



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:35 am GMT

PDB ID : 2JG4  
Title : SUBSTRATE-FREE IDE STRUCTURE IN ITS CLOSED CONFORMATION  
Authors : Malito, E.; Tang, W.J.  
Deposited on : 2007-02-07  
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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
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) : recalc28949

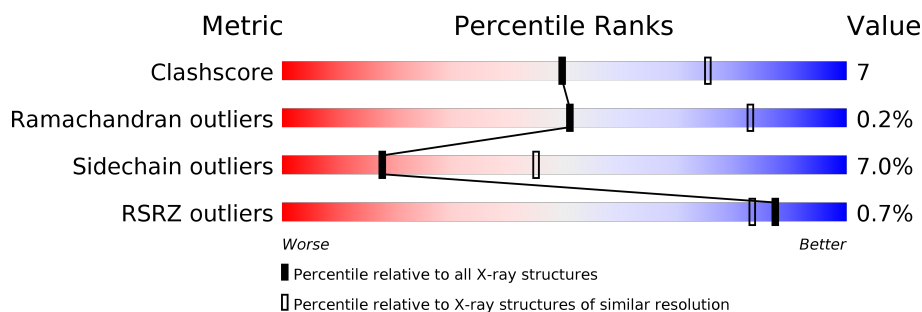
# 1 Overall quality at a glance

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))
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (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	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>79%</span> <span>15%</span> <span>...</span> </div> </div>
1	B	990	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>78%</span> <span>16%</span> <span>...</span> </div> </div>

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	2013	-	-	-	X
3	DIO	A	2014	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DIO	B	2014	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16104 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	961	Total	C	N	O	S	0	1	0
			7850	5048	1320	1448	34			
1	B	958	Total	C	N	O	S	0	0	0
			7801	5020	1308	1439	34			

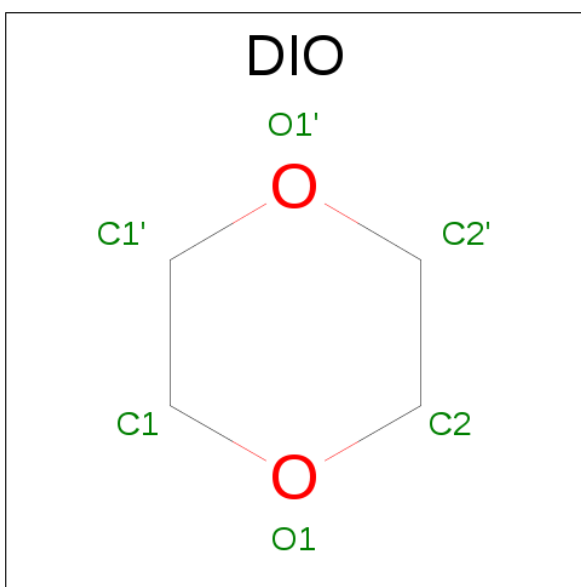
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	ILE	MET	CONFLICT	UNP P14735
A	555	ALA	VAL	CONFLICT	UNP P14735
A	567	PHE	LYS	CONFLICT	UNP P14735
A	568	PHE	LYS	CONFLICT	UNP P14735
A	569	LEU	LYS	CONFLICT	UNP P14735
A	831	PHE	TYR	ENGINEERED MUTATION	UNP P14735
B	78	ILE	MET	CONFLICT	UNP P14735
B	555	ALA	VAL	CONFLICT	UNP P14735
B	567	PHE	LYS	CONFLICT	UNP P14735
B	568	PHE	LYS	CONFLICT	UNP P14735
B	569	LEU	LYS	CONFLICT	UNP P14735
B	831	PHE	TYR	ENGINEERED MUTATION	UNP P14735

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

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



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	242	Total	O	0	0
			242	242		
4	B	185	Total	O	0	0
			185	185		

