Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:13 AM GMT

PDB ID	:	2G54
Title	:	Crystal structure of Zn-bound human insulin-degrading enzyme in complex with insulin B chain
Authors	:	Shen, Y.; Tang, W.-J.
Deposited on	:	2006-02-22
Resolution	:	2.25 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

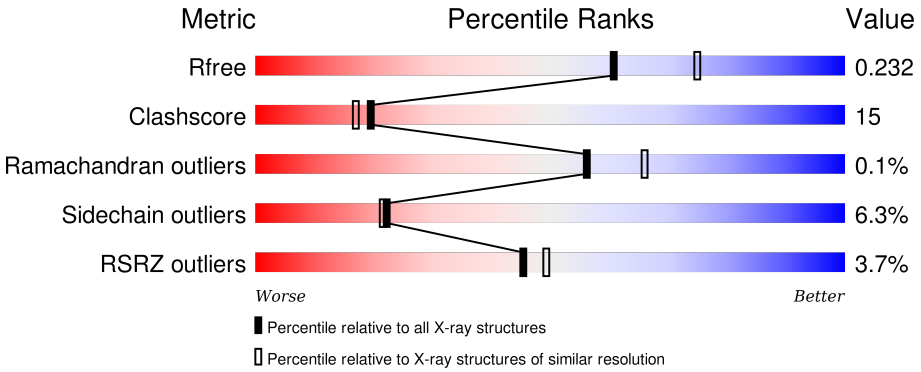
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.25 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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 <=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	3% 71% 23%
1	B	990	3% 66% 28%
2	C	30	23% 13% 23% 7% 57%
2	D	30	30% 20% 13% 7% 60%

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	2000	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16749 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	970	Total	C	N	O	S	0	0	0
			7889	5073	1327	1455	34			
1	B	966	Total	C	N	O	S	0	0	0
			7866	5064	1320	1448	34			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	INITIATING METHIONINE	UNP Q5T5N2
A	31	HIS	-	EXPRESSION TAG	UNP Q5T5N2
A	32	HIS	-	EXPRESSION TAG	UNP Q5T5N2
A	33	HIS	-	EXPRESSION TAG	UNP Q5T5N2
A	34	HIS	-	EXPRESSION TAG	UNP Q5T5N2
A	35	HIS	-	EXPRESSION TAG	UNP Q5T5N2
A	36	HIS	-	EXPRESSION TAG	UNP Q5T5N2
A	37	ALA	-	CLONING ARTIFACT	UNP Q5T5N2
A	38	ALA	-	CLONING ARTIFACT	UNP Q5T5N2
A	39	GLY	-	CLONING ARTIFACT	UNP Q5T5N2
A	40	ILE	-	CLONING ARTIFACT	UNP Q5T5N2
A	41	PRO	-	CLONING ARTIFACT	UNP Q5T5N2
A	111	GLN	GLU	ENGINEERED	UNP Q5T5N2
B	30	MET	-	INITIATING METHIONINE	UNP Q5T5N2
B	31	HIS	-	EXPRESSION TAG	UNP Q5T5N2
B	32	HIS	-	EXPRESSION TAG	UNP Q5T5N2
B	33	HIS	-	EXPRESSION TAG	UNP Q5T5N2
B	34	HIS	-	EXPRESSION TAG	UNP Q5T5N2
B	35	HIS	-	EXPRESSION TAG	UNP Q5T5N2
B	36	HIS	-	EXPRESSION TAG	UNP Q5T5N2
B	37	ALA	-	CLONING ARTIFACT	UNP Q5T5N2
B	38	ALA	-	CLONING ARTIFACT	UNP Q5T5N2
B	39	GLY	-	CLONING ARTIFACT	UNP Q5T5N2
B	40	ILE	-	CLONING ARTIFACT	UNP Q5T5N2
B	41	PRO	-	CLONING ARTIFACT	UNP Q5T5N2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	111	GLN	GLU	ENGINEERED	UNP Q5T5N2

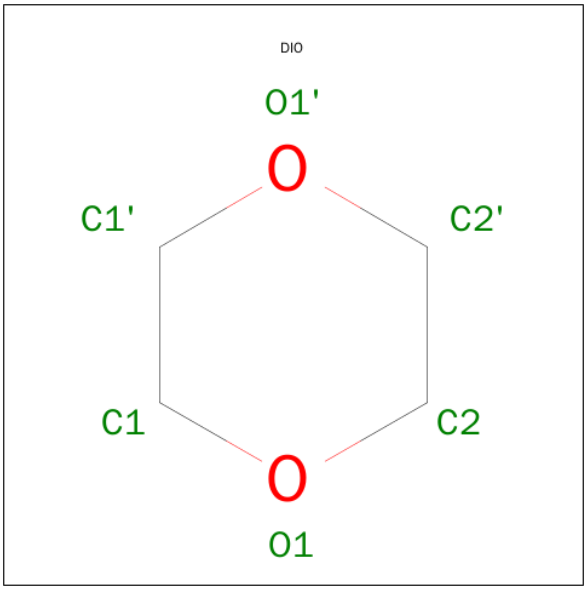
- Molecule 2 is a protein called insulin.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	C	13	Total C N O S 99 65 15 18 1	0	0	0
2	D	12	Total C N O 94 63 14 17	0	0	0

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

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

- Molecule 4 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: $C_4H_8O_2$).



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

- Molecule 5 is water.

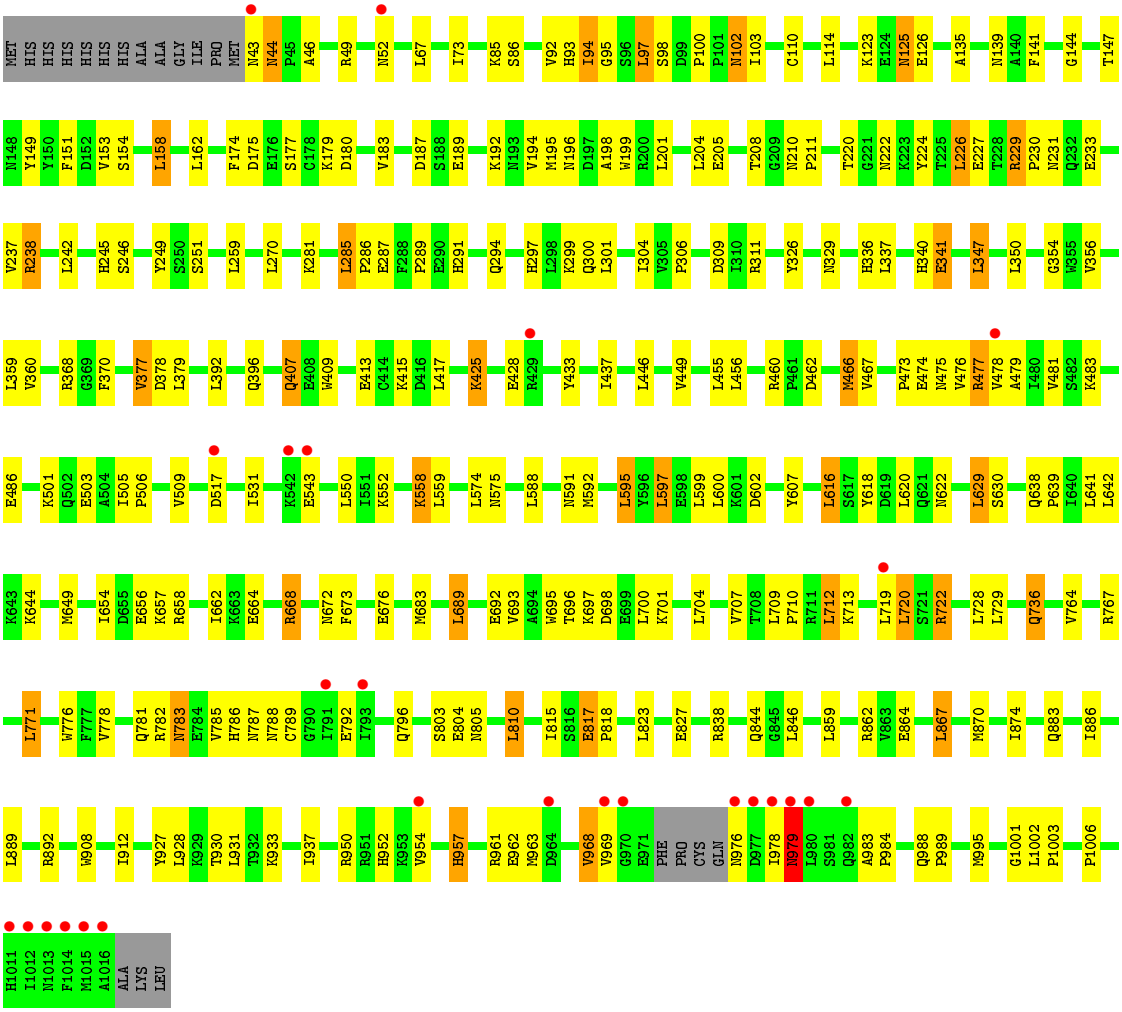
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	432	Total O 432 432	0	0
5	B	352	Total O 352 352	0	0
5	C	2	Total O 2 2	0	0
5	D	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

