



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 08:18 am BST

PDB ID : 3N56  
Title : Crystal Structure of human Insulin-degrading enzyme (IDE) in complex with human B-type natriuretic peptide (BNP)  
Authors : Funke, T.; Guo, Q.; Tang, W.-J.  
Deposited on : 2010-05-24  
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

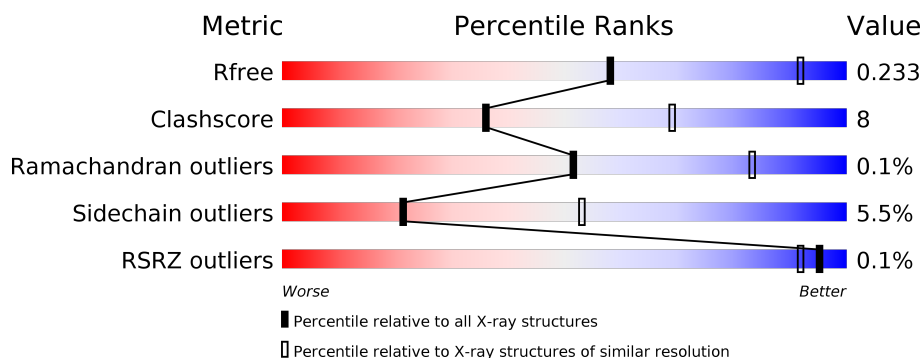
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	990	
1	B	990	
2	C	32	
2	D	32	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15654 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	951	Total	C	N	O	S	0	1	0
			7778	5012	1307	1437	22			
1	B	951	Total	C	N	O	S	0	1	0
			7782	5017	1307	1436	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 Natriuretic peptides B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			13	8	2	3			
2	D	2	Total	C	N	O	0	0	0
			13	8	2	3			

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

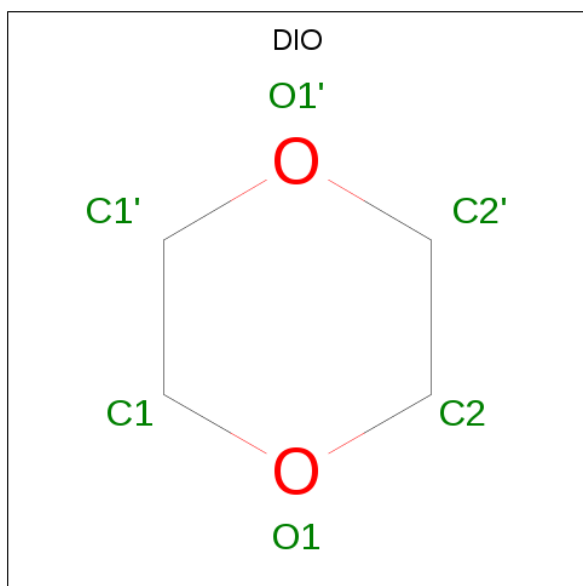
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		

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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: C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>).