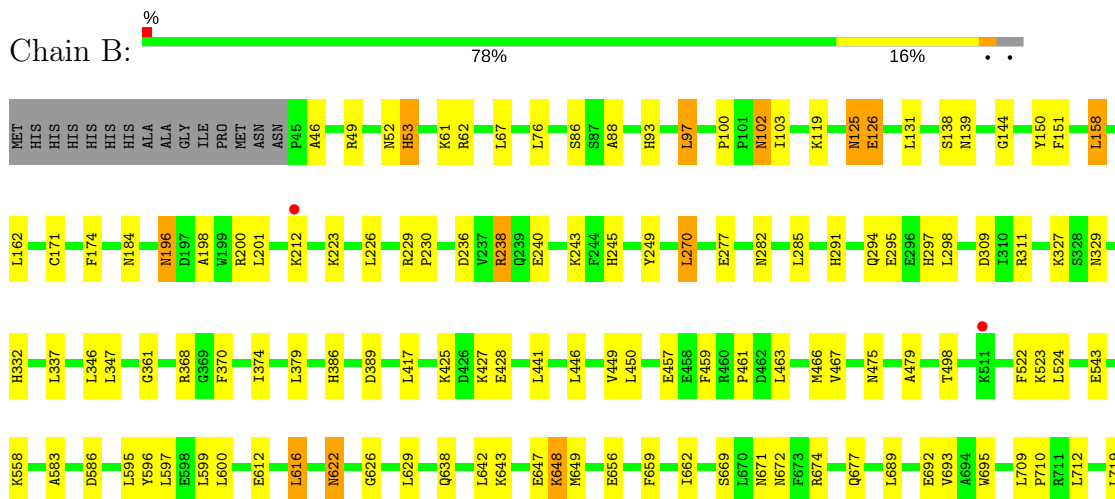
### 3 Residue-property plots

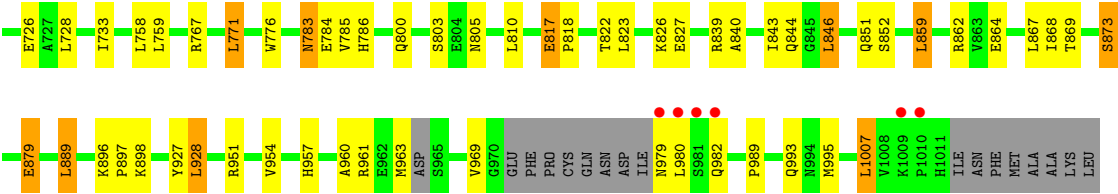
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	263.21Å 263.21Å 90.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.80 29.88 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (15.00-2.80) 99.7 (29.88-2.80)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.91 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.182 , 0.227 0.186 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	39.2	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 50.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16104	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [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	0.59	3/8046 (0.0%)	0.63	4/10883 (0.0%)
1	B	0.49	0/7996	0.60	1/10817 (0.0%)
All	All	0.54	3/16042 (0.0%)	0.62	5/21700 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	GLU	C-N	-22.44	0.82	1.34
1	A	60	ASP	C-N	-10.42	1.10	1.34
1	A	63	GLU	C-N	-8.69	1.14	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	GLU	O-C-N	-5.87	113.30	122.70
1	B	846	LEU	CA-CB-CG	5.78	128.60	115.30
1	A	62	ARG	O-C-N	-5.41	114.04	122.70
1	A	59	GLU	C-N-CA	5.32	134.99	121.70
1	A	285	LEU	CA-CB-CG	5.31	127.52	115.30

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7850	0	7768	105	0
1	B	7801	0	7705	108	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	12	0	16	2	0
3	B	12	0	16	3	0
4	A	242	0	0	11	0
4	B	185	0	0	8	0
All	All	16104	0	15505	209	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 7.