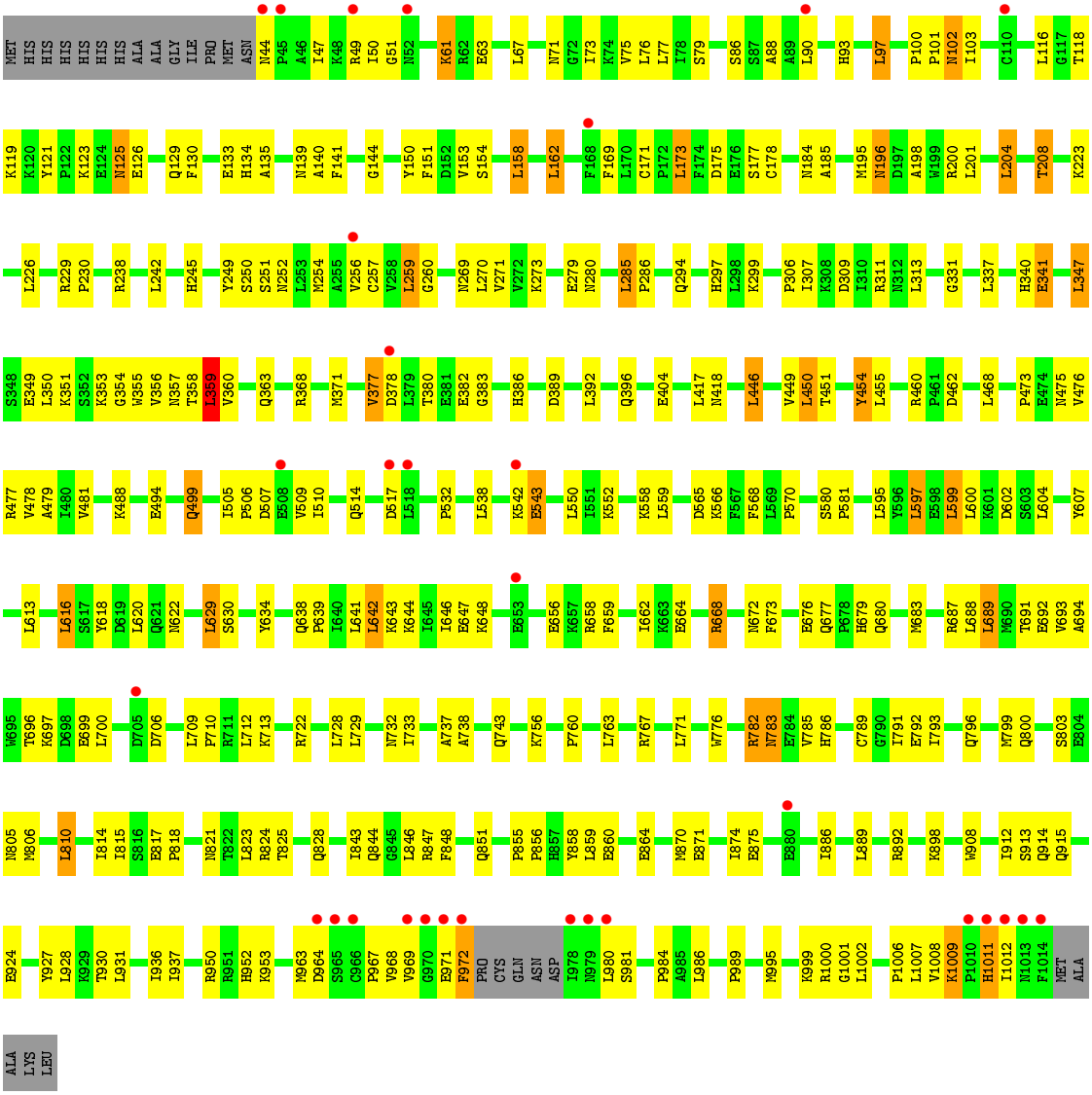
- Molecule 1: Insulin-degrading enzyme

Chain A:

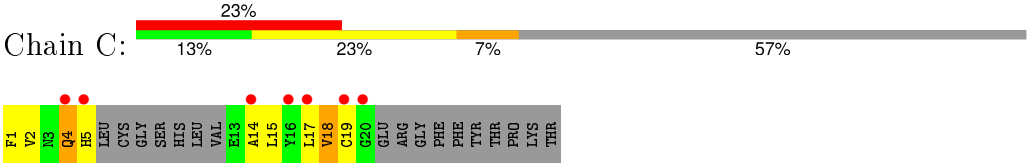


- Molecule 1: Insulin-degrading enzyme

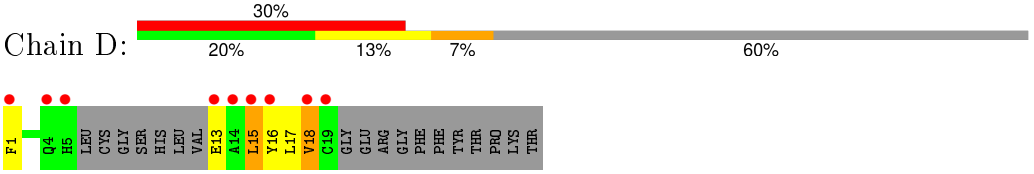
Chain B:



- Molecule 2: insulin



- Molecule 2: insulin



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	262.53Å 262.53Å 90.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.03 – 2.25 28.03 – 2.25	Depositor EDS
% Data completeness (in resolution range)	95.1 (28.03-2.25) 95.0 (28.03-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.78 (at 2.24Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.206 , 0.233 0.206 , 0.232	Depositor DCC
R_{free} test set	15987 reflections (9.97%)	DCC
Wilson B-factor (Å^2)	34.8	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 42.2	EDS
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 165981 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16749	wwPDB-VP
Average B, all atoms (Å^2)	37.0	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.37	0/8085	0.61	5/10938 (0.0%)
1	B	0.38	0/8063	0.60	5/10907 (0.0%)
2	C	1.10	0/99	1.58	2/132 (1.5%)
2	D	1.09	0/94	1.25	0/126
All	All	0.39	0/16341	0.62	12/22103 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	341	GLU	N-CA-C	-6.80	92.64	111.00
1	B	1011	HIS	N-CA-C	-6.76	92.74	111.00
1	A	976	ASN	N-CA-C	-6.37	93.81	111.00
1	A	341	GLU	C-N-CA	-6.08	109.52	122.30
1	A	979	ASN	N-CA-C	-6.04	94.70	111.00
2	C	14	ALA	N-CA-CB	-5.95	101.77	110.10
1	B	341	GLU	N-CA-C	-5.93	95.00	111.00
1	B	341	GLU	C-N-CA	-5.65	110.43	122.30
1	B	782	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	976	ASN	CA-C-N	-5.16	105.85	117.20
1	B	359	LEU	CA-CB-CG	5.16	127.17	115.30
2	C	4	GLN	N-CA-C	-5.02	97.44	111.00

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	7889	0	7792	213	0
1	B	7866	0	7776	264	0
2	C	99	0	94	11	0
2	D	94	0	88	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	6	0	8	2	0
4	B	6	0	8	2	0
5	A	432	0	0	16	0
5	B	352	0	0	15	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
All	All	16749	0	15766	476	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 15.

