Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2022 – 03:19 pm GMT

PDB ID	:	6ZX9
Title	:	Crystal structure of SIV Vpr,fused to T4 lysozyme, isolated from moustached monkey, bound to human DDB1 and human DCAF1 (amino acid residues 1046-1396)
Authors	:	Schwefel, D.; Banchenko, S.
Deposited on	:	2020-07-29
Resolution	:	2.52 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

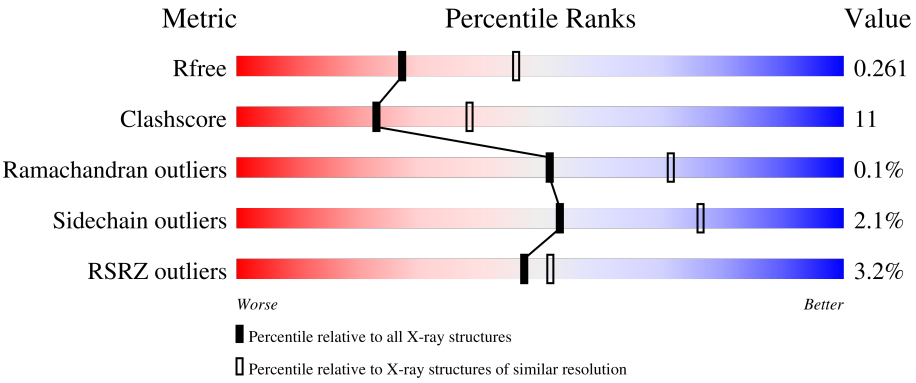
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	1142	3% 76% 22%
2	B	360	2% 69% 24% 7%
3	C	258	5% 73% 25%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13858 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 DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1124	8808	5581	1485	1695	47	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q16531
A	0	SER	-	expression tag	UNP Q16531

- Molecule 2 is a protein called DDB1- and CUL4-associated factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	335	2670	1684	467	501	18	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1045	MET	-	initiating methionine	UNP Q9Y4B6
B	1397	GLU	-	expression tag	UNP Q9Y4B6
B	1398	LEU	-	expression tag	UNP Q9Y4B6
B	1399	ALA	-	expression tag	UNP Q9Y4B6
B	1400	LEU	-	expression tag	UNP Q9Y4B6
B	1401	VAL	-	expression tag	UNP Q9Y4B6
B	1402	PRO	-	expression tag	UNP Q9Y4B6
B	1403	ARG	-	expression tag	UNP Q9Y4B6
B	1404	GLY	-	expression tag	UNP Q9Y4B6

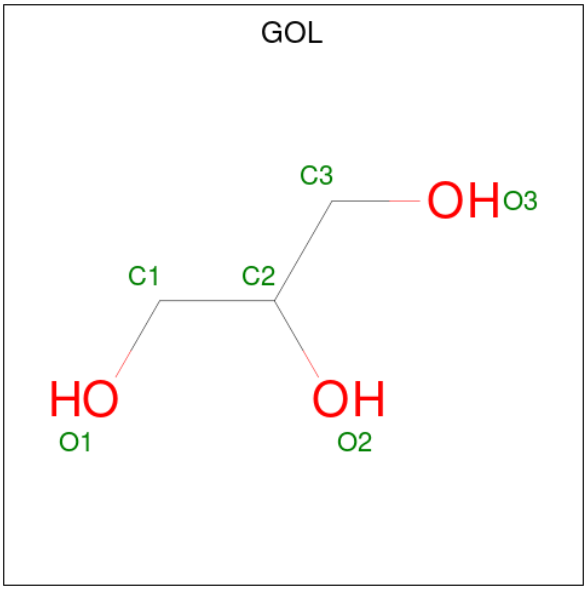
- Molecule 3 is a protein called Vpr protein fused to T4 lysozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	257	Total	C	N	O	S	0	0	0
			2078	1306	384	379	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-156	HIS	GLU	conflict	UNP P00720
C	-155	GLY	ARG	conflict	UNP P00720
C	-113	THR	CYS	conflict	UNP P00720
C	-70	ALA	CYS	conflict	UNP P00720
C	-30	ARG	ILE	conflict	UNP P00720
C	-2	ALA	-	linker	UNP P00720
C	-1	ALA	-	linker	UNP P00720
C	0	ALA	-	linker	UNP P00720

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Zn 1 1	0	0

- Molecule 6 is water.

