEU:O	1:B:760:PRO:C	2.60	0.40
1:B:245:HIS:O	1:B:249:TYR:HB2	2.22	0.40
1:A:628:TYR:OH	1:A:630:SER:HB2	2.21	0.40
1:A:724:HIS:CB	6:A:2139:HOH:O	2.69	0.40
1:B:191:GLU:HG3	1:B:788:ASN:ND2	2.32	0.40
1:A:527:LYS:CD	6:A:2097:HOH:O	2.69	0.40
1:A:311:ARG:HH22	1:A:664:GLU:CD	2.25	0.40
1:A:118:THR:HG22	1:A:172:PRO:HA	2.03	0.40
1:B:538:LEU:H	1:B:538:LEU:HG	1.73	0.40
1:B:363:GLN:HB2	1:B:371:MET:CE	2.52	0.40
1:A:50:ILE:HG22	1:A:51:GLY:O	2.21	0.40
2:C:13:LEU:N	3:D:1:PHE:CE2	2.90	0.40
1:B:915:GLN:O	1:B:1011:HIS:HB3	2.22	0.40
1:B:100:PRO:HA	1:B:101:PRO:HD3	1.89	0.40
1:B:681:HIS:O	1:B:682:ALA:C	2.56	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	945/990 (96%)	882 (93%)	60 (6%)	3 (0%)	46	79
1	B	951/990 (96%)	896 (94%)	51 (5%)	4 (0%)	39	74
2	C	19/21 (90%)	17 (90%)	2 (10%)	0	100	100
2	E	19/21 (90%)	15 (79%)	4 (21%)	0	100	100
3	D	18/30 (60%)	16 (89%)	2 (11%)	0	100	100
3	F	18/30 (60%)	17 (94%)	1 (6%)	0	100	100
All	All	1970/2082 (95%)	1843 (94%)	120 (6%)	7 (0%)	39	74

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	45	PRO
1	A	1011	HIS
1	B	295	GLU
1	B	751	GLU
1	A	488	LYS
1	B	869	THR
1	A	103	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	846/879 (96%)	755 (89%)	91 (11%)	8	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	846/879 (96%)	752 (89%)	94 (11%)	8	23
2	C	19/20 (95%)	15 (79%)	4 (21%)	1	4
2	E	19/20 (95%)	13 (68%)	6 (32%)	0	1
3	D	17/26 (65%)	12 (71%)	5 (29%)	0	1
3	F	17/26 (65%)	13 (76%)	4 (24%)	1	2
All	All	1764/1850 (95%)	1560 (88%)	204 (12%)	7	20

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	54	ILE
1	A	57	SER
1	A	67	LEU
1	A	76	LEU
1	A	96	SER
1	A	97	LEU
1	A	102	ASN
1	A	111	GLN
1	A	125	ASN
1	A	148	ASN
1	A	156	GLU
1	A	158	LEU
1	A	188	SER
1	A	191	GLU
1	A	201	LEU
1	A	223	LYS
1	A	226	LEU
1	A	229	ARG
1	A	243	LYS
1	A	270	LEU
1	A	285	LEU
1	A	316	THR
1	A	329	ASN
1	A	337	LEU
1	A	347	LEU
1	A	356	VAL
1	A	412	GLN
1	A	414	LEU
1	A	417	LEU

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Mol	Chain	Res	Type
1	A	423	ARG
1	A	429	ARG
1	A	446	LEU
1	A	449	VAL
1	A	450	LEU
1	A	466	MET
1	A	488	LYS
1	A	491	ARG
1	A	507	ASP
1	A	512	LYS
1	A	524	LEU
1	A	558	LYS
1	A	595	LEU
1	A	597	LEU
1	A	603	SER
1	A	607	TYR
1	A	616	LEU
1	A	622	ASN
1	A	624	ILE
1	A	629	LEU
1	A	639	PRO
1	A	642	LEU
1	A	644	LYS
1	A	648	LYS
1	A	653	GLU
1	A	656	GLU
1	A	657	LYS
1	A	674	ARG
1	A	677	GLN
1	A	681	HIS
1	A	706	ASP
1	A	711	ARG
1	A	712	LEU
1	A	722	ARG
1	A	728	LEU
1	A	736	GLN
1	A	751	GLU
1	A	759	LEU
1	A	765	ARG
1	A	770	GLN
1	A	771	LEU
1	A	774	ARG

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Mol	Chain	Res	Type
1	A	799	MET
1	A	810	LEU
1	A	817	GLU
1	A	823	LEU
1	A	846	LEU
1	A	853	GLU
1	A	859	LEU
1	A	867	LEU
1	A	883	GLN
1	A	889	LEU
1	A	891	ILE
1	A	928	LEU
1	A	931	LEU
1	A	951	ARG
1	A	982	GLN
1	A	988	GLN
1	A	993	GLN
1	A	1007	LEU
1	A	1011	HIS
1	B	44	ASN
1	B	65	ARG
1	B	74	LYS
1	B	76	LEU
1	B	97	LEU
1	B	111	GLN
1	B	119	LYS
1	B	125	ASN
1	B	128	SER
1	B	131	LEU
1	B	143	SER
1	B	154	SER
1	B	158	LEU
1	B	164	ARG
1	B	171	SER
1	B	177	SER
1	B	196	ASN
1	B	201	LEU
1	B	223	LYS
1	B	226	LEU
1	B	229	ARG
1	B	250	SER
1	B	270	LEU