All (476) 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:782:ARG:NH2	1:B:964:ASP:HA	1.42	1.35
1:B:782:ARG:HH21	1:B:964:ASP:CA	1.67	1.07
1:B:782:ARG:NH2	1:B:964:ASP:CA	2.20	1.05
1:B:782:ARG:HH21	1:B:964:ASP:HA	0.90	1.05
1:A:477:ARG:HB3	1:A:477:ARG:HH11	1.19	1.03
1:B:782:ARG:NH2	1:B:964:ASP:O	1.92	1.02
1:B:208:THR:HG23	1:B:477:ARG:HH22	1.27	1.00
1:B:116:LEU:HD23	1:B:178:CYS:HB3	1.49	0.92
1:B:102:ASN:H	1:B:102:ASN:HD22	1.18	0.91
1:A:817:GLU:HG3	1:A:818:PRO:HD3	1.51	0.91
1:B:356:VAL:HG11	1:B:377:VAL:HG22	1.50	0.91
1:B:864:GLU:HG2	1:B:986:LEU:HD21	1.53	0.87
1:B:119:LYS:HD3	1:B:171:CYS:HB2	1.57	0.87
1:B:354:GLY:O	1:B:380:THR:HG21	1.75	0.86
1:A:93:HIS:HE1	1:A:368:ARG:HH21	1.20	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ILE:HD11	1:A:98:SER:HB2	1.58	0.83
1:A:446:LEU:O	1:A:449:VAL:HG23	1.77	0.83
1:A:477:ARG:HH11	1:A:477:ARG:CB	1.91	0.83
1:B:309:ASP:H	1:B:672:ASN:HD21	1.22	0.83
1:A:102:ASN:HD22	1:A:102:ASN:H	1.24	0.83
1:A:356:VAL:HG11	1:A:377:VAL:HG22	1.61	0.83
1:A:599:LEU:HD13	1:A:662:ILE:HD12	1.59	0.82
1:B:782:ARG:NH2	1:B:964:ASP:C	2.32	0.82
1:A:704:LEU:O	1:A:707:VAL:HG12	1.80	0.82
1:B:782:ARG:HH22	1:B:964:ASP:C	1.83	0.81
1:A:294:GLN:H	1:A:297:HIS:HD2	1.26	0.81
1:B:805:ASN:HD22	1:B:844:GLN:HE22	1.25	0.81
1:B:299:LYS:HD2	1:B:510:ILE:HD13	1.60	0.81
1:A:359:LEU:HD12	1:A:360:VAL:N	1.95	0.80
1:A:505:ILE:HG13	5:A:2141:HOH:O	1.82	0.79
1:B:805:ASN:ND2	1:B:844:GLN:HE22	1.80	0.79
1:B:677:GLN:H	1:B:680:GLN:HE21	1.32	0.78
1:B:309:ASP:H	1:B:672:ASN:ND2	1.82	0.78
1:A:139:ASN:ND2	2:C:18:VAL:HG12	1.99	0.78
1:B:93:HIS:HE1	1:B:368:ARG:HH21	1.33	0.77
1:B:565:ASP:O	1:B:568:PHE:CZ	2.38	0.76
1:B:972:PHE:HD1	1:B:972:PHE:C	1.88	0.76
1:A:477:ARG:HB3	1:A:477:ARG:NH1	1.99	0.76
1:A:778:VAL:HG11	1:A:968:VAL:HG22	1.66	0.76
1:A:764:VAL:HA	1:B:1000:ARG:HH22	1.50	0.76
1:A:309:ASP:H	1:A:672:ASN:HD21	1.35	0.75
1:B:791:ILE:HD11	1:B:793:ILE:HD11	1.69	0.75
1:B:972:PHE:CD1	1:B:972:PHE:C	2.57	0.75
1:B:380:THR:CG2	1:B:383:GLY:H	2.00	0.75
1:B:380:THR:HG22	1:B:383:GLY:H	1.50	0.75
1:A:220:THR:HA	2:C:15:LEU:HD13	1.69	0.74
1:A:886:ILE:HG23	1:A:928:LEU:CD1	2.17	0.73
1:A:125:ASN:HD22	1:A:125:ASN:H	1.35	0.73
1:A:805:ASN:HD22	1:A:844:GLN:HE22	1.36	0.73
1:B:123:LYS:HB2	1:B:126:GLU:HB2	1.71	0.72
1:B:294:GLN:H	1:B:297:HIS:HD2	1.38	0.72
1:A:407:GLN:HG2	1:A:409:TRP:NE1	2.05	0.72
1:B:783:ASN:HD22	1:B:785:VAL:H	1.36	0.71
1:B:599:LEU:HD12	1:B:662:ILE:HD12	1.73	0.71
1:B:550:LEU:HD11	1:B:558:LYS:HG2	1.73	0.69
1:A:407:GLN:HG2	1:A:409:TRP:HE1	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:971:GLU:O	1:B:972:PHE:C	2.29	0.69
1:A:505:ILE:N	5:A:2141:HOH:O	2.25	0.69
1:B:494:GLU:CD	1:B:494:GLU:H	1.96	0.69
1:B:967:PRO:HD3	5:B:2330:HOH:O	1.93	0.69
1:B:783:ASN:ND2	1:B:785:VAL:H	1.92	0.68
1:A:102:ASN:HD22	1:A:102:ASN:N	1.90	0.68
1:A:94:ILE:HD13	1:A:95:GLY:N	2.08	0.68
1:A:815:ILE:HG22	1:A:870:MET:HE2	1.75	0.68
1:B:858:TYR:HA	1:B:972:PHE:CZ	2.29	0.67
1:A:309:ASP:H	1:A:672:ASN:ND2	1.92	0.67
1:B:478:VAL:HG12	1:B:505:ILE:HD11	1.76	0.67
1:B:971:GLU:O	1:B:972:PHE:O	2.11	0.67
1:A:783:ASN:ND2	1:A:786:HIS:H	1.92	0.67
1:A:827:GLU:OE1	1:A:862:ARG:HD3	1.95	0.66
1:A:886:ILE:HG23	1:A:928:LEU:HD13	1.76	0.66
1:B:1008:VAL:HG12	5:B:2302:HOH:O	1.95	0.66
1:B:892:ARG:HG2	5:B:2309:HOH:O	1.97	0.65
1:A:123:LYS:HB3	1:A:126:GLU:HB2	1.78	0.65
1:A:817:GLU:HG3	1:A:818:PRO:CD	2.24	0.64
1:B:102:ASN:N	1:B:102:ASN:HD22	1.87	0.64
1:A:501:LYS:HE3	1:A:503:GLU:OE1	1.96	0.64
1:A:174:PHE:O	1:A:238:ARG:HD3	1.97	0.64
1:B:760:PRO:HA	1:B:763:LEU:HD23	1.80	0.64
1:A:341:GLU:HG2	1:A:347:LEU:HD12	1.80	0.64
1:A:359:LEU:HD12	1:A:360:VAL:H	1.60	0.63
2:C:4:GLN:HG2	2:C:5:HIS:N	2.12	0.63
1:A:93:HIS:CE1	1:A:368:ARG:HH21	2.10	0.63
1:B:692:GLU:HG2	1:B:693:VAL:HG23	1.80	0.63
1:A:204:LEU:O	1:A:208:THR:HG22	1.98	0.63
1:B:643:LYS:O	1:B:647:GLU:HG3	1.99	0.63
1:B:44:ASN:CB	1:B:47:ILE:HD12	2.29	0.63
1:B:49:ARG:HH22	1:B:446:LEU:HD22	1.64	0.63
1:A:102:ASN:ND2	1:A:102:ASN:H	1.97	0.62
1:A:44:ASN:HD22	1:A:46:ALA:H	1.47	0.62
1:B:597:LEU:HG	1:B:620:LEU:HG	1.81	0.62
1:A:135:ALA:HA	1:A:892:ARG:NH2	2.14	0.62
1:A:360:VAL:HG22	2:C:1:PHE:CE2	2.34	0.62
1:A:326:TYR:HA	1:A:329:ASN:ND2	2.14	0.61
1:A:238:ARG:O	1:A:242:LEU:HD23	1.99	0.61
1:B:102:ASN:H	1:B:102:ASN:ND2	1.94	0.61
1:B:259:LEU:HD12	1:B:260:GLY:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ALA:HB3	1:B:151:PHE:CE2	2.35	0.61
1:B:927:TYR:CE2	1:B:931:LEU:HD11	2.35	0.61
1:B:77:LEU:HD21	1:B:271:VAL:HG21	1.82	0.61
1:A:179:LYS:HD2	1:A:237:VAL:HB	1.81	0.61
1:B:93:HIS:CE1	1:B:368:ARG:HH21	2.18	0.60
1:B:980:LEU:HD12	1:B:980:LEU:N	2.16	0.60
1:B:359:LEU:HD13	1:B:360:VAL:N	2.16	0.60
1:B:506:PRO:HG2	1:B:509:VAL:HG23	1.83	0.60
1:A:377:VAL:HG13	1:A:378:ASP:O	2.00	0.60
1:B:908:TRP:CZ2	1:B:912:ILE:HD11	2.37	0.59
1:B:855:PRO:HA	1:B:963:MET:HE1	1.84	0.59
1:A:340:HIS:ND1	1:A:341:GLU:O	2.32	0.59
1:B:44:ASN:CB	1:B:47:ILE:HB	2.32	0.59
1:A:771:LEU:HD21	1:A:954:VAL:HG23	1.83	0.59
1:B:279:GLU:HG3	5:B:2132:HOH:O	2.01	0.59
1:B:196:ASN:ND2	1:B:198:ALA:H	2.00	0.59
1:A:736:GLN:CD	1:A:736:GLN:H	2.05	0.59
1:B:789:CYS:SG	1:B:963:MET:CE	2.91	0.59
1:B:538:LEU:H	1:B:732:ASN:HD21	1.51	0.59
1:B:238:ARG:O	1:B:242:LEU:HD23	2.03	0.58
1:B:118:THR:C	1:B:173:LEU:HD13	2.23	0.58
1:B:950:ARG:HD2	5:B:2284:HOH:O	2.03	0.58
1:A:294:GLN:H	1:A:297:HIS:CD2	2.14	0.58
1:B:340:HIS:ND1	1:B:341:GLU:O	2.35	0.58
1:A:311:ARG:HB3	1:A:379:LEU:HB2	1.86	0.58
1:A:44:ASN:ND2	1:A:46:ALA:H	2.01	0.58
1:A:196:ASN:HD22	1:A:199:TRP:H	1.50	0.58
1:A:220:THR:HA	2:C:15:LEU:CD1	2.34	0.57
1:B:783:ASN:ND2	1:B:786:HIS:H	2.02	0.57
1:A:709:LEU:HB3	1:A:710:PRO:HD3	1.86	0.57
1:A:1006:PRO:HB3	1:B:1002:LEU:C	2.25	0.57
1:B:67:LEU:HD12	1:B:75:VAL:HB	1.86	0.57
1:B:311:ARG:HH22	1:B:664:GLU:CD	2.07	0.57
1:A:359:LEU:HD13	1:A:377:VAL:HG23	1.86	0.57
1:A:478:VAL:CG1	1:A:505:ILE:HD11	2.34	0.57
1:B:679:HIS:HD2	1:B:851:GLN:OE1	1.88	0.57
1:B:204:LEU:O	1:B:208:THR:HB	2.05	0.57
1:B:100:PRO:HG2	1:B:103:ILE:HB	1.86	0.57
1:B:817:GLU:HB3	5:B:2296:HOH:O	2.03	0.57
1:B:125:ASN:H	1:B:125:ASN:HD22	1.53	0.57
1:B:691:THR:CG2	1:B:694:ALA:HB2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:VAL:HG22	2:D:1:PHE:CZ	2.40	0.56
1:A:597:LEU:HG	1:A:620:LEU:HG	1.87	0.56
1:A:360:VAL:HG22	2:C:1:PHE:CZ	2.40	0.56
1:B:517:ASP:HB2	5:B:2225:HOH:O	2.06	0.56
1:A:927:TYR:O	1:A:930:THR:HB	2.05	0.56
1:B:843:ILE:HG22	1:B:844:GLN:N	2.21	0.56
1:B:815:ILE:HG22	1:B:870:MET:CE	2.36	0.56
1:A:94:ILE:CD1	1:A:98:SER:HB2	2.33	0.55
1:B:799:MET:HE1	1:B:1006:PRO:HG2	1.89	0.55
1:B:119:LYS:HD2	1:B:173:LEU:HD12	1.88	0.55
1:B:968:VAL:HG12	1:B:989:PRO:HG3	1.87	0.55
1:B:886:ILE:HG23	1:B:928:LEU:HD13	1.88	0.55
1:A:600:LEU:HD23	1:A:620:LEU:CD2	2.37	0.55
1:B:356:VAL:HG11	1:B:377:VAL:CG2	2.33	0.55
1:A:478:VAL:HG12	1:A:505:ILE:HD11	1.89	0.55
1:A:245:HIS:O	1:A:249:TYR:HB2	2.07	0.54
1:B:208:THR:CG2	1:B:477:ARG:HH12	2.20	0.54
1:B:709:LEU:HG	1:B:713:LYS:HE3	1.89	0.54
1:B:565:ASP:O	1:B:568:PHE:HZ	1.86	0.54
1:B:789:CYS:SG	1:B:963:MET:SD	3.05	0.54
1:A:85:LYS:HE3	5:A:2075:HOH:O	2.06	0.54
1:A:673:PHE:CD1	1:A:697:LYS:HE3	2.41	0.54
1:A:978:ILE:O	1:A:979:ASN:CB	2.55	0.54
1:A:455:LEU:HA	5:A:2195:HOH:O	2.08	0.54
1:B:658:ARG:NH2	5:B:2185:HOH:O	2.41	0.54