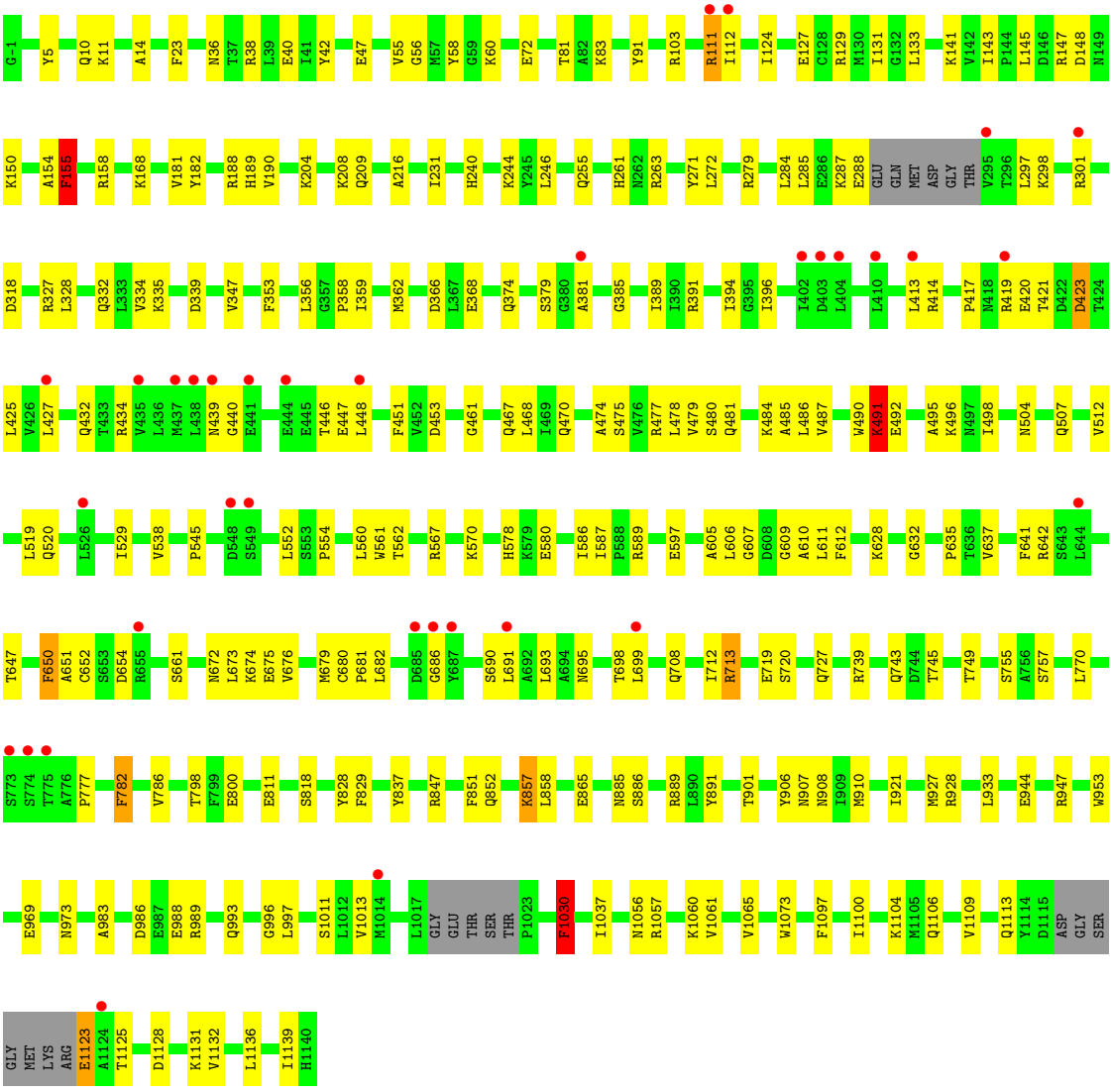
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	202	Total O 202 202	0	0
6	B	37	Total O 37 37	0	0
6	C	14	Total O 14 14	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

