



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2017 – 08:52 AM EDT

PDB ID : 3OFI
Title : Crystal structure of human insulin-degrading enzyme in complex with ubiquitin
Authors : Kalas, V.; Ralat, L.A.; Tang, W.-J.
Deposited on : unknown
Resolution : 2.35 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

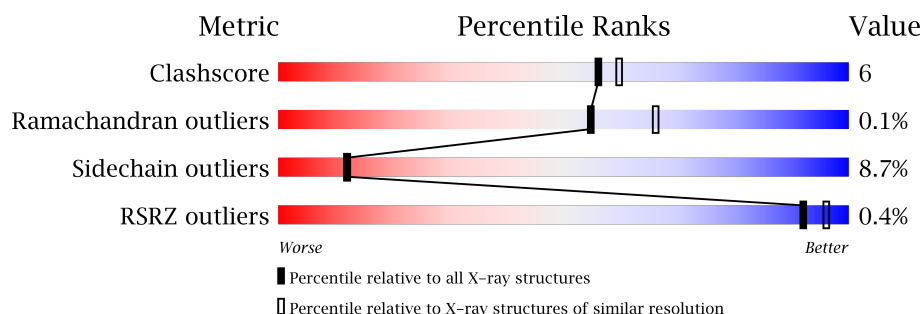
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



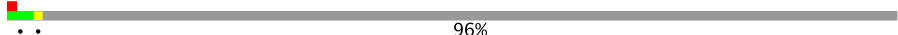
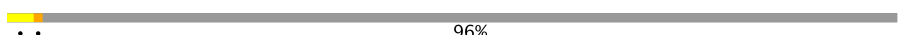
The reported resolution of this entry is 2.35 Å.

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))
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

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 ≥ 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	 78%14% . .
1	B	990	 78%15% . . .
2	C	76	 % ..96%
2	D	76	 ..96%

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
4	DIO	A	2013	-	-	X	X
4	DIO	B	2014	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16016 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	954	Total	C	N	O	S	0	0	0
			7807	5029	1312	1444	22			
1	B	954	Total	C	N	O	S	0	0	0
			7807	5029	1312	1444	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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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 Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	S	0	0	0
			25	16	4	4	1			
2	D	3	Total	C	N	O	S	0	0	0
			25	16	4	4	1			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

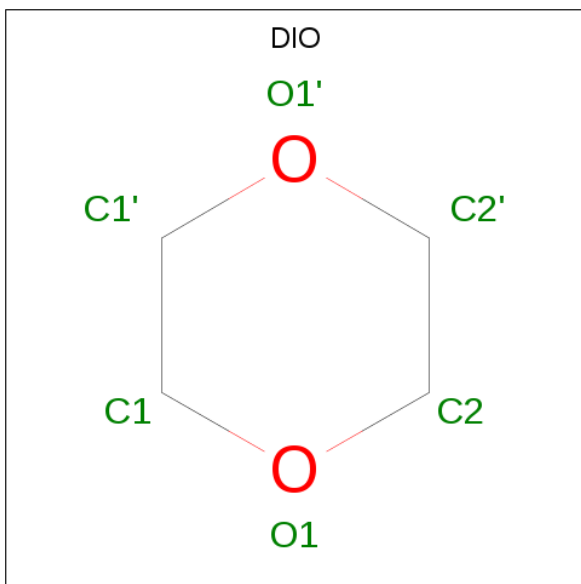
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

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



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

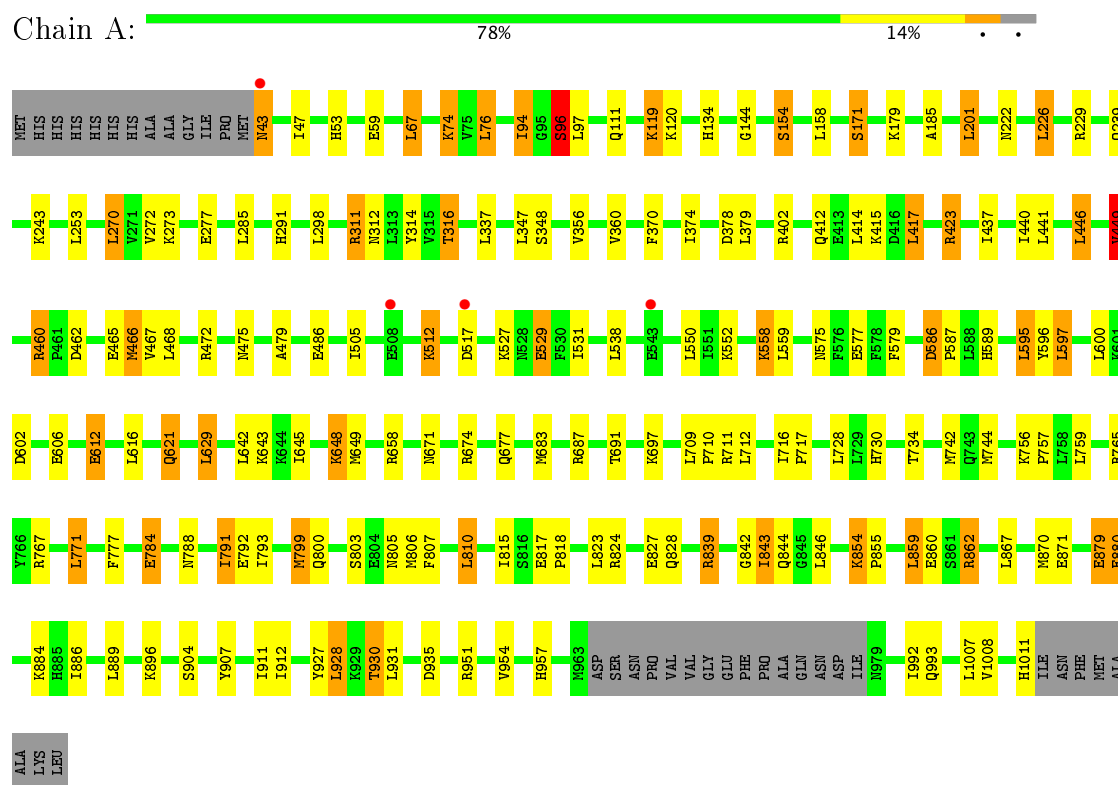
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	218	Total	O	0	0
			218	218		
5	B	113	Total	O	0	0
			113	113		
5	D	1	Total	O	0	0
			1	1		