All (209) 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:59:GLU:O	1:A:60:ASP:N	1.72	1.18
1:A:59:GLU:C	1:A:60:ASP:CA	2.12	1.18
1:A:59:GLU:CA	1:A:60:ASP:N	2.11	1.14
1:A:491:ARG:HG3	1:A:491:ARG:HH11	1.17	1.09
1:A:229:ARG:HG2	1:A:229:ARG:HH11	1.13	1.06
1:B:46:ALA:HA	4:B:3001:HOH:O	1.65	0.95
1:B:622:ASN:H	1:B:622:ASN:HD22	1.19	0.89
1:B:93:HIS:HE1	1:B:368:ARG:HH21	1.15	0.88
1:A:59:GLU:C	1:A:60:ASP:N	0.82	0.87
1:B:441:LEU:HD23	1:B:449:VAL:HG11	1.55	0.86
1:A:309:ASP:H	1:A:672:ASN:HD21	1.25	0.85
1:B:771:LEU:HD21	1:B:954:VAL:HG23	1.58	0.84
1:A:229:ARG:HG2	1:A:229:ARG:NH1	1.90	0.82
1:B:425:LYS:HE2	1:B:428:GLU:OE2	1.81	0.80
1:B:93:HIS:CE1	1:B:368:ARG:HH21	1.99	0.80
1:A:800:GLN:HE22	3:A:2014:DIO:H12	1.46	0.79
1:A:412:GLN:HG2	4:A:3100:HOH:O	1.83	0.77
1:B:102:ASN:H	1:B:102:ASN:HD22	1.33	0.77
1:A:229:ARG:CG	1:A:229:ARG:HH11	1.95	0.74
1:A:491:ARG:CG	1:A:491:ARG:HH11	1.97	0.74
1:A:827:GLU:OE1	1:A:862:ARG:HD3	1.89	0.72
1:B:622:ASN:H	1:B:622:ASN:ND2	1.89	0.71
1:A:622:ASN:H	1:A:622:ASN:HD22	1.39	0.71
1:B:309:ASP:H	1:B:672:ASN:HD21	1.40	0.70
1:A:294:GLN:H	1:A:297:HIS:HD2	1.39	0.69
4:A:3218:HOH:O	1:B:53:HIS:HB3	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:774[A]:ARG:HD3	4:A:3185:HOH:O	1.93	0.68
1:A:934:GLU:HG3	1:B:53:HIS:NE2	2.09	0.67
1:A:389:ASP:O	1:A:393:HIS:HD2	1.78	0.67
1:B:898:LYS:HG2	4:B:3175:HOH:O	1.94	0.67
1:A:93:HIS:HE1	1:A:368:ARG:HH21	1.43	0.67
1:B:827:GLU:OE1	1:B:862:ARG:HD3	1.94	0.66
1:B:184:ASN:HD21	1:B:223:LYS:NZ	1.93	0.66
1:B:783:ASN:ND2	1:B:786:HIS:H	1.93	0.65
1:A:491:ARG:NH1	1:A:491:ARG:HG3	1.98	0.64
1:A:94:ILE:HG13	1:A:248:TYR:HB3	1.78	0.64
1:A:783:ASN:ND2	1:A:786:HIS:H	1.96	0.64
1:A:309:ASP:H	1:A:672:ASN:ND2	1.92	0.63
1:B:656:GLU:HG3	1:B:709:LEU:HD22	1.79	0.62
1:B:174:PHE:O	1:B:238:ARG:HD3	1.99	0.62
1:A:59:GLU:O	1:A:60:ASP:CA	2.38	0.62
1:A:622:ASN:H	1:A:622:ASN:ND2	1.97	0.61
1:B:162:LEU:HD23	1:B:270:LEU:CD1	2.30	0.61
1:A:616:LEU:HD21	1:A:638:GLN:HG2	1.82	0.61
1:B:783:ASN:HD22	1:B:785:VAL:H	1.48	0.61
1:A:880:GLU:CB	1:B:457:GLU:HG2	2.30	0.61
1:B:771:LEU:HD21	1:B:954:VAL:CG2	2.30	0.61
1:B:386:HIS:HE1	4:B:3087:HOH:O	1.83	0.61
1:A:880:GLU:HB3	1:B:457:GLU:HG2	1.83	0.60
1:A:102:ASN:HD22	1:A:102:ASN:H	1.49	0.60
1:B:162:LEU:HD23	1:B:270:LEU:HD13	1.83	0.60
1:A:125:ASN:HD22	1:A:125:ASN:H	1.48	0.60
1:A:53:HIS:HE1	4:A:3005:HOH:O	1.84	0.60