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Mol	Chain	Res	Type
1	B	282	ASN
1	B	285	LEU
1	B	333	TYR
1	B	347	LEU
1	B	356	VAL
1	B	417	LEU
1	B	423	ARG
1	B	440	ILE
1	B	457	GLU
1	B	458	GLU
1	B	466	MET
1	B	483	LYS
1	B	491	ARG
1	B	512	LYS
1	B	519	ASN
1	B	523	LYS
1	B	524	LEU
1	B	534	ASN
1	B	556	MET
1	B	558	LYS
1	B	582	PHE
1	B	586	ASP
1	B	590	SER
1	B	595	LEU
1	B	600	LEU
1	B	616	LEU
1	B	617	SER
1	B	622	ASN
1	B	627	MET
1	B	629	LEU
1	B	635	ASN
1	B	642	LEU
1	B	653	GLU
1	B	674	ARG
1	B	677	GLN
1	B	712	LEU
1	B	719	LEU
1	B	722	ARG
1	B	728	LEU
1	B	733	ILE
1	B	736	GLN
1	B	751	GLU

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Mol	Chain	Res	Type
1	B	759	LEU
1	B	764	VAL
1	B	771	LEU
1	B	780	GLN
1	B	783	ASN
1	B	791	ILE
1	B	799	MET
1	B	817	GLU
1	B	823	LEU
1	B	846	LEU
1	B	854	LYS
1	B	859	LEU
1	B	867	LEU
1	B	870	MET
1	B	873	SER
1	B	875	GLU
1	B	896	LYS
1	B	899	LYS
1	B	906	LYS
1	B	912	ILE
1	B	914	GLN
1	B	928	LEU
1	B	931	LEU
1	B	934	GLU
1	B	941	LYS
1	B	951	ARG
1	B	981	SER
1	B	996	THR
1	B	1007	LEU
2	C	3	VAL
2	C	10	ILE
2	C	13	LEU
2	C	19	TYR
3	D	2	VAL
3	D	4	GLN
3	D	13	GLU
3	D	15	LEU
3	D	16	TYR
2	E	2	ILE
2	E	3	VAL
2	E	4	GLU
2	E	5	GLN

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Mol	Chain	Res	Type
2	E	13	LEU
2	E	20	CYS
3	F	1	PHE
3	F	2	VAL
3	F	4	GLN
3	F	18	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	53	HIS
1	A	93	HIS
1	A	102	ASN
1	A	125	ASN
1	A	148	ASN
1	A	157	HIS
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	393	HIS
1	A	502	GLN
1	A	515	ASN
1	A	575	ASN
1	A	589	HIS
1	A	605	ASN
1	A	622	ASN
1	A	672	ASN
1	A	730	HIS
1	A	770	GLN
1	A	780	GLN
1	A	783	ASN
1	A	786	HIS
1	A	805	ASN
1	A	828	GLN
1	A	841	ASN
1	A	883	GLN

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Mol	Chain	Res	Type
1	A	957	HIS
1	A	979	ASN
1	A	988	GLN
1	B	52	ASN
1	B	53	HIS
1	B	93	HIS
1	B	111	GLN
1	B	125	ASN
1	B	184	ASN
1	B	190	HIS
1	B	196	ASN
1	B	239	GLN
1	B	294	GLN
1	B	363	GLN
1	B	386	HIS
1	B	393	HIS
1	B	407	GLN
1	B	475	ASN
1	B	502	GLN
1	B	534	ASN
1	B	589	HIS
1	B	622	ASN
1	B	672	ASN
1	B	730	HIS
1	B	783	ASN
1	B	788	ASN
1	B	805	ASN
1	B	828	GLN
1	B	883	GLN
1	B	914	GLN
1	B	922	ASN
1	B	957	HIS
3	D	4	GLN
3	D	5	HIS
2	E	15	GLN
2	E	18	ASN
3	F	5	HIS