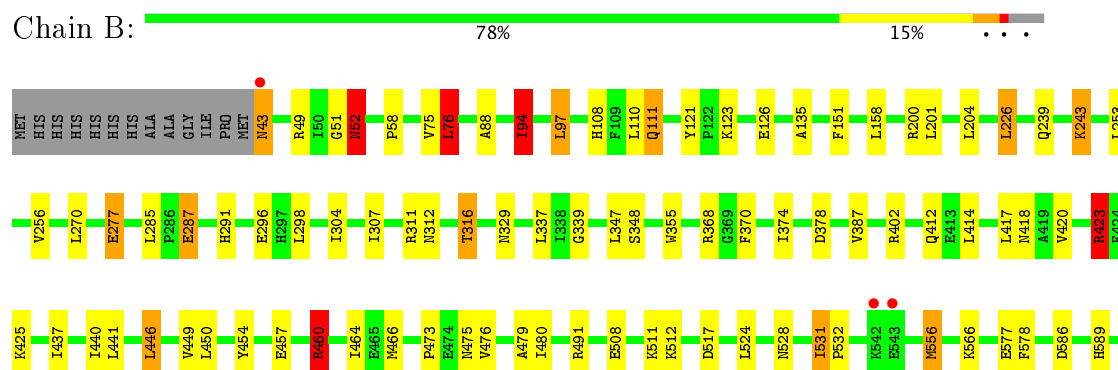
3 Residue-property plots

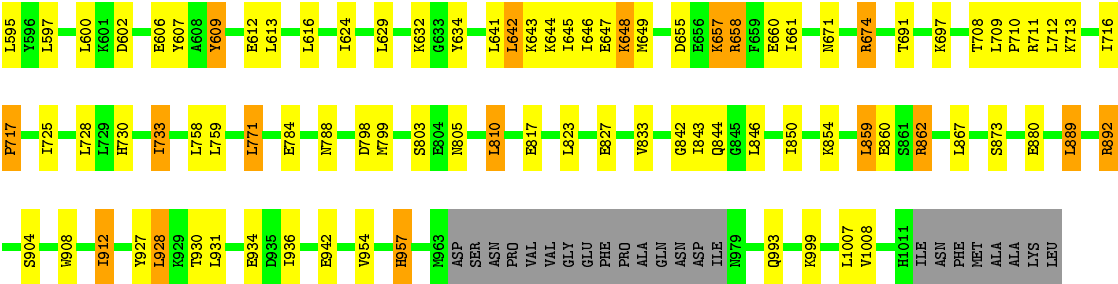
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Insulin-degrading enzyme