1:A:671:ASN:O	1:A:674:ARG:HG2	2.03	0.59
1:B:805:ASN:HD22	1:B:844:GLN:HE22	1.51	0.58
1:B:298:LEU:HD13	1:B:475:ASN:HB2	1.85	0.57
1:B:297:HIS:HE1	4:B:3059:HOH:O	1.86	0.57
1:B:309:ASP:H	1:B:672:ASN:ND2	2.01	0.57
1:A:771:LEU:HD21	1:A:954:VAL:CG2	2.35	0.57
1:B:896:LYS:HD3	1:B:897:PRO:HD2	1.86	0.57
1:A:294:GLN:H	1:A:297:HIS:CD2	2.21	0.56
1:B:600:LEU:HD21	1:B:649:MET:HB3	1.86	0.56
1:A:632:LYS:HD2	4:A:3154:HOH:O	2.06	0.56
1:A:196:ASN:HD21	1:A:198:ALA:HB3	1.70	0.56
1:A:415:LYS:HE3	4:A:3099:HOH:O	2.06	0.56
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.88	0.55
1:B:817:GLU:HG3	1:B:818:PRO:HD3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:600:LEU:HD11	1:B:648:LYS:HB3	1.88	0.55
1:A:979:ASN:HA	4:A:3236:HOH:O	2.05	0.55
1:A:196:ASN:HD22	1:A:199:TRP:H	1.53	0.55
1:B:689:LEU:HD23	1:B:995:MET:HG2	1.88	0.54
1:A:602:ASP:OD1	1:A:658:ARG:HD3	2.08	0.54
1:B:125:ASN:H	1:B:125:ASN:HD22	1.56	0.54
1:B:368:ARG:HD2	4:B:3057:HOH:O	2.07	0.54
1:B:52:ASN:O	1:B:53:HIS:C	2.46	0.53
1:A:123:LYS:HB3	1:A:126:GLU:HB2	1.90	0.53
1:B:294:GLN:H	1:B:297:HIS:CD2	2.27	0.52
1:B:196:ASN:ND2	1:B:198:ALA:H	2.07	0.52
1:B:295:GLU:OE1	1:B:295:GLU:HA	2.10	0.52
1:B:616:LEU:HD21	1:B:638:GLN:HG2	1.91	0.52
1:A:852:SER:HB3	1:A:859:LEU:HD21	1.92	0.52
1:B:184:ASN:HD21	1:B:223:LYS:HZ1	1.58	0.52
1:A:709:LEU:HB3	1:A:710:PRO:HD3	1.91	0.52
1:A:691:THR:O	1:A:999:LYS:HE3	2.10	0.51
1:A:577:GLU:OE2	1:A:912:ILE:HG22	2.10	0.51
1:B:294:GLN:H	1:B:297:HIS:HD2	1.59	0.50
1:A:460:ARG:NH1	1:A:462:ASP:OD1	2.44	0.50
1:A:389:ASP:O	1:A:393:HIS:CD2	2.62	0.50
1:B:298:LEU:HD13	1:B:475:ASN:CB	2.42	0.50
1:A:102:ASN:HD22	1:A:102:ASN:N	2.08	0.50
1:A:229:ARG:HD2	1:A:233:GLU:OE2	2.12	0.50
1:A:759:LEU:HB2	1:A:762:GLN:HG3	1.94	0.50
1:A:595:LEU:HD12	1:A:662:ILE:HG22	1.94	0.50
1:A:446:LEU:O	1:A:449:VAL:HG22	2.12	0.50
1:B:62:ARG:HD3	1:B:427:LYS:HE3	1.93	0.49
1:B:979:ASN:ND2	1:B:980:LEU:HG	2.27	0.49
1:B:229:ARG:HB3	1:B:230:PRO:HD3	1.94	0.49
1:A:577:GLU:HG3	4:A:3142:HOH:O	2.13	0.49
1:B:600:LEU:CD2	1:B:649:MET:HB3	2.42	0.49
1:B:599:LEU:HD23	1:B:662:ILE:HD12	1.95	0.49
1:A:455:LEU:HA	4:A:3101:HOH:O	2.13	0.49
1:A:880:GLU:HG3	1:B:327:LYS:HD3	1.95	0.48
1:B:783:ASN:ND2	1:B:785:VAL:H	2.11	0.48
1:A:100:PRO:HB2	1:A:102:ASN:ND2	2.29	0.48
1:A:311:ARG:HB3	1:A:379:LEU:HB2	1.95	0.48
1:A:245:HIS:O	1:A:249:TYR:HB2	2.13	0.48
1:B:97:LEU:HB2	1:B:144:GLY:O	2.14	0.48