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		

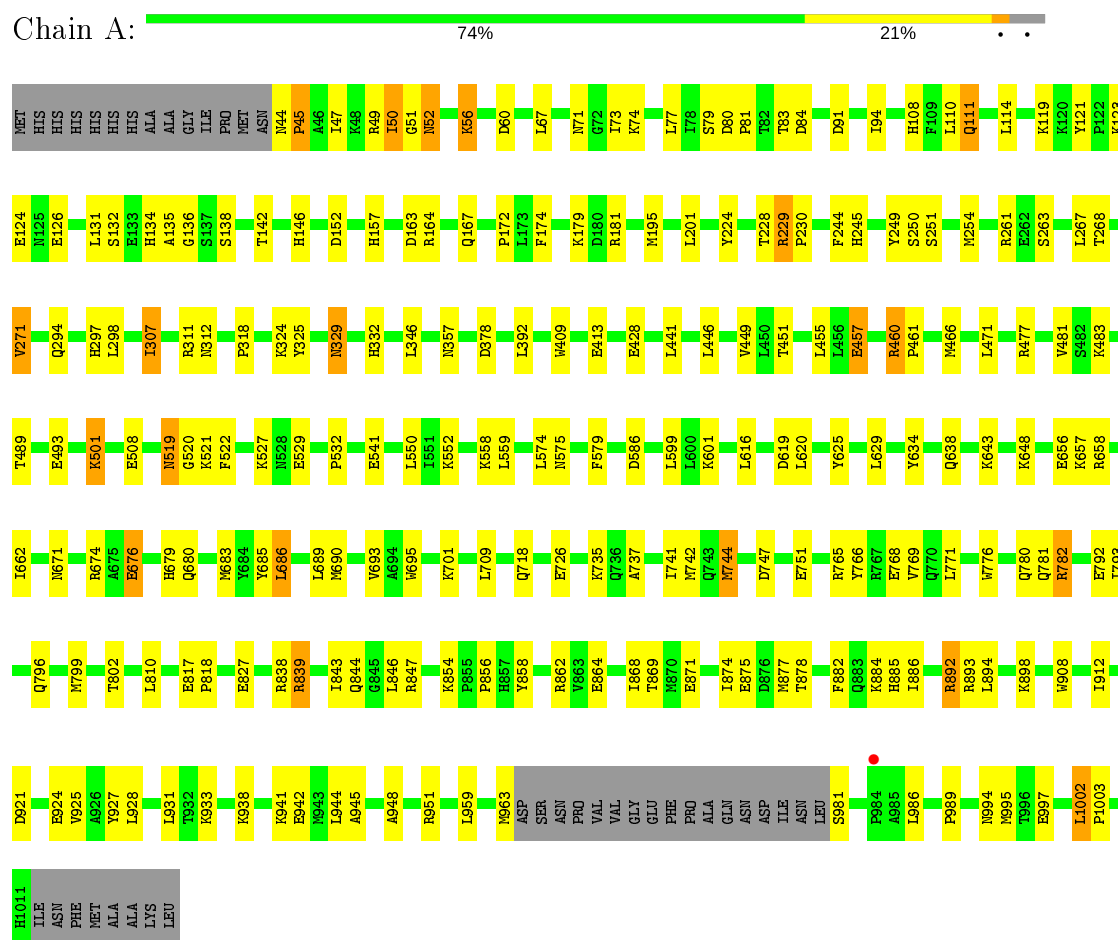
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	21	Total	O	0	0
			21	21		
5	B	33	Total	O	0	0
			33	33		

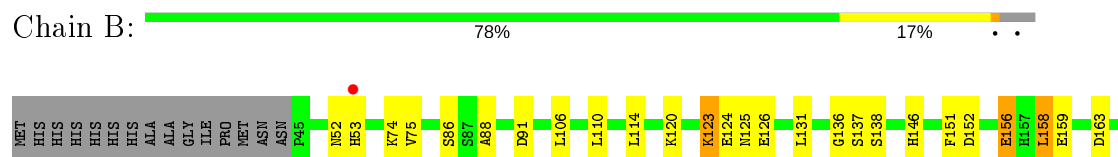
### 3 Residue-property plots

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, $\alpha$ , $\beta$ , $\gamma$	264.04 Å   264.04 Å   90.64 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	50.00 – 3.10 49.90 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.5 (50.00-3.10) 96.5 (49.90-3.10)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 3.12 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.202 , 0.243 0.198 , 0.233	Depositor DCC
$R_{free}$ test set	1206 reflections (1.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.1	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 15.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15654	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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	0.40	0/7977	0.58	0/10793
1	B	0.39	0/7981	0.57	0/10796
2	C	0.76	0/13	0.54	0/17
2	D	0.78	0/13	0.54	0/17
All	All	0.40	0/15984	0.57	0/21623

There are no bond length outliers.

There are no bond angle outliers.

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	7778	0	7709	137	0
1	B	7782	0	7726	110	0
2	C	13	0	14	0	0
2	D	13	0	14	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
5	A	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	33	0	0	6	0
All	All	15654	0	15479	247	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 8.