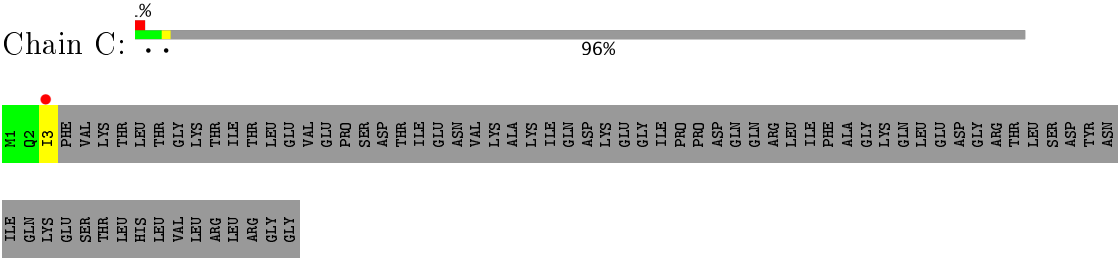


- Molecule 1: Insulin-degrading enzyme

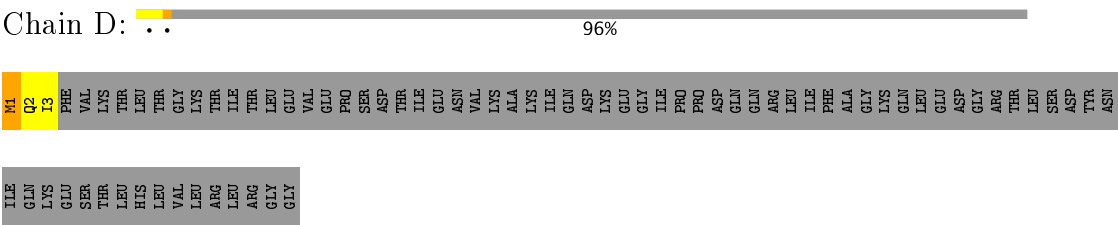




● Molecule 2: Ubiquitin



● Molecule 2: Ubiquitin



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	262.94 Å 262.94 Å 90.97 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.35 49.69 – 2.35	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.35) 94.7 (49.69-2.35)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 2.34 Å)	Xtriage
Refinement program	REFMAC, CNS 1.1	Depositor
R, R_{free}	0.210 , 0.240 0.184 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.020 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16016	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% 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

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	1.12	17/8002 (0.2%)	0.98	22/10824 (0.2%)
1	B	1.08	13/8002 (0.2%)	0.98	21/10824 (0.2%)
2	C	0.93	0/24	1.06	0/30
2	D	1.19	0/24	1.41	0/30
All	All	1.10	30/16052 (0.2%)	0.98	43/21708 (0.2%)

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	B	0	2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	880	GLU	CG-CD	7.16	1.62	1.51
1	A	784	GLU	CG-CD	6.91	1.62	1.51
1	A	577	GLU	CG-CD	6.90	1.62	1.51
1	A	74	LYS	CE-NZ	6.39	1.65	1.49
1	A	612	GLU	CB-CG	-6.37	1.40	1.52
1	A	465	GLU	CG-CD	6.25	1.61	1.51
1	B	277	GLU	CG-CD	6.03	1.60	1.51
1	A	185	ALA	CA-CB	5.98	1.65	1.52
1	A	74	LYS	CD-CE	5.96	1.66	1.51
1	B	121	TYR	CD1-CE1	5.90	1.48	1.39
1	A	579	PHE	CE2-CZ	5.88	1.48	1.37
1	A	879	GLU	CD-OE1	5.80	1.32	1.25
1	A	880	GLU	CG-CD	5.66	1.60	1.51
1	B	511	LYS	CB-CG	5.56	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	687	ARG	CG-CD	5.53	1.65	1.51
1	B	784	GLU	CG-CD	5.51	1.60	1.51
1	A	96	SER	CB-OG	-5.42	1.35	1.42
1	A	529	GLU	CB-CG	-5.40	1.41	1.52
1	B	287	GLU	CG-CD	5.33	1.59	1.51
1	B	880	GLU	CB-CG	5.33	1.62	1.52
1	A	880	GLU	CD-OE1	5.30	1.31	1.25
1	B	355	TRP	CB-CG	-5.27	1.40	1.50
1	B	784	GLU	CD-OE2	5.26	1.31	1.25
1	A	871	GLU	CD-OE1	5.26	1.31	1.25
1	A	854	LYS	CD-CE	5.17	1.64	1.51
1	B	296	GLU	CG-CD	5.12	1.59	1.51
1	B	508	GLU	CG-CD	5.10	1.59	1.51
1	A	880	GLU	CD-OE2	5.04	1.31	1.25
1	B	609	TYR	CE1-CZ	5.03	1.45	1.38
1	B	660	GLU	CG-CD	5.01	1.59	1.51