1:A:934:GLU:HG3	1:B:53:HIS:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:GLY:HA3	1:A:152:ASP:O	2.14	0.48
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.49	0.48
1:B:88:ALA:HB3	1:B:151:PHE:CE2	2.48	0.48
1:B:960:ALA:HB3	1:B:963:MET:HG3	1.96	0.48
1:B:767:ARG:HG2	1:B:1007:LEU:HD13	1.96	0.48
1:A:314:TYR:HB2	1:A:479:ALA:HB3	1.94	0.47
1:B:692:GLU:HG2	1:B:693:VAL:HG23	1.97	0.47
1:A:114:LEU:HD13	1:A:168:PHE:HB3	1.96	0.47
1:B:839:ARG:HB3	3:B:2014:DIO:H12	1.96	0.47
1:B:583:ALA:CB	1:B:626:GLY:HA2	2.44	0.47
1:B:869:THR:O	1:B:873:SER:HB2	2.15	0.47
1:A:655:ASP:OD1	1:A:657:LYS:HB2	2.14	0.47
1:A:824:ARG:O	1:A:828:GLN:HA	2.15	0.47
1:B:236:ASP:O	1:B:240:GLU:HG2	2.15	0.47
1:B:346:LEU:HA	1:B:522:PHE:CE2	2.49	0.47
1:B:93:HIS:HE1	1:B:368:ARG:NH2	1.98	0.46
1:A:960:ALA:HB3	1:A:963:MET:HG3	1.97	0.46
1:A:620:LEU:HD13	1:A:629:LEU:HG	1.98	0.46
1:A:927:TYR:O	1:A:930:THR:HB	2.15	0.45
1:B:643:LYS:O	1:B:647:GLU:HB2	2.16	0.45
1:B:596:TYR:OH	1:B:649:MET:HB2	2.16	0.45
1:A:196:ASN:ND2	1:A:199:TRP:H	2.13	0.45
1:B:776:TRP:CE3	1:B:989:PRO:HB3	2.52	0.45
1:A:817:GLU:HG3	1:A:818:PRO:HD3	1.97	0.45
1:A:711:ARG:HD2	4:A:3174:HOH:O	2.17	0.45
1:A:783:ASN:HD22	1:A:786:HIS:H	1.63	0.45
1:B:100:PRO:HG2	1:B:103:ILE:HB	1.98	0.45
1:B:622:ASN:N	1:B:622:ASN:ND2	2.61	0.45
1:A:838:ARG:O	1:A:844:GLN:HA	2.17	0.45
1:B:245:HIS:O	1:B:249:TYR:HB2	2.17	0.44
1:B:119:LYS:HB2	1:B:171:CYS:SG	2.56	0.44
1:A:596:TYR:OH	1:A:649:MET:HB2	2.17	0.44
1:B:86:SER:HB3	1:B:158:LEU:HG	2.00	0.44
1:B:671:ASN:O	1:B:674:ARG:HG2	2.17	0.44
1:B:125:ASN:N	1:B:125:ASN:HD22	2.16	0.44
1:A:491:ARG:CG	1:A:491:ARG:NH1	2.66	0.43
1:A:591:ASN:O	1:A:595:LEU:HD22	2.17	0.43
1:A:860:GLU:OE2	1:A:957:HIS:HE1	2.02	0.43
1:B:479:ALA:HB2	3:B:2013:DIO:H22	2.00	0.43
1:B:361:GLY:HA2	1:B:374:ILE:O	2.18	0.43
1:B:459:PHE:CE2	1:B:461:PRO:HG3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LEU:CD1	1:A:138:SER:HB2	2.48	0.43
1:A:88:ALA:HB3	1:A:151:PHE:CE2	2.53	0.43
1:B:311:ARG:HB3	1:B:379:LEU:HB2	1.99	0.43
1:B:329:ASN:HB3	1:B:332:HIS:HB2	2.00	0.43
1:A:118:THR:HG22	1:A:172:PRO:HA	2.01	0.43
1:A:107:SER:HB3	1:A:244:PHE:CZ	2.54	0.43
1:A:329:ASN:HB3	1:A:332:HIS:HB2	2.01	0.43
1:B:822:THR:O	1:B:827:GLU:HG3	2.19	0.43
1:B:889:LEU:HB3	1:B:928:LEU:HD11	2.01	0.43
1:B:960:ALA:O	1:B:961:ARG:C	2.57	0.43
1:A:229:ARG:HB3	1:A:230:PRO:HD3	2.01	0.43
1:B:852:SER:HB3	1:B:859:LEU:HD21	2.00	0.43