### 5.3.3 RNA ⓘ

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](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	$\# Z  > 2$
5	DIO	A	3013	-	6,6,6	0.53	0	6,6,6	1.26	1 (16%)
5	DIO	A	3014	-	6,6,6	0.64	0	6,6,6	0.47	0
5	DIO	A	3015	-	6,6,6	0.61	0	6,6,6	1.24	1 (16%)
5	DIO	A	3016	-	6,6,6	0.45	0	6,6,6	0.95	0
5	DIO	B	3013	-	6,6,6	0.63	0	6,6,6	0.92	1 (16%)
5	DIO	B	3014	-	6,6,6	0.82	0	6,6,6	1.53	2 (33%)
5	DIO	B	3015	-	6,6,6	0.61	0	6,6,6	1.63	1 (16%)
5	DIO	B	3016	-	6,6,6	0.58	0	6,6,6	1.20	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
5	DIO	A	3013	-	-	0/0/6/6	0/1/1/1
5	DIO	A	3014	-	-	0/0/6/6	0/1/1/1
5	DIO	A	3015	-	-	0/0/6/6	0/1/1/1
5	DIO	A	3016	-	-	0/0/6/6	0/1/1/1
5	DIO	B	3013	-	-	0/0/6/6	0/1/1/1
5	DIO	B	3014	-	-	0/0/6/6	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DIO	B	3015	-	-	0/0/6/6	0/1/1/1
5	DIO	B	3016	-	-	0/0/6/6	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	3013	DIO	C2'-O1'-C1'	2.04	116.77	109.89
5	A	3013	DIO	C2'-O1'-C1'	2.29	117.60	109.89
5	A	3015	DIO	C2'-O1'-C1'	2.35	117.79	109.89
5	B	3014	DIO	C2-O1-C1	2.42	118.05	109.89
5	B	3014	DIO	C2'-O1'-C1'	2.72	119.06	109.89
5	B	3015	DIO	C2'-O1'-C1'	2.85	119.48	109.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	3014	DIO	1	0
5	B	3013	DIO	3	0
5	B	3014	DIO	1	0
5	B	3015	DIO	2	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	953/990 (96%)	-0.51	2 (0%) 95 94	23, 35, 51, 70	0
1	B	955/990 (96%)	-0.43	8 (0%) 87 81	25, 41, 57, 76	0
2	C	21/21 (100%)	2.72	14 (66%) 0 0	34, 53, 56, 57	0
2	E	21/21 (100%)	2.93	11 (52%) 0 0	33, 46, 65, 67	0
3	D	20/30 (66%)	3.05	12 (60%) 0 0	33, 62, 73, 75	0
3	F	20/30 (66%)	2.80	11 (55%) 0 0	43, 54, 58, 59	0
All	All	1990/2082 (95%)	-0.33	58 (2%) 55 43	23, 38, 56, 76	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	21	ASN	6.8
2	E	16	LEU	6.5
3	F	20	GLY	6.2
3	F	19	CYS	6.2
2	E	20	CYS	6.1
3	D	19	CYS	6.1
3	D	16	TYR	5.9
2	C	20	CYS	5.9
2	E	19	TYR	5.8
3	D	14	ALA	5.8
2	C	21	ASN	5.6
2	E	13	LEU	5.6
2	C	16	LEU	5.5
2	C	19	TYR	5.4
3	D	15	LEU	5.3
3	D	18	VAL	5.2
2	E	17	GLU	5.0
3	F	18	VAL	4.9
3	D	13	GLU	4.8

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Mol	Chain	Res	Type	RSRZ
3	F	15	LEU	4.8
3	F	12	VAL	4.6
3	F	16	TYR	4.4
3	F	14	ALA	4.4
3	D	17	LEU	4.3
2	C	18	ASN	4.3
3	F	1	PHE	4.2
3	F	17	LEU	4.2
3	D	12	VAL	4.1
2	E	15	GLN	3.9
2	E	18	ASN	3.9
2	C	13	LEU	3.9
1	B	43	ASN	3.8
2	E	14	TYR	3.6
3	D	11	LEU	3.6
3	D	9	SER	3.4
2	C	17	GLU	3.4
3	D	20	GLY	3.3
1	A	43	ASN	3.2
2	C	15	GLN	2.9
3	F	11	LEU	2.9
1	B	44	ASN	2.9
2	C	1	GLY	2.5
1	B	1011	HIS	2.5
2	C	5	GLN	2.5
3	F	13	GLU	2.4
1	B	656	GLU	2.4
1	B	1010	PRO	2.3
2	C	14	TYR	2.3
1	A	980	LEU	2.3
2	C	6	CYS	2.2
1	B	212	LYS	2.2
2	C	12	SER	2.2
2	E	6	CYS	2.1
1	B	508	GLU	2.1
1	B	979	ASN	2.1
3	D	8	GLY	2.1
2	E	2	ILE	2.0
2	C	9	SER	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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	DIO	B	3015	6/6	0.91	0.28	6.44	68,73,74,74	0
5	DIO	A	3015	6/6	0.97	0.32	3.06	69,70,70,71	0
5	DIO	B	3016	6/6	0.95	0.28	1.91	81,83,84,85	0
4	ZN	A	3012	1/1	0.94	0.28	1.62	2,2,2,2	0
5	DIO	B	3013	6/6	0.97	0.23	1.08	50,53,54,55	0
5	DIO	A	3013	6/6	0.95	0.17	0.73	61,63,65,66	0
5	DIO	A	3016	6/6	0.96	0.20	0.73	71,72,74,74	0
5	DIO	B	3014	6/6	0.94	0.16	0.31	64,66,67,67	0
4	ZN	B	3012	1/1	0.91	0.29	0.19	2,2,2,2	0
5	DIO	A	3014	6/6	0.95	0.25	-	54,57,59,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.