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	311	ARG	NE-CZ-NH2	-10.78	114.91	120.30
1	B	862	ARG	NE-CZ-NH2	-9.86	115.37	120.30
1	B	311	ARG	NE-CZ-NH2	-8.97	115.82	120.30
1	B	94	ILE	CG1-CB-CG2	-8.70	92.27	111.40
1	B	658	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	A	94	ILE	CG1-CB-CG2	-7.87	94.08	111.40
1	B	862	ARG	NE-CZ-NH1	7.81	124.21	120.30
1	A	311	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	B	423	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	B	460	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	B	311	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	B	52	ASN	N-CA-C	-7.09	91.86	111.00
1	A	460	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	A	67	LEU	CA-CB-CG	6.37	129.96	115.30
1	B	733	ILE	CB-CA-C	-6.17	99.27	111.60
1	A	859	LEU	CB-CG-CD1	6.03	121.25	111.00
1	A	862	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	A	595	LEU	CB-CG-CD1	5.95	121.12	111.00
1	A	843	ILE	CG1-CB-CG2	-5.90	98.42	111.40
1	A	415	LYS	CD-CE-NZ	-5.85	98.24	111.70
1	A	810	LEU	CB-CG-CD2	5.80	120.86	111.00
1	B	798	ASP	CB-CG-OD1	5.78	123.50	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	472	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	A	629	LEU	CB-CG-CD2	5.67	120.65	111.00
1	A	744	MET	CG-SD-CE	5.65	109.24	100.20
1	B	76	LEU	CB-CG-CD1	5.63	120.57	111.00
1	B	892	ARG	NE-CZ-NH2	5.55	123.07	120.30
1	A	449	VAL	CB-CA-C	-5.41	101.12	111.40
1	B	460	ARG	CG-CD-NE	-5.36	100.55	111.80
1	A	824	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	839	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	A	270	LEU	CB-CG-CD2	5.24	119.90	111.00
1	B	928	LEU	CA-CB-CG	5.24	127.34	115.30
1	B	889	LEU	CB-CG-CD2	5.22	119.88	111.00
1	A	529	GLU	CB-CA-C	-5.20	100.01	110.40
1	B	697	LYS	CD-CE-NZ	-5.16	99.84	111.70
1	A	76	LEU	CB-CG-CD2	5.16	119.77	111.00
1	B	226	LEU	CB-CG-CD1	5.09	119.66	111.00
1	B	674	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	B	226	LEU	CA-CB-CG	5.07	126.96	115.30
1	A	767	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	B	97	LEU	CA-CB-CG	5.01	126.82	115.30
1	A	586	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	43	ASN	Peptide
1	B	51	GLY	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	7807	0	7751	93	0
1	B	7807	0	7751	89	0
2	C	25	0	30	0	0
2	D	25	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	6	0	8	7	0
4	B	12	0	16	2	0
5	A	218	0	0	8	0
5	B	113	0	0	9	0
5	D	1	0	0	0	0
All	All	16016	0	15586	181	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 6.