1:B:121:TYR:HB3	1:B:126:GLU:HG2	1.89	0.54
1:A:479:ALA:HB2	4:A:2000:DIO:H12	1.90	0.54
1:B:473:PRO:O	1:B:476:VAL:HG12	2.07	0.54
2:C:17:LEU:HG	2:C:17:LEU:O	2.06	0.54
1:B:208:THR:HG23	1:B:477:ARG:NH2	2.11	0.54
1:A:147:THR:HG22	1:A:149:TYR:CE1	2.42	0.54
1:B:815:ILE:HA	1:B:870:MET:HE1	1.90	0.54
1:B:542:LYS:HG3	1:B:543:GLU:HG3	1.90	0.53
1:B:356:VAL:CG1	1:B:377:VAL:HG22	2.31	0.53
1:B:380:THR:HG23	1:B:382:GLU:H	1.73	0.53
1:A:771:LEU:HD21	1:A:954:VAL:CG2	2.39	0.53
1:B:696:THR:OG1	1:B:699:GLU:HG3	2.09	0.53
1:A:692:GLU:HG2	1:A:693:VAL:HG23	1.90	0.53
1:A:787:ASN:HB2	1:A:961:ARG:NH2	2.23	0.53
1:A:86:SER:HB3	1:A:158:LEU:HG	1.91	0.53
1:A:1002:LEU:C	1:B:1006:PRO:HB3	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:886:ILE:HG23	1:B:928:LEU:CD1	2.39	0.53
1:A:224:TYR:O	1:A:229:ARG:HB2	2.09	0.53
1:A:805:ASN:HD22	1:A:844:GLN:NE2	2.06	0.52
1:A:696:THR:O	1:A:700:LEU:HD13	2.09	0.52
1:A:517:ASP:HB2	5:A:2232:HOH:O	2.09	0.52
1:A:707:VAL:HG13	1:A:707:VAL:O	2.10	0.52
1:A:139:ASN:HD21	2:C:18:VAL:HG12	1.73	0.52
1:B:599:LEU:HD12	1:B:662:ILE:CD1	2.40	0.52
1:B:871:GLU:O	1:B:875:GLU:HG2	2.09	0.52
1:B:356:VAL:HG12	1:B:357:ASN:N	2.24	0.52
1:B:677:GLN:HB2	1:B:680:GLN:HG3	1.92	0.51
1:B:386:HIS:HD2	1:B:389:ASP:OD2	1.93	0.51
1:B:119:LYS:HB2	1:B:171:CYS:SG	2.50	0.51
1:B:347:LEU:HG	1:B:359:LEU:HB3	1.92	0.51
1:B:478:VAL:CG1	1:B:505:ILE:HD11	2.40	0.51
1:A:287:GLU:HG2	1:A:289:PRO:HD3	1.92	0.51
1:B:309:ASP:N	1:B:672:ASN:HD21	2.01	0.51
1:A:326:TYR:HA	1:A:329:ASN:HD21	1.74	0.51
1:A:550:LEU:HD11	1:A:558:LYS:HG3	1.92	0.51
1:A:285:LEU:HD23	1:A:286:PRO:HD2	1.92	0.51
1:B:821:ASN:O	1:B:825:THR:HB	2.11	0.51
1:B:928:LEU:HA	1:B:931:LEU:HD13	1.92	0.51
1:B:49:ARG:NH2	1:B:446:LEU:HD22	2.26	0.51
1:B:196:ASN:HD22	1:B:198:ALA:N	2.09	0.51
1:B:311:ARG:NH2	1:B:664:GLU:OE2	2.43	0.51
2:C:1:PHE:HE1	2:C:5:HIS:O	1.94	0.51
1:A:908:TRP:CE2	1:A:912:ILE:HD11	2.46	0.51
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.93	0.51
1:B:359:LEU:HD22	1:B:377:VAL:HG23	1.93	0.50
1:A:196:ASN:HD21	1:A:198:ALA:HB3	1.75	0.50
1:B:380:THR:HG23	1:B:382:GLU:N	2.25	0.50
1:A:141:PHE:HA	2:C:15:LEU:O	2.12	0.50
1:B:506:PRO:HG2	1:B:509:VAL:CG2	2.41	0.50
1:B:691:THR:HG21	1:B:694:ALA:HB2	1.92	0.50
1:B:377:VAL:HG13	1:B:378:ASP:O	2.12	0.50
1:A:600:LEU:HD23	1:A:620:LEU:HD21	1.92	0.50
1:B:499:GLN:HG3	5:B:2217:HOH:O	2.10	0.50
1:A:205:GLU:HA	1:A:208:THR:CG2	2.42	0.50
1:A:654:ILE:HD13	1:A:712:LEU:HD13	1.93	0.50
1:A:97:LEU:HB2	1:A:144:GLY:O	2.12	0.50
1:A:506:PRO:HG2	1:A:509:VAL:CG2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:TRP:HB2	1:A:700:LEU:HD11	1.93	0.50
1:A:591:ASN:O	1:A:595:LEU:HD22	2.11	0.50
1:A:446:LEU:HD23	5:A:2201:HOH:O	2.11	0.50
1:B:510:ILE:O	1:B:514:GLN:HG3	2.12	0.50
1:B:629:LEU:HD22	1:B:630:SER:N	2.26	0.50
1:A:44:ASN:HD22	1:A:44:ASN:C	2.14	0.50
1:A:602:ASP:OD1	1:A:658:ARG:HD3	2.11	0.50
1:B:687:ARG:O	1:B:691:THR:HG22	2.12	0.50
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.47	0.50
1:B:805:ASN:ND2	1:B:844:GLN:NE2	2.55	0.49
1:A:425:LYS:HE2	1:A:428:GLU:OE2	2.12	0.49
1:B:97:LEU:HB2	1:B:144:GLY:O	2.12	0.49
1:A:94:ILE:HD11	1:A:98:SER:CB	2.37	0.49
1:A:810:LEU:HG	1:A:928:LEU:HD21	1.92	0.49
1:B:709:LEU:HB3	1:B:710:PRO:HD3	1.94	0.49
1:A:908:TRP:CZ2	1:A:912:ILE:HD11	2.47	0.49
1:B:313:LEU:HB3	1:B:377:VAL:HG12	1.95	0.49
1:A:805:ASN:ND2	1:A:844:GLN:HE22	2.06	0.49
1:B:767:ARG:NH1	1:B:1006:PRO:HA	2.27	0.49
1:A:789:CYS:SG	1:A:963:MET:CE	3.01	0.49
1:A:300:GLN:CA	5:A:2141:HOH:O	2.59	0.49
1:A:776:TRP:CE3	1:A:989:PRO:HB3	2.47	0.49
1:A:658:ARG:NH2	5:A:2179:HOH:O	2.46	0.49
1:A:483:LYS:O	1:A:486:GLU:HB2	2.11	0.49
1:B:129:GLN:O	1:B:133:GLU:HG3	2.12	0.49
1:B:61:LYS:N	1:B:61:LYS:HD2	2.28	0.49
1:A:67:LEU:C	1:A:67:LEU:HD12	2.33	0.49
1:B:683:MET:HA	1:B:792:GLU:OE2	2.12	0.49
1:B:815:ILE:HG22	1:B:870:MET:HE2	1.93	0.48
1:B:604:LEU:CD2	1:B:648:LYS:HD2	2.43	0.48
1:B:565:ASP:OD2	1:B:566:LYS:HE3	2.13	0.48
1:B:153:VAL:HG22	1:B:154:SER:N	2.28	0.48
1:A:300:GLN:HA	5:A:2141:HOH:O	2.11	0.48
1:B:538:LEU:H	1:B:538:LEU:HD22	1.79	0.48
1:B:543:GLU:CD	1:B:543:GLU:H	2.17	0.48
1:A:194:VAL:HG12	1:A:195:MET:HE2	1.96	0.48
1:A:676:GLU:OE2	1:A:676:GLU:HA	2.12	0.48
1:B:688:LEU:O	1:B:999:LYS:HE2	2.14	0.48
1:B:874:ILE:HG22	1:B:937:ILE:HD11	1.95	0.48
1:B:196:ASN:HD22	1:B:198:ALA:H	1.58	0.48
1:B:799:MET:CE	1:B:1006:PRO:HG2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:722:ARG:NH1	1:B:756:LYS:HD3	2.29	0.48
1:B:196:ASN:HD22	1:B:196:ASN:C	2.17	0.48
1:B:604:LEU:HD21	1:B:648:LYS:HD2	1.96	0.48
1:A:950:ARG:HD2	5:A:2344:HOH:O	2.13	0.48
1:A:368:ARG:HD2	5:A:2182:HOH:O	2.13	0.48
1:A:988:GLN:NE2	1:A:989:PRO:HD2	2.29	0.48
1:B:73:ILE:HG13	1:B:251:SER:HB2	1.94	0.48
1:A:100:PRO:HG2	1:A:103:ILE:HB	1.95	0.48
1:B:898:LYS:HE3	5:B:2030:HOH:O	2.13	0.48
1:A:783:ASN:ND2	1:A:785:VAL:H	2.12	0.48
1:A:194:VAL:HG12	1:A:195:MET:CE	2.44	0.48
1:A:803:SER:HA	1:A:927:TYR:CE2	2.49	0.47
1:B:358:THR:HG23	5:B:2186:HOH:O	2.14	0.47
1:B:141:PHE:HA	2:D:15:LEU:O	2.14	0.47
1:A:43:ASN:O	1:A:44:ASN:C	2.53	0.47
1:A:656:GLU:HG3	1:A:709:LEU:HD22	1.97	0.47
1:B:810:LEU:HD13	1:B:936:ILE:HD11	1.96	0.47
1:A:306:PRO:HB3	1:A:481:VAL:CG1	2.44	0.47
1:A:796:GLN:HB3	1:A:952:HIS:HB2	1.97	0.47
1:A:783:ASN:HD22	1:A:785:VAL:H	1.63	0.47
1:B:139:ASN:HB3	1:B:150:TYR:CZ	2.49	0.47
1:B:309:ASP:O	1:B:668:ARG:HG2	2.15	0.47
1:B:449:VAL:HG13	1:B:450:LEU:HD13	1.97	0.47
1:A:781:GLN:HE21	1:A:782:ARG:H	1.62	0.47
1:B:552:LYS:HB3	1:B:559:LEU:HB3	1.96	0.47
1:B:803:SER:HA	1:B:927:TYR:CE2	2.50	0.47
1:B:196:ASN:HD21	1:B:198:ALA:HB3	1.79	0.47
1:A:392:LEU:O	1:A:396:GLN:HG3	2.14	0.47
1:B:843:ILE:HG22	1:B:844:GLN:H	1.80	0.47
1:A:827:GLU:OE1	1:A:862:ARG:CD	2.63	0.47
1:A:927:TYR:CE2	1:A:931:LEU:HD11	2.50	0.47
1:B:204:LEU:HD13	4:B:2001:DIO:H2'2	1.97	0.47
1:A:764:VAL:HA	1:B:1000:ARG:NH2	2.24	0.47
1:A:789:CYS:SG	1:A:963:MET:HE1	2.55	0.47
1:A:804:GLU:HG3	5:A:2355:HOH:O	2.15	0.47
1:A:883:GLN:NE2	5:A:2042:HOH:O	2.47	0.47
1:A:356:VAL:HG11	1:A:377:VAL:CG2	2.37	0.46
1:B:927:TYR:O	1:B:930:THR:HB	2.15	0.46
1:A:983:ALA:HA	1:A:984:PRO:HD2	1.74	0.46
1:B:805:ASN:HD22	1:B:844:GLN:NE2	2.02	0.46
1:A:205:GLU:HA	1:A:208:THR:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1001:GLY:O	1:B:1002:LEU:HD12	2.15	0.46
1:A:125:ASN:HD22	1:A:125:ASN:N	2.02	0.46
2:D:17:LEU:HB3	2:D:18:VAL:HG22	1.98	0.46
1:B:299:LYS:HD2	1:B:510:ILE:CD1	2.38	0.46
1:A:309:ASP:O	1:A:668:ARG:HG2	2.16	0.46
1:A:49:ARG:NH1	5:A:2057:HOH:O	2.46	0.46
1:B:451:THR:HB	1:B:455:LEU:HD12	1.96	0.46
1:B:349:GLU:HA	1:B:349:GLU:OE2	2.15	0.46
1:B:306:PRO:HB3	1:B:481:VAL:CG1	2.46	0.46
1:A:622:ASN:H	1:A:622:ASN:HD22	1.63	0.46
1:A:407:GLN:HG2	1:A:409:TRP:CD1	2.50	0.46
1:A:607:TYR:CE2	1:A:644:LYS:HG2	2.51	0.46
1:B:294:GLN:H	1:B:297:HIS:CD2	2.26	0.45
1:A:1003:PRO:HB3	1:B:1006:PRO:HD3	1.98	0.45
1:B:475:ASN:HB3	5:B:2155:HOH:O	2.15	0.45
1:B:793:ILE:HD12	1:B:860:GLU:OE1	2.16	0.45
1:A:311:ARG:HH22	1:A:664:GLU:CD	2.20	0.45
1:A:771:LEU:CD2	1:A:954:VAL:HG23	2.46	0.45
1:A:180:ASP:O	1:A:183:VAL:HG12	2.16	0.45
1:A:689:LEU:HD13	1:A:995:MET:CE	2.47	0.45
1:A:187:ASP:OD1	1:A:222:ASN:HB2	2.16	0.45
1:A:886:ILE:HG23	1:A:928:LEU:HD11	1.97	0.45
1:B:559:LEU:HD11	1:B:729:LEU:HD22	1.98	0.45