All (247) 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:517:ASP:HB2	5:B:1035:HOH:O	1.35	1.22
1:A:579:PHE:HE1	1:A:765:ARG:NH2	1.44	1.15
1:A:460:ARG:HH21	1:A:460:ARG:HG2	1.09	1.06
1:B:517:ASP:OD1	5:B:1023:HOH:O	1.79	0.99
1:B:688:LEU:HB3	1:B:995:MET:HE1	1.47	0.97
1:A:579:PHE:CE1	1:A:765:ARG:NH2	2.35	0.93
1:A:579:PHE:HE1	1:A:765:ARG:HH21	1.15	0.88
1:A:601:LYS:HE2	1:A:620:LEU:O	1.74	0.88
1:A:864:GLU:HG2	1:A:986:LEU:HD21	1.56	0.87
1:B:601:LYS:HE2	1:B:620:LEU:O	1.74	0.86
1:A:780:GLN:HE21	1:A:959:LEU:HD11	1.46	0.79
1:A:460:ARG:HG2	1:A:460:ARG:NH2	1.89	0.78
1:B:843:ILE:HG22	1:B:844:GLN:H	1.49	0.77
1:B:782:ARG:HH12	1:B:963:MET:H	1.32	0.77
1:B:877:MET:O	1:B:933:LYS:NZ	2.20	0.75
1:B:688:LEU:HB3	1:B:995:MET:CE	2.17	0.75
1:A:599:LEU:HD23	1:A:662:ILE:HD12	1.68	0.74
1:A:579:PHE:HE1	1:A:765:ARG:HH22	1.36	0.73
1:B:312:ASN:HD22	1:B:378:ASP:HA	1.54	0.73
1:B:213:HIS:HD2	1:B:215:PHE:H	1.36	0.71
1:B:441:LEU:HD23	1:B:449:VAL:HG11	1.73	0.71
1:B:357:ASN:ND2	1:B:658:ARG:HH22	1.90	0.70
1:B:813:GLN:HE21	1:B:885:HIS:HD2	1.41	0.69
1:B:827:GLU:OE1	1:B:862:ARG:HD3	1.93	0.69
1:A:893:ARG:NH2	1:A:924:GLU:OE1	2.25	0.68
1:B:862:ARG:NH2	1:B:981:SER:O	2.24	0.68
1:A:771:LEU:H	1:A:796:GLN:HE22	1.41	0.67
1:B:428:GLU:HG3	1:B:433:TYR:CD1	2.28	0.67
1:B:727:ALA:HB3	1:B:742:MET:CE	2.25	0.67
1:B:222:ASN:HB3	1:B:225:THR:H	1.61	0.66
1:B:517:ASP:CB	5:B:1035:HOH:O	2.12	0.65
1:A:737:ALA:O	1:A:741:ILE:HG12	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ASP:OD2	1:B:146:HIS:HD2	1.80	0.65
1:A:47:ILE:HG21	1:A:50:ILE:HD11	1.78	0.65
1:A:47:ILE:HG21	1:A:50:ILE:CD1	2.26	0.65
1:A:44:ASN:N	1:A:45:PRO:HD3	2.10	0.64
1:A:164:ARG:HH11	1:A:164:ARG:HG3	1.62	0.63
1:A:312:ASN:HD22	1:A:378:ASP:HA	1.62	0.63
1:A:77:LEU:HD21	1:A:271:VAL:HG11	1.80	0.63
1:B:213:HIS:HE1	1:B:290:GLU:O	1.81	0.63
1:B:572:ALA:HB3	1:B:638:GLN:HE22	1.64	0.63
1:A:893:ARG:NH1	1:A:921:ASP:OD1	2.32	0.62
1:A:817:GLU:HB3	1:A:818:PRO:HD3	1.79	0.62
1:B:357:ASN:ND2	1:B:658:ARG:NH2	2.47	0.62
1:B:780:GLN:NE2	1:B:959:LEU:HD11	2.15	0.62
1:A:67:LEU:HD21	1:A:268:THR:HG23	1.82	0.62
1:A:44:ASN:N	1:A:45:PRO:CD	2.63	0.61
1:A:294:GLN:H	1:A:297:HIS:HD2	1.49	0.61
1:B:361:GLY:O	2:D:1:SER:HA	2.01	0.60
1:A:229:ARG:HB3	1:A:230:PRO:HD3	1.83	0.59
1:A:839:ARG:HH11	1:A:839:ARG:CG	2.15	0.59
1:B:322:LEU:HD12	1:B:363:GLN:HE21	1.67	0.59
1:B:677:GLN:HG3	1:B:678:PRO:HD2	1.85	0.58
1:B:780:GLN:HE21	1:B:959:LEU:HD11	1.68	0.58
1:B:600:LEU:HD11	1:B:648:LYS:HB3	1.86	0.58
1:B:806:MET:HE1	1:B:893:ARG:HH12	1.69	0.58
1:B:550:LEU:HD11	1:B:558:LYS:HG3	1.84	0.58
1:A:874:ILE:O	1:A:933:LYS:HE2	2.03	0.58
1:B:123:LYS:HB3	1:B:126:GLU:HB2	1.86	0.58
1:A:80:ASP:O	1:A:83:THR:HG22	2.04	0.58
1:A:679:HIS:O	1:A:683:MET:HG3	2.04	0.57
1:A:460:ARG:CG	1:A:460:ARG:HH21	1.97	0.57