All (181) 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:A:800:GLN:HE22	4:A:2013:DIO:H12	1.19	1.03
1:A:94:ILE:HD11	1:A:253:LEU:CD1	1.89	1.02
1:B:243:LYS:HE2	1:B:243:LYS:HA	1.52	0.90
1:A:777:PHE:HB3	1:A:992:ILE:HD11	1.53	0.89
1:B:368:ARG:HD3	5:B:3057:HOH:O	1.73	0.89
1:A:94:ILE:HD11	1:A:253:LEU:HD13	1.54	0.89
1:A:94:ILE:HD11	1:A:253:LEU:HD12	1.59	0.85
1:A:879:GLU:OE2	5:A:3220:HOH:O	1.94	0.82
1:B:827:GLU:OE1	1:B:862:ARG:HD3	1.81	0.81
1:B:339:GLY:O	2:D:1:MET:HA	1.79	0.81
1:A:777:PHE:HB3	1:A:992:ILE:CD1	2.14	0.78
1:B:312:ASN:HD22	1:B:378:ASP:HA	1.46	0.78
1:A:53:HIS:HE1	5:A:3005:HOH:O	1.68	0.76
1:B:927:TYR:O	1:B:930:THR:HB	1.88	0.74
1:A:59:GLU:OE2	1:A:423:ARG:NH1	2.22	0.73
1:B:810:LEU:HD12	1:B:936:ILE:HD11	1.71	0.73
1:B:441:LEU:HD23	1:B:449:VAL:HG11	1.71	0.72
1:B:316:THR:CG2	5:B:3063:HOH:O	2.37	0.72
1:B:94:ILE:CD1	1:B:253:LEU:CD1	2.70	0.69
1:B:94:ILE:HD12	1:B:253:LEU:HD13	1.72	0.68
1:B:479:ALA:HB2	4:B:2013:DIO:H22	1.74	0.68
1:B:691:THR:O	1:B:999:LYS:HE3	1.94	0.67
1:B:771:LEU:HD21	1:B:954:VAL:HG23	1.76	0.67
1:B:602:ASP:OD1	1:B:658:ARG:HD3	1.96	0.66
1:A:843:ILE:N	1:A:843:ILE:HD12	2.11	0.65
1:B:243:LYS:HE2	1:B:243:LYS:CA	2.25	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ILE:CD1	1:B:253:LEU:HD13	2.27	0.63
1:B:457:GLU:OE2	5:B:4042:HOH:O	2.15	0.63
1:B:440:ILE:HD11	1:B:449:VAL:O	1.99	0.63
1:A:119:LYS:HB2	1:A:171:SER:HB2	1.81	0.62
1:B:578:PHE:CD2	1:B:725:ILE:HD12	2.34	0.62
1:A:94:ILE:CD1	1:A:253:LEU:HD13	2.28	0.62
1:A:842:GLY:H	4:A:2013:DIO:H1'2	1.64	0.62
1:A:709:LEU:HB3	1:A:710:PRO:HD3	1.83	0.60
1:B:799:MET:HE3	1:B:1008:VAL:HG22	1.82	0.60
1:A:460:ARG:NH1	1:A:462:ASP:OD1	2.35	0.60
1:A:312:ASN:HD22	1:A:378:ASP:HA	1.65	0.60
1:A:586:ASP:OD1	1:A:589:HIS:HD2	1.85	0.59
1:B:827:GLU:OE1	1:B:862:ARG:CD	2.50	0.59
1:B:805:ASN:HD22	1:B:844:GLN:HE22	1.50	0.58
1:B:643:LYS:HE3	1:B:647:GLU:OE2	2.03	0.58
1:B:316:THR:HG23	5:B:3063:HOH:O	2.00	0.58
1:A:602:ASP:OD1	1:A:658:ARG:HD3	2.04	0.58
1:A:815:ILE:HG22	1:A:870:MET:HG3	1.86	0.58
1:A:43:ASN:C	1:A:43:ASN:ND2	2.57	0.58
1:A:316:THR:HB	1:A:374:ILE:HG22	1.86	0.57
1:B:771:LEU:HD21	1:B:954:VAL:CG2	2.34	0.57
1:A:799:MET:HE3	1:A:1008:VAL:HG22	1.86	0.57
1:A:600:LEU:HD11	1:A:648:LYS:HB3	1.87	0.57
1:A:298:LEU:HD13	1:A:475:ASN:HB3	1.87	0.56
1:A:827:GLU:OE1	1:A:862:ARG:HD3	2.05	0.56
1:B:632:LYS:NZ	5:B:3141:HOH:O	2.38	0.56
1:B:110:LEU:HD23	1:B:110:LEU:C	2.26	0.56
1:A:800:GLN:NE2	4:A:2013:DIO:H12	2.03	0.56
1:B:123:LYS:HB3	1:B:126:GLU:HB2	1.88	0.56
1:A:466:MET:HE2	1:A:467:VAL:HA	1.88	0.56
1:A:730:HIS:HD2	1:A:904:SER:OG	1.90	0.54
1:B:908:TRP:O	1:B:912:ILE:HG13	2.08	0.53
1:A:402:ARG:NH1	1:A:468:LEU:O	2.42	0.53
1:B:709:LEU:HB3	1:B:710:PRO:HD3	1.90	0.53
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.43	0.53
1:A:671:ASN:O	1:A:674:ARG:HG2	2.09	0.53
1:B:387:VAL:HG21	1:B:480:ILE:HD12	1.91	0.53
1:B:671:ASN:O	1:B:674:ARG:HG2	2.09	0.52
1:B:491:ARG:HD2	5:B:3114:HOH:O	2.09	0.52
1:A:805:ASN:HD22	1:A:844:GLN:HE22	1.56	0.52
4:A:2013:DIO:H22	5:A:3213:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:827:GLU:OE1	1:A:862:ARG:CD	2.58	0.52
1:A:586:ASP:OD1	1:A:589:HIS:CD2	2.63	0.51
1:A:927:TYR:O	1:A:930:THR:HB	2.10	0.51
1:B:657:LYS:O	1:B:661:ILE:HG12	2.09	0.51
1:A:94:ILE:CD1	1:A:253:LEU:CD1	2.78	0.51
1:A:817:GLU:HB3	1:A:818:PRO:HD3	1.93	0.51
1:A:119:LYS:HB2	1:A:171:SER:CB	2.41	0.51
1:B:312:ASN:ND2	1:B:378:ASP:HA	2.21	0.51
1:B:810:LEU:HD12	1:B:936:ILE:CD1	2.41	0.51
1:A:43:ASN:C	1:A:43:ASN:HD22	2.15	0.51
1:B:58:PRO:HG2	1:B:423:ARG:HG3	1.93	0.50
1:B:298:LEU:HD13	1:B:475:ASN:HB3	1.92	0.50
1:A:314:TYR:HB2	1:A:479:ALA:HB3	1.93	0.50
1:B:348:SER:OG	1:B:606:GLU:OE2	2.20	0.50
1:A:559:LEU:HD22	1:A:742:MET:HB2	1.94	0.50
1:A:446:LEU:O	1:A:449:VAL:HG22	2.11	0.49
1:A:222:ASN:O	1:A:226:LEU:HB2	2.13	0.49
1:B:368:ARG:CD	5:B:3057:HOH:O	2.44	0.49
1:B:803:SER:HA	1:B:927:TYR:CE2	2.48	0.49
1:A:239:GLN:O	1:A:243:LYS:HG3	2.13	0.49
1:A:886:ILE:HG23	1:A:928:LEU:HD13	1.94	0.49
1:A:777:PHE:CB	1:A:992:ILE:HD11	2.34	0.49
1:B:291:HIS:CD2	1:B:370:PHE:HB2	2.48	0.48
1:B:88:ALA:HB3	1:B:151:PHE:CE2	2.47	0.48
1:B:716:ILE:HB	1:B:717:PRO:CD	2.44	0.48
1:A:860:GLU:OE2	1:A:957:HIS:HE1	1.96	0.48
1:A:800:GLN:HE22	4:A:2013:DIO:C1	2.08	0.48