1:B:659:PHE:CE1	1:B:712:LEU:HD12	2.52	0.45
1:B:86:SER:HB3	1:B:158:LEU:HG	1.98	0.45
1:B:250:SER:O	1:B:254:MET:HG3	2.16	0.45
1:A:189:GLU:O	1:A:192:LYS:HG2	2.17	0.45
1:A:110:CYS:O	1:A:114:LEU:HG	2.16	0.45
1:B:479:ALA:HB2	4:B:2001:DIO:H12	1.98	0.45
1:A:93:HIS:HE1	1:A:368:ARG:NH2	2.00	0.45
1:A:1001:GLY:O	1:A:1002:LEU:HD12	2.16	0.45
1:A:229:ARG:HH11	1:A:229:ARG:HG3	1.82	0.45
1:A:433:TYR:O	1:A:437:ILE:HG12	2.16	0.45
1:A:559:LEU:HD11	1:A:729:LEU:HG	1.99	0.45
1:B:251:SER:OG	1:B:280:ASN:HB2	2.17	0.45
1:B:140:ALA:O	2:D:16:TYR:HA	2.17	0.45
1:B:538:LEU:N	1:B:538:LEU:HD22	2.32	0.45
1:A:175:ASP:OD2	1:A:177:SER:HB3	2.16	0.45
1:B:600:LEU:HD23	1:B:620:LEU:HD21	1.99	0.45
1:B:796:GLN:HB3	1:B:952:HIS:HB2	1.99	0.45
1:B:368:ARG:HD2	5:B:2158:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:776:TRP:CE3	1:B:989:PRO:HB3	2.51	0.44
1:B:602:ASP:OD1	1:B:658:ARG:HD3	2.17	0.44
1:A:222:ASN:O	1:A:226:LEU:HB2	2.16	0.44
1:B:200:ARG:CZ	1:B:307:ILE:HD11	2.46	0.44
1:B:245:HIS:O	1:B:249:TYR:HB2	2.17	0.44
1:B:269:ASN:O	1:B:273:LYS:HG2	2.17	0.44
1:A:73:ILE:HG13	1:A:251:SER:HB2	2.00	0.44
1:B:119:LYS:CD	1:B:171:CYS:HB2	2.40	0.44
1:A:722:ARG:HH11	1:A:722:ARG:HG3	1.82	0.44
1:B:1009:LYS:HA	1:B:1009:LYS:HD2	1.76	0.44
1:A:683:MET:HA	1:A:792:GLU:OE2	2.17	0.44
1:B:855:PRO:CA	1:B:963:MET:HE1	2.48	0.44
1:B:729:LEU:HD23	1:B:738:ALA:HA	1.99	0.44
1:B:175:ASP:OD2	1:B:177:SER:HB3	2.18	0.44
1:B:792:GLU:HA	1:B:848:PHE:O	2.18	0.44
1:B:673:PHE:CG	1:B:697:LYS:HE3	2.52	0.44
1:B:776:TRP:CD2	1:B:989:PRO:HB3	2.53	0.44
1:A:474:GLU:C	1:A:475:ASN:HD22	2.21	0.44
1:B:642:LEU:O	1:B:646:ILE:HG12	2.17	0.44
1:B:931:LEU:HD12	1:B:931:LEU:N	2.33	0.44
1:B:810:LEU:O	1:B:814:ILE:HG13	2.18	0.44
1:A:354:GLY:HA3	1:A:657:LYS:HE2	1.99	0.44
1:A:933:LYS:O	1:A:937:ILE:HG12	2.18	0.44
1:B:285:LEU:HD23	1:B:286:PRO:HD2	2.00	0.44
1:B:360:VAL:HG22	2:D:1:PHE:CE2	2.52	0.43
1:B:915:GLN:O	1:B:1011:HIS:HB2	2.18	0.43
1:B:622:ASN:H	1:B:622:ASN:HD22	1.66	0.43
1:A:231:ASN:C	1:A:233:GLU:H	2.22	0.43
1:A:709:LEU:HG	1:A:713:LYS:HE3	2.01	0.43
1:A:153:VAL:HG22	1:A:154:SER:N	2.34	0.43
1:B:800:GLN:HA	1:B:844:GLN:NE2	2.34	0.43
1:B:855:PRO:HA	1:B:856:PRO:HD3	1.91	0.43
1:B:673:PHE:CD1	1:B:697:LYS:HE3	2.53	0.43
1:A:867:LEU:HD12	1:A:867:LEU:HA	1.85	0.43
1:B:151:PHE:CD1	1:B:151:PHE:C	2.91	0.43
1:A:638:GLN:HB2	1:A:639:PRO:HD3	2.01	0.43
1:B:771:LEU:HD23	1:B:796:GLN:OE1	2.19	0.43
1:A:588:LEU:O	1:A:592:MET:HG3	2.18	0.43
1:B:499:GLN:HE21	1:B:499:GLN:CA	2.31	0.43
1:B:356:VAL:CG1	1:B:357:ASN:N	2.82	0.43
1:A:466:MET:HE1	1:A:467:VAL:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:SER:O	1:A:281:LYS:HE3	2.18	0.43
1:A:259:LEU:HD23	1:A:259:LEU:C	2.39	0.43
1:B:908:TRP:CE2	1:B:912:ILE:HD11	2.54	0.42
1:B:392:LEU:O	1:B:396:GLN:HG3	2.18	0.42
1:A:204:LEU:HD23	4:A:2000:DIO:H2'2	2.01	0.42
1:B:75:VAL:HG12	1:B:76:LEU:N	2.34	0.42
1:A:415:LYS:HE2	1:A:456:LEU:O	2.19	0.42
1:A:616:LEU:HD22	1:A:641:LEU:CD2	2.49	0.42
1:A:968:VAL:HG13	1:A:989:PRO:HG3	2.00	0.42
1:A:620:LEU:HD13	1:A:629:LEU:HG	2.00	0.42
1:B:130:PHE:O	1:B:134:HIS:HD2	2.02	0.42
1:B:90:LEU:HD13	1:B:169:PHE:CE2	2.54	0.42
1:A:473:PRO:O	1:A:476:VAL:HG12	2.19	0.42
1:A:618:TYR:HA	1:A:630:SER:O	2.19	0.42
1:B:196:ASN:ND2	1:B:198:ALA:N	2.67	0.42
1:A:864:GLU:HB3	1:A:984:PRO:CG	2.50	0.42
1:B:638:GLN:HB2	1:B:639:PRO:HD3	2.01	0.42
1:B:913:SER:O	1:B:914:GLN:HB2	2.19	0.42
1:B:185:ALA:HB2	1:B:828:GLN:HE22	1.85	0.42
1:B:864:GLU:HG3	1:B:984:PRO:HG3	2.02	0.42
1:A:301:LEU:HA	1:A:478:VAL:HG13	2.01	0.42
1:B:259:LEU:C	1:B:259:LEU:HD12	2.39	0.42
1:B:981:SER:HB2	5:B:2332:HOH:O	2.20	0.42
1:B:460:ARG:NH1	1:B:462:ASP:OD1	2.52	0.42
1:A:698:ASP:HA	1:A:701:LYS:HE2	2.02	0.42
1:A:460:ARG:NH1	1:A:462:ASP:OD1	2.53	0.42
1:A:719:LEU:HD12	1:A:720:LEU:HD13	2.01	0.42
1:A:151:PHE:C	1:A:151:PHE:CD1	2.93	0.42
1:A:476:VAL:HG22	1:A:477:ARG:N	2.34	0.42
1:B:806:MET:SD	1:B:924:GLU:HB3	2.60	0.42
1:B:418:ASN:HB3	1:B:454:TYR:O	2.19	0.42
1:A:838:ARG:O	1:A:844:GLN:HA	2.20	0.42
1:B:817:GLU:CB	1:B:818:PRO:HD3	2.49	0.42
1:B:968:VAL:HG12	1:B:989:PRO:CG	2.50	0.42
1:A:205:GLU:CA	1:A:208:THR:HG22	2.50	0.41
1:B:799:MET:HE1	1:B:1006:PRO:CG	2.50	0.41
1:B:184:ASN:HD21	1:B:223:LYS:NZ	2.17	0.41
1:A:299:LYS:HB2	1:A:299:LYS:NZ	2.35	0.41
1:B:229:ARG:N	1:B:230:PRO:HD2	2.35	0.41
1:A:789:CYS:SG	1:A:963:MET:HE3	2.60	0.41
1:B:733:ILE:HG13	1:B:737:ALA:HB3	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:957:HIS:HD2	5:A:2348:HOH:O	2.02	0.41
1:B:135:ALA:HA	1:B:892:ARG:CZ	2.50	0.41
1:B:71:ASN:HB2	1:B:251:SER:OG	2.20	0.41
1:B:570:PRO:O	1:B:634:TYR:HA	2.21	0.41
1:B:63:GLU:HB2	1:B:79:SER:HB3	2.01	0.41
1:A:227:GLU:O	1:A:230:PRO:HG2	2.21	0.41
1:A:210:ASN:HA	1:A:211:PRO:HD2	1.91	0.41
1:B:208:THR:O	1:B:208:THR:HG23	2.20	0.41
1:A:354:GLY:CA	1:A:657:LYS:HE2	2.51	0.41
1:B:616:LEU:HD22	1:B:641:LEU:CD2	2.50	0.41
1:A:92:VAL:HG12	1:A:94:ILE:HG22	2.02	0.41
1:A:478:VAL:HG11	1:A:505:ILE:HD11	2.03	0.41
1:B:550:LEU:CD1	1:B:558:LYS:HG2	2.46	0.41
1:B:50:ILE:HG12	1:B:51:GLY:N	2.35	0.41
1:B:618:TYR:HA	1:B:630:SER:O	2.20	0.41
1:B:331:GLY:HA3	1:B:363:GLN:OE1	2.21	0.41
1:B:793:ILE:O	1:B:847:ARG:HA	2.20	0.41
1:B:928:LEU:O	1:B:928:LEU:HD22	2.21	0.41
1:A:874:ILE:HG22	1:A:937:ILE:HD11	2.01	0.41
1:B:638:GLN:N	1:B:639:PRO:CD	2.84	0.41
1:B:824:ARG:O	1:B:828:GLN:HA	2.21	0.41
1:A:52:ASN:ND2	5:A:2058:HOH:O	2.53	0.41
1:B:195:MET:HG2	5:B:2095:HOH:O	2.20	0.41
1:A:817:GLU:N	1:A:818:PRO:CD	2.84	0.41
1:B:49:ARG:HG2	1:B:50:ILE:N	2.35	0.41
1:A:413:GLU:CG	1:A:531:ILE:HD11	2.51	0.41
1:B:371:MET:HE2	1:B:371:MET:HB3	1.89	0.41
1:B:196:ASN:ND2	1:B:198:ALA:HB3	2.36	0.41
1:B:100:PRO:HA	1:B:101:PRO:HD3	1.95	0.41
1:B:656:GLU:HG3	1:B:709:LEU:HD22	2.02	0.41
1:A:204:LEU:CD2	1:A:304:ILE:HG12	2.51	0.40
1:B:689:LEU:HD13	1:B:995:MET:SD	2.61	0.40
1:B:353:LYS:HD3	1:B:355:TRP:CH2	2.56	0.40
1:B:580:SER:HA	1:B:581:PRO:HD3	1.93	0.40
1:B:676:GLU:HA	1:B:676:GLU:OE2	2.21	0.40
1:A:600:LEU:HD21	1:A:649:MET:HG3	2.03	0.40
1:B:1011:HIS:HB3	1:B:1012:ILE:H	1.69	0.40
1:B:532:PRO:HG3	1:B:634:TYR:CD2	2.56	0.40
1:A:336:HIS:HA	2:C:2:VAL:HG22	2.03	0.40
1:B:208:THR:HG21	1:B:477:ARG:HH12	1.85	0.40
1:B:789:CYS:SG	1:B:963:MET:HE1	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:776:TRP:HA	1:B:953:LYS:O	2.21	0.40
1:A:550:LEU:CD1	1:A:558:LYS:HG3	2.51	0.40
1:B:252:ASN:HB3	1:B:280:ASN:OD1	2.20	0.40
1:A:574:LEU:C	1:A:575:ASN:HD22	2.25	0.40
1:B:162:LEU:HA	1:B:162:LEU:HD23	1.88	0.40
1:A:767:ARG:NH1	1:A:1006:PRO:HA	2.37	0.40
1:A:622:ASN:H	1:A:622:ASN:ND2	2.20	0.40
1:A:474:GLU:HG2	1:A:475:ASN:ND2	2.36	0.40
1:B:607:TYR:CE2	1:B:644:LYS:HG2	2.56	0.40
1:B:256:VAL:HG12	1:B:257:CYS:N	2.37	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	966/990 (98%)	931 (96%)	34 (4%)	1 (0%)	56	66
1	B	962/990 (97%)	919 (96%)	43 (4%)	0	100	100
2	C	9/30 (30%)	8 (89%)	1 (11%)	0	100	100
2	D	8/30 (27%)	8 (100%)	0	0	100	100
All	All	1945/2040 (95%)	1866 (96%)	78 (4%)	1 (0%)	56	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	979	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	857/883 (97%)	807 (94%)	50 (6%)	25 25
1	B	855/883 (97%)	801 (94%)	54 (6%)	22 21
2	C	10/26 (38%)	8 (80%)	2 (20%)	1 0
2	D	9/26 (35%)	6 (67%)	3 (33%)	0 0
All	All	1731/1818 (95%)	1622 (94%)	109 (6%)	22 21