1:A:944:LEU:O	1:A:951:ARG:NH1	2.38	0.57
1:A:519:ASN:C	1:A:519:ASN:HD22	2.08	0.56
1:A:451:THR:HB	1:A:455:LEU:HD12	1.87	0.56
1:A:111:GLN:HG2	1:A:142:THR:OG1	2.06	0.56
1:B:689:LEU:CD2	1:B:995:MET:HG2	2.36	0.56
1:A:656:GLU:HG3	1:A:709:LEU:HD22	1.87	0.55
1:A:780:GLN:NE2	1:A:959:LEU:HD11	2.20	0.55
1:A:519:ASN:HD22	1:A:521:LYS:H	1.54	0.54
1:A:945:ALA:O	1:A:951:ARG:HD2	2.07	0.54
1:A:908:TRP:O	1:A:912:ILE:HG12	2.08	0.54
1:B:156:GLU:O	1:B:156:GLU:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:MET:HA	1:A:792:GLU:OE1	2.08	0.54
1:B:767:ARG:HD3	1:B:1005:PHE:O	2.07	0.54
1:B:137:SER:H	1:B:152:ASP:HB3	1.73	0.53
1:B:727:ALA:HB3	1:B:742:MET:HE1	1.88	0.53
1:B:677:GLN:HB2	1:B:680:GLN:NE2	2.23	0.53
1:A:409:TRP:HB3	1:B:120:LYS:HE3	1.89	0.53
1:B:428:GLU:HG3	1:B:433:TYR:CG	2.44	0.53
1:A:827:GLU:OE2	1:A:862:ARG:NH1	2.41	0.53
1:A:346:LEU:HA	1:A:522:PHE:CE1	2.43	0.53
1:A:839:ARG:HH11	1:A:839:ARG:HG3	1.72	0.53
1:A:428:GLU:CD	1:A:428:GLU:H	2.12	0.52
1:A:91:ASP:OD2	1:A:146:HIS:ND1	2.41	0.52
1:A:489:THR:HA	1:A:501:LYS:HG3	1.91	0.52
1:A:73:ILE:HG13	1:A:251:SER:HB2	1.92	0.52
1:B:583:ALA:CB	1:B:626:GLY:HA2	2.40	0.52
1:B:771:LEU:HD11	1:B:954:VAL:CG2	2.39	0.52
1:B:635:ASN:HD21	1:B:732:ASN:HD22	1.57	0.52
1:B:213:HIS:CD2	1:B:215:PHE:H	2.23	0.52
1:B:689:LEU:HD23	1:B:995:MET:HG2	1.90	0.52
1:A:298:LEU:HD21	1:A:318:PRO:HG3	1.92	0.51
1:B:559:LEU:HB2	1:B:742:MET:HE2	1.91	0.51
1:A:245:HIS:O	1:A:249:TYR:HB2	2.10	0.51
1:A:413:GLU:OE2	1:A:527:LYS:HE2	2.10	0.51
1:A:643:LYS:HB2	1:A:744:MET:SD	2.49	0.51
1:A:558:LYS:HB3	1:A:726:GLU:HG3	1.93	0.51
1:A:519:ASN:ND2	1:A:521:LYS:H	2.09	0.51
1:B:727:ALA:HB3	1:B:742:MET:HE3	1.93	0.51
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.93	0.50
1:A:782:ARG:HH12	1:A:963:MET:H	1.59	0.50
1:A:51:GLY:C	1:A:52:ASN:O	2.49	0.50
1:A:862:ARG:NH2	1:A:981:SER:O	2.42	0.50
1:B:238:ARG:HG2	1:B:238:ARG:O	2.11	0.50
1:A:768:GLU:HB3	1:A:843:ILE:HG13	1.93	0.50
1:B:299:LYS:HD2	1:B:510:ILE:HD13	1.94	0.50
1:A:77:LEU:HD22	1:A:267:LEU:HB3	1.94	0.50
1:B:771:LEU:HD11	1:B:954:VAL:HG23	1.94	0.50
1:A:172:PRO:HG2	1:A:174:PHE:CE2	2.47	0.50
1:A:769:VAL:CG1	1:A:1002:LEU:HD13	2.42	0.50
1:A:689:LEU:CD2	1:A:995:MET:HG2	2.42	0.50
1:A:625:TYR:CZ	1:A:765:ARG:HD3	2.47	0.49
1:B:817:GLU:HB3	1:B:818:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:843:ILE:HG22	1:B:844:GLN:N	2.24	0.49
1:A:994:ASN:HB3	1:A:997:GLU:HB2	1.93	0.49
1:B:298:LEU:HD21	1:B:318:PRO:HG2	1.94	0.49
1:A:250:SER:O	1:A:254:MET:HG3	2.13	0.49
1:A:793:ILE:O	1:A:847:ARG:HA	2.13	0.49
1:B:245:HIS:O	1:B:249:TYR:HB2	2.12	0.49
1:A:769:VAL:HG13	1:A:1002:LEU:CD1	2.43	0.48
1:A:123:LYS:HG3	1:A:126:GLU:HB2	1.94	0.48
1:A:574:LEU:C	1:A:575:ASN:HD22	2.16	0.48
1:B:646:ILE:HG12	1:B:745:VAL:HG13	1.95	0.48
1:B:948:ALA:HB3	1:B:951:ARG:HB2	1.94	0.48