1:B:420:VAL:HG12	1:B:634:TYR:OH	2.14	0.48
1:A:621:GLN:HB3	1:A:621:GLN:HE21	1.53	0.47
1:B:402:ARG:HD3	5:B:3108:HOH:O	2.13	0.47
1:B:528:ASN:HB3	1:B:531:ILE:CD1	2.45	0.47
1:B:609:TYR:CE2	1:B:613:LEU:HD11	2.50	0.47
1:A:880:GLU:HG3	1:B:457:GLU:HG2	1.95	0.47
1:A:311:ARG:HB3	1:A:379:LEU:HB2	1.96	0.47
1:B:473:PRO:O	1:B:476:VAL:HG12	2.15	0.47
1:B:200:ARG:CZ	1:B:307:ILE:HD11	2.45	0.47
1:B:843:ILE:HG22	1:B:844:GLN:N	2.29	0.47
1:B:94:ILE:HD11	1:B:253:LEU:CD1	2.46	0.46
1:A:348:SER:OG	1:A:606:GLU:OE2	2.23	0.46
1:A:417:LEU:HD11	1:A:531:ILE:HG12	1.96	0.46
1:B:607:TYR:CE2	1:B:644:LYS:HG2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:PHE:HD2	1:B:725:ILE:HD12	1.80	0.46
1:B:423:ARG:CG	1:B:423:ARG:HH11	2.29	0.46
1:B:460:ARG:O	1:B:464:ILE:HD13	2.16	0.46
1:A:803:SER:O	1:A:807:PHE:HD2	1.99	0.45
1:A:807:PHE:CE1	1:A:935:ASP:HB3	2.52	0.45
1:A:842:GLY:H	4:A:2013:DIO:C1'	2.30	0.45
1:A:466:MET:HE3	1:A:466:MET:O	2.17	0.45
1:A:709:LEU:HB3	1:A:710:PRO:CD	2.46	0.45
1:A:47:ILE:HD11	1:A:272:VAL:HG21	1.99	0.44
1:B:691:THR:O	1:B:999:LYS:CE	2.64	0.44
1:B:854:LYS:HB2	1:B:859:LEU:HD13	1.99	0.44
1:A:96:SER:HB2	1:A:144:GLY:HA2	2.00	0.44
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.98	0.44
1:A:575:ASN:N	1:A:575:ASN:HD22	2.15	0.44
1:B:586:ASP:OD1	1:B:589:HIS:CD2	2.70	0.44
1:A:842:GLY:N	4:A:2013:DIO:H1'2	2.32	0.44
1:A:854:LYS:HE2	1:A:855:PRO:HD2	2.00	0.44
1:B:600:LEU:HD11	1:B:648:LYS:HB3	2.00	0.44
1:B:204:LEU:HD21	1:B:304:ILE:HD12	1.99	0.43
1:A:586:ASP:HB2	1:A:587:PRO:CD	2.48	0.43
1:B:108:HIS:O	1:B:111:GLN:HB3	2.19	0.43
1:B:316:THR:HG22	5:B:3063:HOH:O	2.10	0.43
1:A:791:ILE:CD1	1:A:793:ILE:HG13	2.49	0.43
1:B:860:GLU:OE2	1:B:957:HIS:HE1	2.01	0.43
1:B:730:HIS:HD2	1:B:904:SER:OG	2.01	0.43
1:A:538:LEU:HD13	1:A:734:THR:HG23	1.99	0.43
1:A:440:ILE:HD12	1:A:449:VAL:HG12	2.00	0.43
1:A:842:GLY:C	1:A:843:ILE:HD12	2.39	0.43
1:B:528:ASN:HB3	1:B:531:ILE:HD13	2.01	0.43
1:B:135:ALA:HA	1:B:892:ARG:NH2	2.33	0.43
1:B:532:PRO:HG3	1:B:634:TYR:CD2	2.54	0.43
1:A:437:ILE:HD13	1:A:437:ILE:N	2.34	0.42
1:B:842:GLY:HA3	1:B:1008:VAL:HG23	2.02	0.42
1:B:641:LEU:O	1:B:645:ILE:HG12	2.19	0.42
1:B:842:GLY:H	4:B:2014:DIO:H21	1.84	0.42
1:A:683:MET:HA	1:A:792:GLU:OE2	2.20	0.42
1:A:806:MET:HE3	1:A:928:LEU:HG	2.02	0.42
1:B:418:ASN:ND2	1:B:454:TYR:O	2.53	0.42
1:A:716:ILE:HB	1:A:717:PRO:HD3	2.02	0.42
1:B:387:VAL:HG11	1:B:480:ILE:HD11	2.00	0.42
1:A:441:LEU:HD23	1:A:449:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:LEU:HA	1:A:201:LEU:HD12	1.68	0.41
1:A:645:ILE:HG22	1:A:649:MET:HE3	2.01	0.41
1:A:896:LYS:HB2	1:A:896:LYS:HE2	1.80	0.41
1:B:708:THR:HB	1:B:710:PRO:HD2	2.01	0.41
1:A:134:HIS:O	1:A:154:SER:HB3	2.19	0.41
1:A:53:HIS:CE1	5:A:3005:HOH:O	2.54	0.41
1:A:559:LEU:HD22	1:A:742:MET:CB	2.50	0.41
1:A:862:ARG:HD2	5:A:3202:HOH:O	2.19	0.41
1:B:423:ARG:HG2	1:B:423:ARG:HH11	1.84	0.41
1:B:76:LEU:HD12	1:B:437:ILE:HG21	2.02	0.41
1:A:756:LYS:HB3	1:A:757:PRO:HD2	2.01	0.41
1:A:907:TYR:O	1:A:911:ILE:HG12	2.20	0.41
1:A:550:LEU:HD11	1:A:558:LYS:HG2	2.02	0.41
1:A:884:LYS:NZ	5:A:3222:HOH:O	2.53	0.41
1:A:771:LEU:HD21	1:A:954:VAL:HG23	2.02	0.41
1:B:441:LEU:CD2	1:B:449:VAL:HG11	2.45	0.41
1:B:75:VAL:HA	1:B:256:VAL:O	2.21	0.41
1:A:674:ARG:HD2	1:A:784:GLU:OE2	2.21	0.41
1:A:697:LYS:NZ	5:A:3171:HOH:O	2.54	0.41
1:B:49:ARG:HH12	1:B:446:LEU:HD22	1.86	0.41
1:A:512:LYS:HE3	1:A:512:LYS:HB3	2.00	0.41
1:B:52:ASN:HD22	1:B:52:ASN:HA	1.50	0.41
1:B:556:MET:HG3	1:B:556:MET:O	2.20	0.41
1:A:596:TYR:CD2	1:A:597:LEU:HD13	2.55	0.41
1:B:713:LYS:O	1:B:717:PRO:HD2	2.20	0.40
1:B:94:ILE:CD1	1:B:253:LEU:HD12	2.50	0.40
1:A:791:ILE:HD13	1:A:793:ILE:HG13	2.03	0.40
1:A:828:GLN:NE2	5:A:3203:HOH:O	2.54	0.40
1:B:600:LEU:HD21	1:B:649:MET:HB3	2.03	0.40
1:B:642:LEU:O	1:B:646:ILE:HG12	2.21	0.40
1:B:833:VAL:HG22	1:B:850:ILE:HD12	2.03	0.40
1:A:880:GLU:CG	1:B:457:GLU:HG2	2.51	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	950/990 (96%)	924 (97%)	25 (3%)	1 (0%)	55	66
1	B	950/990 (96%)	923 (97%)	27 (3%)	0	100	100
2	C	1/76 (1%)	1 (100%)	0	0	100	100
2	D	1/76 (1%)	1 (100%)	0	0	100	100
All	All	1902/2132 (89%)	1849 (97%)	52 (3%)	1 (0%)	55	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	SER