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	94	ILE
1	A	97	LEU
1	A	102	ASN
1	A	125	ASN
1	A	158	LEU
1	A	162	LEU
1	A	201	LEU
1	A	226	LEU
1	A	229	ARG
1	A	238	ARG
1	A	270	LEU
1	A	285	LEU
1	A	337	LEU
1	A	347	LEU
1	A	350	LEU
1	A	377	VAL
1	A	407	GLN
1	A	417	LEU
1	A	425	LYS
1	A	466	MET
1	A	477	ARG
1	A	543	GLU
1	A	558	LYS

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Mol	Chain	Res	Type
1	A	595	LEU
1	A	597	LEU
1	A	616	LEU
1	A	629	LEU
1	A	642	LEU
1	A	668	ARG
1	A	689	LEU
1	A	712	LEU
1	A	720	LEU
1	A	722	ARG
1	A	728	LEU
1	A	736	GLN
1	A	771	LEU
1	A	783	ASN
1	A	788	ASN
1	A	810	LEU
1	A	817	GLU
1	A	823	LEU
1	A	846	LEU
1	A	859	LEU
1	A	867	LEU
1	A	889	LEU
1	A	957	HIS
1	A	962	GLU
1	A	968	VAL
1	A	969	VAL
1	B	61	LYS
1	B	97	LEU
1	B	102	ASN
1	B	125	ASN
1	B	158	LEU
1	B	162	LEU
1	B	173	LEU
1	B	196	ASN
1	B	201	LEU
1	B	204	LEU
1	B	208	THR
1	B	226	LEU
1	B	259	LEU
1	B	270	LEU
1	B	285	LEU
1	B	337	LEU