1:A:948:ALA:HA	1:A:949:PRO:HD2	1.73	0.42
1:B:622:ASN:N	1:B:622:ASN:HD22	2.01	0.42
1:B:139:ASN:HB3	1:B:150:TYR:CZ	2.54	0.42
1:B:803:SER:HA	1:B:927:TYR:CE2	2.54	0.42
1:A:441:LEU:HD23	1:A:449:VAL:HG11	2.01	0.42
1:B:677:GLN:HG2	1:B:851:GLN:HE22	1.84	0.42
1:A:311:ARG:NH1	1:A:379:LEU:O	2.50	0.42
1:A:491:ARG:HB2	1:A:500:TYR:O	2.19	0.42
1:B:689:LEU:CD2	1:B:995:MET:HG2	2.50	0.42
1:A:185:ALA:HB2	1:A:828:GLN:HE22	1.83	0.42
1:B:386:HIS:HD2	1:B:389:ASP:OD2	2.03	0.42
1:B:200:ARG:NH2	1:B:498:THR:HA	2.34	0.42
1:B:709:LEU:HB3	1:B:710:PRO:HD3	2.01	0.42
1:A:93:HIS:HD2	1:A:145:GLU:O	2.02	0.42
1:A:805:ASN:HD22	1:A:844:GLN:HE22	1.67	0.42
1:A:886:ILE:HG23	1:A:928:LEU:HD13	2.02	0.41
1:B:805:ASN:ND2	1:B:844:GLN:HE22	2.16	0.41
1:A:239:GLN:O	1:A:243:LYS:HG2	2.20	0.41
1:A:715:PHE:O	1:A:718:GLN:HB3	2.20	0.41
1:B:583:ALA:HB2	1:B:626:GLY:HA2	2.02	0.41
1:B:800:GLN:HA	1:B:844:GLN:NE2	2.36	0.41
3:A:2014:DIO:H22	4:A:3213:HOH:O	2.20	0.41
1:B:131:LEU:CD1	1:B:138:SER:HB2	2.50	0.41
1:B:49:ARG:NH2	1:B:446:LEU:HD23	2.36	0.41
1:B:558:LYS:HB2	1:B:726:GLU:HG3	2.02	0.41
1:A:125:ASN:HD22	1:A:125:ASN:N	2.17	0.41
1:A:673:PHE:CG	1:A:697:LYS:HE3	2.55	0.41
1:A:736:GLN:CD	1:A:736:GLN:N	2.74	0.41
1:B:599:LEU:HD21	1:B:659:PHE:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:GLU:HG3	4:B:3018:HOH:O	2.20	0.41
1:A:140:ALA:HA	1:A:148:ASN:O	2.21	0.41
1:A:179:LYS:HD2	1:A:237:VAL:HB	2.01	0.41
1:A:236:ASP:OD2	1:A:239:GLN:HG2	2.20	0.41
1:A:940:TYR:CE1	1:A:945:ALA:HB2	2.55	0.41
1:B:368:ARG:HD3	4:B:3065:HOH:O	2.20	0.41
1:B:864:GLU:OE1	1:B:951:ARG:NH2	2.48	0.41
1:A:604:LEU:HA	1:A:604:LEU:HD23	1.92	0.41
1:A:796:GLN:HB3	1:A:952:HIS:HB2	2.03	0.41
1:A:793:ILE:O	1:A:847:ARG:HA	2.21	0.41
1:B:840:ALA:HA	3:B:2014:DIO:H1'1	2.03	0.41
1:B:291:HIS:CD2	1:B:370:PHE:HB2	2.56	0.40
1:B:843:ILE:HG22	1:B:844:GLN:N	2.36	0.40
1:B:463:LEU:O	1:B:467:VAL:HG23	2.22	0.40
1:B:879:GLU:OE1	1:B:879:GLU:HA	2.20	0.40
1:A:62:ARG:HG2	1:A:80:ASP:HB2	2.04	0.40
1:B:784:GLU:O	1:B:961:ARG:HG3	2.22	0.40
1:B:586:ASP:HA	1:B:695:TRP:CZ2	2.56	0.40
1:B:864:GLU:HG3	4:B:3174:HOH:O	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	958/990 (97%)	929 (97%)	27 (3%)	2 (0%)	51	83
1	B	952/990 (96%)	914 (96%)	37 (4%)	1 (0%)	55	86
All	All	1910/1980 (96%)	1843 (96%)	64 (3%)	3 (0%)	51	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	964	ASP
1	B	53	HIS
1	A	295	GLU