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	850/879 (97%)	777 (91%)	73 (9%)	12	12
1	B	850/879 (97%)	779 (92%)	71 (8%)	13	13
2	C	3/68 (4%)	2 (67%)	1 (33%)	0	0
2	D	3/68 (4%)	0	3 (100%)	0	0
All	All	1706/1894 (90%)	1558 (91%)	148 (9%)	12	12

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	67	LEU
1	A	74	LYS
1	A	76	LEU
1	A	97	LEU

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Mol	Chain	Res	Type
1	A	111	GLN
1	A	119	LYS
1	A	120	LYS
1	A	154	SER
1	A	158	LEU
1	A	171	SER
1	A	179	LYS
1	A	201	LEU
1	A	226	LEU
1	A	229	ARG
1	A	270	LEU
1	A	273	LYS
1	A	277	GLU
1	A	285	LEU
1	A	316	THR
1	A	337	LEU
1	A	347	LEU
1	A	356	VAL
1	A	360	VAL
1	A	412	GLN
1	A	414	LEU
1	A	417	LEU
1	A	423	ARG
1	A	446	LEU
1	A	449	VAL
1	A	466	MET
1	A	486	GLU
1	A	505	ILE
1	A	512	LYS
1	A	517	ASP
1	A	527	LYS
1	A	529	GLU
1	A	558	LYS
1	A	595	LEU
1	A	597	LEU
1	A	612	GLU
1	A	616	LEU
1	A	621	GLN
1	A	629	LEU
1	A	642	LEU
1	A	643	LYS
1	A	648	LYS

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Mol	Chain	Res	Type
1	A	677	GLN
1	A	691	THR
1	A	711	ARG
1	A	712	LEU
1	A	728	LEU
1	A	759	LEU
1	A	765	ARG
1	A	771	LEU
1	A	788	ASN
1	A	791	ILE
1	A	799	MET
1	A	810	LEU
1	A	823	LEU
1	A	839	ARG
1	A	846	LEU
1	A	859	LEU
1	A	867	LEU
1	A	889	LEU
1	A	912	ILE
1	A	928	LEU
1	A	930	THR
1	A	931	LEU
1	A	951	ARG
1	A	993	GLN
1	A	1007	LEU
1	A	1011	HIS
1	B	43	ASN
1	B	52	ASN
1	B	76	LEU
1	B	94	ILE
1	B	97	LEU
1	B	111	GLN
1	B	158	LEU
1	B	201	LEU
1	B	226	LEU
1	B	239	GLN
1	B	243	LYS
1	B	270	LEU
1	B	277	GLU
1	B	285	LEU
1	B	287	GLU
1	B	316	THR