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Mol	Chain	Res	Type
1	B	347	LEU
1	B	350	LEU
1	B	351	LYS
1	B	359	LEU
1	B	377	VAL
1	B	404	GLU
1	B	417	LEU
1	B	446	LEU
1	B	450	LEU
1	B	454	TYR
1	B	468	LEU
1	B	488	LYS
1	B	499	GLN
1	B	507	ASP
1	B	543	GLU
1	B	595	LEU
1	B	597	LEU
1	B	599	LEU
1	B	613	LEU
1	B	616	LEU
1	B	629	LEU
1	B	642	LEU
1	B	668	ARG
1	B	689	LEU
1	B	700	LEU
1	B	706	ASP
1	B	728	LEU
1	B	743	GLN
1	B	783	ASN
1	B	810	LEU
1	B	823	LEU
1	B	846	LEU
1	B	859	LEU
1	B	889	LEU
1	B	969	VAL
1	B	972	PHE
1	B	1007	LEU
1	B	1009	LYS
2	C	18	VAL
2	C	19	CYS
2	D	13	GLU
2	D	15	LEU

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Mol	Chain	Res	Type
2	D	18	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	52	ASN
1	A	93	HIS
1	A	102	ASN
1	A	125	ASN
1	A	184	ASN
1	A	196	ASN
1	A	231	ASN
1	A	294	GLN
1	A	297	HIS
1	A	300	GLN
1	A	329	ASN
1	A	332	HIS
1	A	393	HIS
1	A	475	ASN
1	A	502	GLN
1	A	575	ASN
1	A	589	HIS
1	A	622	ASN
1	A	672	ASN
1	A	680	GLN
1	A	743	GLN
1	A	770	GLN
1	A	781	GLN
1	A	783	ASN
1	A	805	ASN
1	A	828	GLN
1	A	883	GLN
1	A	914	GLN
1	A	922	ASN
1	A	988	GLN
1	B	93	HIS
1	B	102	ASN
1	B	125	ASN
1	B	134	HIS
1	B	184	ASN
1	B	196	ASN