### 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	858/883 (97%)	799 (93%)	59 (7%)	18	46
1	B	850/883 (96%)	790 (93%)	60 (7%)	17	44
All	All	1708/1766 (97%)	1589 (93%)	119 (7%)	18	45

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LYS
1	A	97	LEU
1	A	102	ASN
1	A	125	ASN
1	A	158	LEU
1	A	196	ASN
1	A	201	LEU
1	A	226	LEU
1	A	229	ARG
1	A	270	LEU
1	A	281	LYS
1	A	285	LEU
1	A	337	LEU
1	A	347	LEU
1	A	352	SER
1	A	412	GLN
1	A	415	LYS
1	A	417	LEU
1	A	431	ARG
1	A	446	LEU
1	A	449	VAL

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Mol	Chain	Res	Type
1	A	450	LEU
1	A	466	MET
1	A	491	ARG
1	A	521	LYS
1	A	595	LEU
1	A	597	LEU
1	A	600	LEU
1	A	616	LEU
1	A	622	ASN
1	A	629	LEU
1	A	632	LYS
1	A	642	LEU
1	A	674	ARG
1	A	691	THR
1	A	711	ARG
1	A	712	LEU
1	A	719	LEU
1	A	728	LEU
1	A	736	GLN
1	A	756	LYS
1	A	759	LEU
1	A	765	ARG
1	A	771	LEU
1	A	784	GLU
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	889	LEU
1	A	928	LEU
1	A	931	LEU
1	A	957	HIS
1	A	964	ASP
1	A	969	VAL
1	A	1007	LEU
1	B	61	LYS
1	B	67	LEU
1	B	76	LEU
1	B	97	LEU