1:A:135:ALA:HA	1:A:892:ARG:NH1	2.28	0.48
1:A:110:LEU:HD23	1:A:114:LEU:HD13	1.95	0.48
1:A:229:ARG:CB	1:A:230:PRO:HD3	2.44	0.48
1:A:357:ASN:HD22	1:A:658:ARG:HH22	1.60	0.48
1:A:164:ARG:HH11	1:A:164:ARG:CG	2.27	0.47
1:A:616:LEU:HD11	1:A:638:GLN:HG2	1.94	0.47
1:B:213:HIS:CE1	1:B:290:GLU:O	2.65	0.47
1:A:224:TYR:HA	1:A:228:THR:HB	1.95	0.47
1:B:760:PRO:HA	1:B:763:LEU:HD22	1.96	0.47
1:A:457:GLU:HG2	1:B:880:GLU:HB3	1.95	0.47
1:B:741:ILE:O	1:B:745:VAL:HG23	2.14	0.47
1:A:550:LEU:HD11	1:A:558:LYS:HG2	1.96	0.47
1:A:676:GLU:HG3	1:A:680:GLN:OE1	2.15	0.47
1:A:874:ILE:O	1:A:933:LYS:CE	2.61	0.47
1:A:693:VAL:HB	1:A:766:TYR:CE1	2.50	0.47
1:A:131:LEU:CD1	1:A:138:SER:HB2	2.45	0.46
1:B:806:MET:HE1	1:B:893:ARG:NH1	2.30	0.46
1:B:357:ASN:HD21	1:B:658:ARG:HH22	1.60	0.46
1:A:868:ILE:HG13	1:A:869:THR:N	2.30	0.46
1:A:871:GLU:O	1:A:875:GLU:HG2	2.15	0.46
1:B:151:PHE:CD1	1:B:151:PHE:C	2.89	0.46
1:A:686:LEU:HD21	1:A:838:ARG:NE	2.30	0.46
1:B:188:SER:HB3	1:B:831:TYR:HB2	1.98	0.46
1:A:856:PRO:C	1:A:858:TYR:N	2.69	0.46
1:A:927:TYR:CE2	1:A:931:LEU:HD11	2.51	0.46
1:B:331:GLY:HA3	1:B:363:GLN:NE2	2.31	0.46
1:B:327:LYS:HB2	5:B:14:HOH:O	2.16	0.45
1:A:686:LEU:HD21	1:A:838:ARG:HE	1.82	0.45
1:B:604:LEU:HD13	1:B:648:LYS:HG3	1.98	0.45
1:A:121:TYR:HB3	1:A:126:GLU:HG2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:ASN:N	1:A:575:ASN:HD22	2.13	0.45
1:B:422:PHE:CZ	1:B:451:THR:HG22	2.52	0.45
1:B:74:LYS:HD2	5:B:15:HOH:O	2.15	0.45
1:A:839:ARG:NH1	1:A:839:ARG:HG3	2.32	0.45
1:B:75:VAL:HG13	1:B:256:VAL:HG13	1.98	0.45
1:B:75:VAL:HG22	1:B:256:VAL:HG12	1.99	0.45
1:B:88:ALA:HB3	1:B:151:PHE:CE2	2.51	0.45
1:A:56:LYS:HG3	1:A:60:ASP:HB3	1.99	0.45
1:A:307:ILE:O	1:A:483:LYS:NZ	2.50	0.44
1:A:671:ASN:OD1	1:A:701:LYS:HD3	2.16	0.44
1:A:685:TYR:CZ	1:A:781:GLN:HG2	2.52	0.44
1:A:928:LEU:O	1:A:931:LEU:HB2	2.17	0.44
1:A:81:PRO:O	1:A:261:ARG:HD3	2.18	0.44
1:A:827:GLU:OE1	1:A:862:ARG:HD3	2.16	0.44
1:B:693:VAL:HB	1:B:766:TYR:CE1	2.52	0.44
1:A:894:LEU:CD1	1:A:925:VAL:HG11	2.48	0.44
1:A:769:VAL:HG13	1:A:1002:LEU:HD13	1.97	0.44
1:B:873:SER:O	1:B:877:MET:HB2	2.18	0.44
1:B:291:HIS:CD2	1:B:370:PHE:HB2	2.53	0.44
1:B:581:PRO:HG2	1:B:582:PHE:HD2	1.81	0.44
1:A:769:VAL:CG1	1:A:1002:LEU:CD1	2.96	0.44
1:A:441:LEU:HD23	1:A:449:VAL:HG11	1.99	0.44
1:A:689:LEU:HD23	1:A:995:MET:HG2	2.00	0.43
1:B:110:LEU:HD23	1:B:114:LEU:HD13	1.99	0.43
1:A:460:ARG:HA	1:A:461:PRO:HD2	1.86	0.43
1:A:735:LYS:CG	1:A:735:LYS:O	2.66	0.43
1:B:86:SER:HB3	1:B:158:LEU:HG	1.99	0.43
1:A:877:MET:CE	1:A:885:HIS:CD2	3.02	0.43
1:B:229:ARG:HB3	1:B:230:PRO:HD3	1.99	0.43
1:A:163:ASP:O	1:A:167:GLN:HG2	2.18	0.43
1:A:776:TRP:CE3	1:A:989:PRO:HB3	2.52	0.43
1:A:110:LEU:CD1	1:A:244:PHE:HD2	2.32	0.43
1:B:124:GLU:OE2	1:B:181:ARG:NH2	2.52	0.43