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Mol	Chain	Res	Type
1	B	297	HIS
1	B	300	GLN
1	B	386	HIS
1	B	475	ASN
1	B	499	GLN
1	B	502	GLN
1	B	605	ASN
1	B	621	GLN
1	B	622	ASN
1	B	672	ASN
1	B	679	HIS
1	B	680	GLN
1	B	718	GLN
1	B	732	ASN
1	B	781	GLN
1	B	783	ASN
1	B	788	ASN
1	B	805	ASN
1	B	828	GLN
1	B	887	GLN
1	B	914	GLN
1	B	922	ASN
1	B	993	GLN

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 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	A	2000	-	6,6,6	0.79	0	6,6,6	0.18	0
4	DIO	B	2001	-	6,6,6	0.72	0	6,6,6	0.26	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	2000	-	-	0/0/6/6	0/1/1/1
4	DIO	B	2001	-	-	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.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2000	DIO	2	0
4	B	2001	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^{th} 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	970/990 (97%)	-0.10	26 (2%)	58	62	20, 33, 50, 73	0
1	B	966/990 (97%)	0.01	31 (3%)	51	56	25, 38, 56, 76	0
2	C	13/30 (43%)	2.87	7 (53%)	0	0	38, 63, 72, 74	0
2	D	12/30 (40%)	2.90	9 (75%)	0	0	42, 66, 69, 70	0
All	All	1961/2040 (96%)	-0.00	73 (3%)	45	49	20, 35, 55, 76	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	5	HIS	9.5
1	B	964	ASP	9.3
1	A	1014	PHE	7.9
1	B	1012	ILE	7.4
1	A	1015	MET	7.0
1	A	977	ASP	6.6
2	D	19	CYS	6.5
2	C	19	CYS	6.2
1	B	1013	ASN	6.1
1	B	972	PHE	6.0
1	B	979	ASN	5.6
2	C	20	GLY	5.3
1	B	1014	PHE	5.3
1	A	976	ASN	5.1
1	B	1011	HIS	5.1
1	B	980	LEU	5.0
2	D	4	GLN	4.9
2	D	5	HIS	4.8
1	A	979	ASN	4.7
1	B	971	GLU	4.7
1	A	43	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	1012	ILE	4.1
1	A	970	GLY	3.9
2	D	16	TYR	3.9
1	B	978	ILE	3.7
1	A	978	ILE	3.7
2	D	14	ALA	3.6
1	B	508	GLU	3.6
1	A	542	LYS	3.5
1	A	1013	ASN	3.3
2	C	16	TYR	3.3
1	A	1016	ALA	3.2
2	D	13	GLU	3.2
1	B	542	LYS	3.1
1	B	880	GLU	3.1
2	C	14	ALA	3.0
1	B	970	GLY	2.9
1	B	52	ASN	2.9
2	C	4	GLN	2.9
1	B	966	CYS	2.7
1	A	982	GLN	2.7
1	B	256	VAL	2.7
1	B	45	PRO	2.7
1	A	791	ILE	2.6
2	C	17	LEU	2.6
1	A	964	ASP	2.6
1	B	44	ASN	2.5
1	A	543	GLU	2.5
1	B	965	SER	2.5
1	A	517	ASP	2.4
1	B	378	ASP	2.4
1	A	1011	HIS	2.4
1	B	110	CYS	2.4
1	A	793	ILE	2.3
1	B	705	ASP	2.3
1	B	168	PHE	2.3
2	D	18	VAL	2.3
1	B	517	ASP	2.2
2	D	15	LEU	2.2
2	D	1	PHE	2.2
1	A	969	VAL	2.2
1	B	969	VAL	2.2
1	B	90	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	653	GLU	2.2
1	A	719	LEU	2.1
1	A	429	ARG	2.1
1	A	478	VAL	2.1
1	B	518	LEU	2.1
1	A	52	ASN	2.0
1	B	49	ARG	2.0
1	A	980	LEU	2.0
1	A	954	VAL	2.0
1	B	1010	PRO	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^{th} 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	A	2000	6/6	0.96	0.22	2.02	52,53,53,54	0
4	DIO	B	2001	6/6	0.94	0.20	1.42	43,45,46,48	0
3	ZN	A	1100	1/1	0.99	0.02	-2.21	36,36,36,36	0
3	ZN	B	1200	1/1	0.99	0.03	-2.63	43,43,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.