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Mol	Chain	Res	Type
1	B	329	ASN
1	B	337	LEU
1	B	347	LEU
1	B	374	ILE
1	B	412	GLN
1	B	414	LEU
1	B	417	LEU
1	B	423	ARG
1	B	425	LYS
1	B	446	LEU
1	B	450	LEU
1	B	460	ARG
1	B	466	MET
1	B	512	LYS
1	B	517	ASP
1	B	524	LEU
1	B	531	ILE
1	B	556	MET
1	B	566	LYS
1	B	577	GLU
1	B	595	LEU
1	B	597	LEU
1	B	612	GLU
1	B	616	LEU
1	B	624	ILE
1	B	629	LEU
1	B	642	LEU
1	B	648	LYS
1	B	655	ASP
1	B	657	LYS
1	B	711	ARG
1	B	712	LEU
1	B	717	PRO
1	B	728	LEU
1	B	733	ILE
1	B	758	LEU
1	B	759	LEU
1	B	771	LEU
1	B	788	ASN
1	B	810	LEU
1	B	817	GLU
1	B	823	LEU

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Mol	Chain	Res	Type
1	B	846	LEU
1	B	859	LEU
1	B	867	LEU
1	B	873	SER
1	B	889	LEU
1	B	912	ILE
1	B	928	LEU
1	B	931	LEU
1	B	934	GLU
1	B	942	GLU
1	B	957	HIS
1	B	993	GLN
1	B	1007	LEU
2	C	3	ILE
2	D	1	MET
2	D	2	GLN
2	D	3	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	53	HIS
1	A	231	ASN
1	A	232	GLN
1	A	312	ASN
1	A	336	HIS
1	A	499	GLN
1	A	575	ASN
1	A	589	HIS
1	A	621	GLN
1	A	730	HIS
1	A	770	GLN
1	A	805	ASN
1	A	828	GLN
1	A	841	ASN
1	A	883	GLN
1	A	957	HIS
1	A	979	ASN
1	B	52	ASN
1	B	231	ASN
1	B	232	GLN

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Mol	Chain	Res	Type
1	B	294	GLN
1	B	312	ASN
1	B	329	ASN
1	B	363	GLN
1	B	412	GLN
1	B	575	ASN
1	B	589	HIS
1	B	730	HIS
1	B	770	GLN
1	B	805	ASN
1	B	828	GLN
1	B	841	ASN
1	B	914	GLN
1	B	922	ASN
1	B	957	HIS
1	B	979	ASN
1	B	993	GLN
2	C	2	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\# Z > 2$
4	DIO	A	2013	-	6,6,6	0.54	0	6,6,6	1.97	3 (50%)
4	DIO	B	2013	-	6,6,6	0.62	0	6,6,6	1.09	1 (16%)
4	DIO	B	2014	-	6,6,6	0.54	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
4	DIO	A	2013	-	-	0/0/6/6	0/1/1/1
4	DIO	B	2013	-	-	0/0/6/6	0/1/1/1
4	DIO	B	2014	-	-	0/0/6/6	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2013	DIO	O1-C1-C1'	-2.92	96.36	110.89
4	A	2013	DIO	O1-C2-C2'	-2.58	98.06	110.89
4	B	2013	DIO	C2'-O1'-C1'	2.09	116.95	109.89
4	A	2013	DIO	C2'-O1'-C1'	2.22	117.39	109.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2013	DIO	7	0
4	B	2013	DIO	1	0
4	B	2014	DIO	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	954/990 (96%)	-0.41	4 (0%) 92 96	16, 29, 44, 64	0
1	B	954/990 (96%)	-0.39	3 (0%) 93 97	21, 32, 47, 72	0
2	C	3/76 (3%)	1.34	1 (33%) 0 0	45, 45, 45, 46	0
2	D	3/76 (3%)	0.96	0 100 100	43, 43, 43, 45	0
All	All	1914/2132 (89%)	-0.39	8 (0%) 92 96	16, 30, 46, 72	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	43	ASN	3.4
1	B	543	GLU	3.2
1	A	543	GLU	3.0
1	B	542	LYS	2.8
1	B	43	ASN	2.8
1	A	517	ASP	2.7
1	A	508	GLU	2.2
2	C	3	ILE	2.1

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, 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	LLDF	B-factors(Å ²)	Q<0.9
4	DIO	B	2014	6/6	0.91	0.23	12.82	49,55,59,60	0
4	DIO	A	2013	6/6	0.94	0.23	6.38	47,50,53,55	0
4	DIO	B	2013	6/6	0.97	0.08	-2.06	40,42,44,44	0
3	ZN	B	2012	1/1	0.96	0.11	-	36,36,36,36	0
3	ZN	A	2012	1/1	0.99	0.11	-	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.