1:B:396:GLN:OE1	1:B:519:ASN:HB2	2.18	0.43
1:A:136:GLY:HA3	1:A:152:ASP:O	2.18	0.43
1:B:131:LEU:CD1	1:B:138:SER:HB2	2.48	0.43
1:B:756:LYS:HB2	1:B:756:LYS:HE2	1.69	0.43
1:B:932:THR:HG23	1:B:935:ASP:H	1.84	0.43
2:D:1:SER:HA	2:D:2:PRO:HD3	1.88	0.43
1:A:877:MET:O	1:A:933:LYS:HE3	2.19	0.43
1:B:796:GLN:HB3	1:B:952:HIS:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:801:SER:HB3	1:B:804:GLU:HB2	2.01	0.42
1:B:510:ILE:O	1:B:514:GLN:HG3	2.19	0.42
1:B:579:PHE:CE1	1:B:765:ARG:NH1	2.87	0.42
1:A:519:ASN:HD22	1:A:520:GLY:N	2.18	0.42
1:B:136:GLY:CA	1:B:152:ASP:O	2.67	0.42
1:B:124:GLU:OE1	1:B:181:ARG:NH2	2.52	0.42
1:A:877:MET:CE	1:A:885:HIS:HD2	2.32	0.42
1:B:778:VAL:HG22	1:B:955:SER:HB2	2.02	0.42
1:A:324:LYS:HE2	1:A:325:TYR:CZ	2.53	0.42
1:B:197:ASP:O	1:B:201:LEU:HG	2.20	0.42
1:A:108:HIS:O	1:A:111:GLN:HG3	2.19	0.42
1:A:747:ASP:O	1:A:751:GLU:HB2	2.20	0.42
1:B:871:GLU:O	1:B:875:GLU:HG3	2.20	0.42
1:A:802:THR:HG23	1:A:924:GLU:HG2	2.02	0.42
5:B:21:HOH:O	2:D:1:SER:CB	2.68	0.42
1:B:294:GLN:H	1:B:297:HIS:HD2	1.67	0.41
1:B:91:ASP:OD2	1:B:146:HIS:CD2	2.68	0.41
1:B:942:GLU:HG2	1:B:943:MET:HG2	2.02	0.41
1:B:771:LEU:HB2	1:B:952:HIS:HB3	2.01	0.41
1:B:683:MET:HA	1:B:792:GLU:OE1	2.21	0.41
1:B:808:LEU:HD22	1:B:844:GLN:HG2	2.01	0.41
1:B:771:LEU:CD1	1:B:954:VAL:HG23	2.50	0.41
1:B:688:LEU:CB	1:B:995:MET:HE1	2.35	0.41
1:A:134:HIS:HD2	1:A:157:HIS:CD2	2.38	0.41
1:A:47:ILE:HG21	1:A:50:ILE:HD13	2.01	0.41
1:A:311:ARG:HA	1:A:481:VAL:O	2.21	0.41
1:A:856:PRO:C	1:A:858:TYR:H	2.24	0.41
1:A:882:PHE:CE2	1:A:886:ILE:HD11	2.56	0.41
1:B:594:TYR:CE2	1:B:598:GLU:HG3	2.56	0.41
1:A:307:ILE:HA	1:A:307:ILE:HD12	1.94	0.41
1:A:619:ASP:O	1:A:629:LEU:HA	2.21	0.41
1:B:163:ASP:O	1:B:167:GLN:HG2	2.21	0.41
1:A:47:ILE:CG2	1:A:50:ILE:HD13	2.51	0.41
1:B:459:PHE:CE2	1:B:461:PRO:HG3	2.56	0.41
1:B:807:PHE:HE1	1:B:935:ASP:HB3	1.85	0.41
1:A:294:GLN:H	1:A:297:HIS:CD2	2.35	0.41
1:A:948:ALA:HB3	1:A:951:ARG:HB2	2.02	0.41
1:B:679:HIS:O	1:B:683:MET:HG3	2.20	0.41
1:A:229:ARG:HD3	1:A:229:ARG:HA	1.96	0.41
1:A:329:ASN:HB3	1:A:332:HIS:HB3	2.03	0.41
1:A:532:PRO:HG3	1:A:634:TYR:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LEU:HD21	1:A:271:VAL:CG1	2.50	0.41
1:A:877:MET:HE2	1:A:885:HIS:CD2	2.56	0.40
1:B:451:THR:O	1:B:452:ALA:C	2.59	0.40
1:A:124:GLU:OE2	1:A:181:ARG:NH2	2.54	0.40
1:A:1002:LEU:CB	1:A:1003:PRO:CD	3.00	0.40
1:B:52:ASN:O	1:B:53:HIS:C	2.59	0.40
1:A:586:ASP:HA	1:A:695:TRP:CZ2	2.56	0.40
1:A:843:ILE:HG22	1:A:844:GLN:N	2.36	0.40
1:B:722:ARG:HB2	1:B:758:LEU:HD12	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	948/990 (96%)	902 (95%)	44 (5%)	2 (0%)	47	79
1	B	948/990 (96%)	905 (96%)	43 (4%)	0	100	100
All	All	1896/1980 (96%)	1807 (95%)	87 (5%)	2 (0%)	51	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	PRO
1	A	52	ASN