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Mol	Chain	Res	Type
1	B	102	ASN
1	B	125	ASN
1	B	126	GLU
1	B	158	LEU
1	B	196	ASN
1	B	201	LEU
1	B	212	LYS
1	B	226	LEU
1	B	238	ARG
1	B	243	LYS
1	B	270	LEU
1	B	277	GLU
1	B	282	ASN
1	B	285	LEU
1	B	337	LEU
1	B	347	LEU
1	B	417	LEU
1	B	450	LEU
1	B	466	MET
1	B	523	LYS
1	B	524	LEU
1	B	543	GLU
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	648	LYS
1	B	669	SER
1	B	712	LEU
1	B	719	LEU
1	B	728	LEU
1	B	733	ILE
1	B	758	LEU
1	B	759	LEU
1	B	771	LEU
1	B	783	ASN
1	B	810	LEU
1	B	817	GLU
1	B	823	LEU

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Mol	Chain	Res	Type
1	B	826	LYS
1	B	846	LEU
1	B	859	LEU
1	B	867	LEU
1	B	868	ILE
1	B	873	SER
1	B	879	GLU
1	B	889	LEU
1	B	928	LEU
1	B	957	HIS
1	B	969	VAL
1	B	982	GLN
1	B	993	GLN
1	B	1007	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) 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	196	ASN
1	A	231	ASN
1	A	232	GLN
1	A	294	GLN
1	A	297	HIS
1	A	300	GLN
1	A	336	HIS
1	A	393	HIS
1	A	407	GLN
1	A	502	GLN
1	A	575	ASN
1	A	589	HIS
1	A	605	ASN
1	A	622	ASN
1	A	672	ASN
1	A	783	ASN
1	A	805	ASN
1	A	828	GLN
1	A	857	HIS

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Mol	Chain	Res	Type
1	A	922	ASN
1	A	957	HIS
1	A	979	ASN
1	B	52	ASN
1	B	93	HIS
1	B	102	ASN
1	B	125	ASN
1	B	184	ASN
1	B	196	ASN
1	B	231	ASN
1	B	294	GLN
1	B	297	HIS
1	B	300	GLN
1	B	336	HIS
1	B	386	HIS
1	B	393	HIS
1	B	475	ASN
1	B	502	GLN
1	B	575	ASN
1	B	605	ASN
1	B	622	ASN
1	B	672	ASN
1	B	783	ASN
1	B	805	ASN
1	B	828	GLN
1	B	914	GLN
1	B	922	ASN
1	B	957	HIS
1	B	979	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	A	2013	-	6,6,6	0.61	0	6,6,6	0.68	0
3	DIO	A	2014	-	6,6,6	0.38	0	6,6,6	1.08	0
3	DIO	B	2013	-	6,6,6	0.51	0	6,6,6	0.77	0
3	DIO	B	2014	-	6,6,6	0.45	0	6,6,6	0.97	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DIO	A	2013	-	-	0/0/6/6	0/1/1/1
3	DIO	A	2014	-	-	0/0/6/6	0/1/1/1
3	DIO	B	2013	-	-	0/0/6/6	0/1/1/1
3	DIO	B	2014	-	-	0/0/6/6	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2014	DIO	2	0
3	B	2013	DIO	1	0
3	B	2014	DIO	2	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, 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	961/990 (97%)	-0.52	5 (0%) 90 88	18, 30, 46, 61	0
1	B	958/990 (96%)	-0.39	8 (0%) 86 81	23, 37, 56, 75	0
All	All	1919/1980 (96%)	-0.46	13 (0%) 87 83	18, 34, 52, 75	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	980	LEU	4.3
1	B	979	ASN	3.9
1	A	43	ASN	3.3
1	B	1010	PRO	2.8
1	A	965	SER	2.7
1	A	964	ASP	2.5
1	A	52	ASN	2.5
1	B	981	SER	2.4
1	A	982	GLN	2.3
1	B	982	GLN	2.2
1	B	212	LYS	2.1
1	B	1009	LYS	2.1
1	B	511	LYS	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
3	DIO	A	2014	6/6	0.92	0.32	18.14	52,53,54,55	0
3	DIO	A	2013	6/6	0.90	0.20	15.63	53,54,55,55	0
3	DIO	B	2014	6/6	0.93	0.25	7.76	51,52,53,54	0
3	DIO	B	2013	6/6	0.98	0.17	0.86	40,41,42,42	0
2	ZN	B	2012	1/1	0.95	0.06	-3.55	42,42,42,42	1
2	ZN	A	2012	1/1	0.97	0.08	-	32,32,32,32	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.