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.



The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	845/879 (96%)	790 (94%)	55 (6%)	17	47
1	B	846/879 (96%)	810 (96%)	36 (4%)	29	62
2	C	2/27 (7%)	1 (50%)	1 (50%)	0	0
2	D	2/27 (7%)	1 (50%)	1 (50%)	0	0
All	All	1695/1812 (94%)	1602 (94%)	93 (6%)	21	53

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	50	ILE
1	A	56	LYS
1	A	71	ASN
1	A	74	LYS
1	A	79	SER
1	A	84	ASP
1	A	94	ILE
1	A	111	GLN
1	A	119	LYS
1	A	132	SER
1	A	179	LYS
1	A	195	MET
1	A	201	LEU
1	A	229	ARG
1	A	263	SER
1	A	271	VAL
1	A	307	ILE
1	A	329	ASN
1	A	392	LEU
1	A	446	LEU
1	A	457	GLU
1	A	460	ARG
1	A	466	MET
1	A	471	LEU
1	A	477	ARG
1	A	493	GLU
1	A	501	LYS
1	A	508	GLU
1	A	519	ASN

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Mol	Chain	Res	Type
1	A	529	GLU
1	A	541	GLU
1	A	648	LYS
1	A	657	LYS
1	A	674	ARG
1	A	676	GLU
1	A	686	LEU
1	A	690	MET
1	A	718	GLN
1	A	742	MET
1	A	744	MET
1	A	782	ARG
1	A	799	MET
1	A	810	LEU
1	A	839	ARG
1	A	846	LEU
1	A	854	LYS
1	A	878	THR
1	A	884	LYS
1	A	892	ARG
1	A	898	LYS
1	A	938	LYS
1	A	941	LYS
1	A	942	GLU
1	A	1002	LEU
1	B	106	LEU
1	B	123	LYS
1	B	125	ASN
1	B	156	GLU
1	B	158	LEU
1	B	159	GLU
1	B	170	LEU
1	B	188	SER
1	B	273	LYS
1	B	281	LYS
1	B	324	LYS
1	B	389	ASP
1	B	425	LYS
1	B	450	LEU
1	B	466	MET
1	B	471	LEU
1	B	475	ASN

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Mol	Chain	Res	Type
1	B	476	VAL
1	B	510	ILE
1	B	511	LYS
1	B	523	LYS
1	B	562	LYS
1	B	574	LEU
1	B	603	SER
1	B	612	GLU
1	B	637	LYS
1	B	674	ARG
1	B	677	GLN
1	B	697	LYS
1	B	756	LYS
1	B	763	LEU
1	B	767	ARG
1	B	824	ARG
1	B	872	LYS
1	B	943	MET
1	B	980	LEU
2	C	1	SER
2	D	1	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	93	HIS
1	A	129	GLN
1	A	297	HIS
1	A	312	ASN
1	A	357	ASN
1	A	519	ASN
1	A	575	ASN
1	A	677	GLN
1	A	752	HIS
1	A	780	GLN
1	A	788	ASN
1	A	796	GLN
1	A	885	HIS
1	A	922	ASN
1	B	111	GLN
1	B	125	ASN

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Mol	Chain	Res	Type
1	B	146	HIS
1	B	213	HIS
1	B	232	GLN
1	B	297	HIS
1	B	312	ASN
1	B	357	ASN
1	B	363	GLN
1	B	442	HIS
1	B	499	GLN
1	B	514	GLN
1	B	635	ASN
1	B	638	GLN
1	B	680	GLN
1	B	885	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	B	4006	-	6,6,6	0.54	0	6,6,6	0.70	0
4	DIO	A	4001	-	6,6,6	0.55	0	6,6,6	0.84	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	B	4006	-	-	-	0/1/1/1
4	DIO	A	4001	-	-	-	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.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	951/990 (96%)	-0.20	1 (0%) 95 92	41, 55, 71, 85	0
1	B	951/990 (96%)	-0.25	1 (0%) 95 92	38, 49, 65, 80	0
2	C	2/32 (6%)	1.11	0 100 100	87, 87, 87, 87	0
2	D	2/32 (6%)	1.60	0 100 100	86, 86, 86, 86	0
All	All	1906/2044 (93%)	-0.22	2 (0%) 95 92	38, 53, 69, 87	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	984	PRO	2.2
1	B	53	HIS	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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	A	2001	1/1	0.89	0.25	72,72,72,72	0
3	ZN	B	2002	1/1	0.93	0.27	60,60,60,60	0
4	DIO	A	4001	6/6	0.95	0.35	89,89,89,89	0
4	DIO	B	4006	6/6	0.97	0.29	94,94,94,94	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.