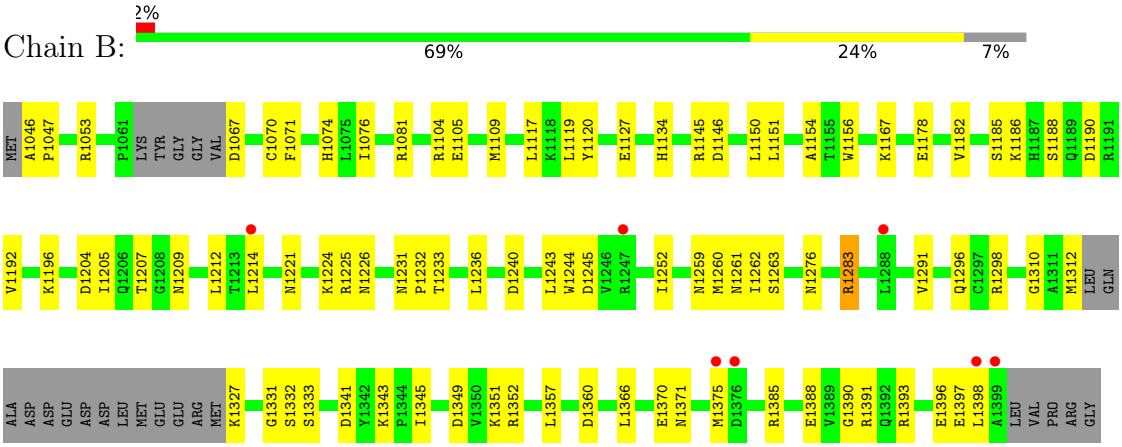
• Molecule 1: DNA damage-binding protein 1

Chain A:



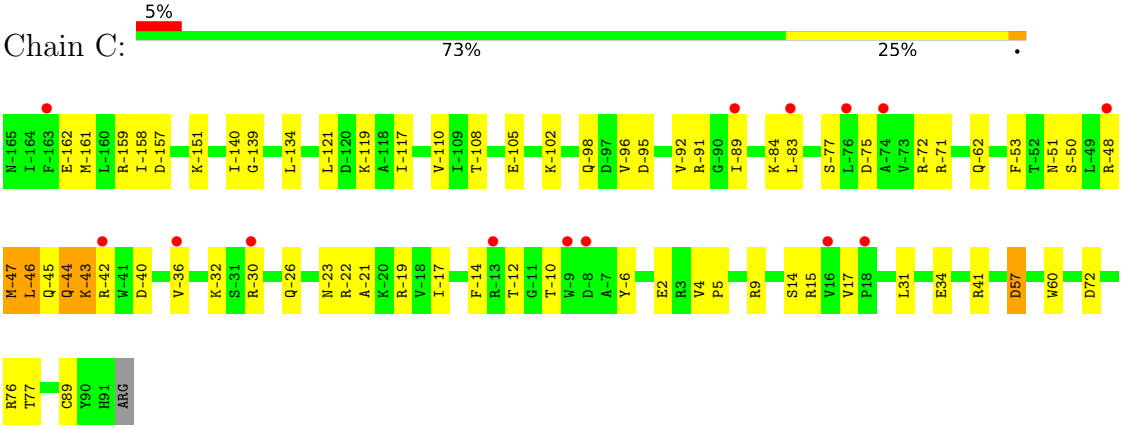
• Molecule 2: DDB1- and CUL4-associated factor 1

Chain B:



• Molecule 3: Vpr protein fused to T4 lysozyme

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	265.90Å 95.54Å 98.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.07 – 2.52 79.07 – 2.52	Depositor EDS
% Data completeness (in resolution range)	99.2 (79.07-2.52) 89.0 (79.07-2.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.81 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.12_2829, PHENIX 1.12_2829	Depositor
R, R_{free}	0.216 , 0.260 0.216 , 0.261	Depositor DCC
R_{free} test set	3948 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å^2)	46.3	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -h,l,k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13858	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, GOL

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	0.29	0/8973	0.58	3/12154 (0.0%)
2	B	0.28	0/2731	0.50	0/3696
3	C	0.31	0/2124	0.48	0/2878
All	All	0.29	0/13828	0.55	3/18728 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1030	PHE	CB-CG-CD1	5.67	124.77	120.80
1	A	491	LYS	CD-CE-NZ	5.34	123.97	111.70
1	A	155	PHE	CB-CG-CD1	5.03	124.32	120.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	928	ARG	Peptide

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	8808	0	8782	195	0
2	B	2670	0	2568	71	0
3	C	2078	0	2059	51	0
4	A	36	0	48	2	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
5	C	1	0	0	0	0
6	A	202	0	0	8	0
6	B	37	0	0	1	0
6	C	14	0	0	2	0
All	All	13858	0	13473	309	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 11.

All (309) 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)
2:B:1393:ARG:HD2	2:B:1398:LEU:CD2	1.28	1.56
2:B:1393:ARG:CD	2:B:1398:LEU:HD21	1.30	1.55
1:A:111:ARG:NH1	1:A:112:ILE:CG2	1.68	1.54
1:A:111:ARG:NH1	1:A:112:ILE:HG22	0.83	1.15
1:A:906:TYR:OH	2:B:1396:GLU:OE1	1.71	1.07
2:B:1393:ARG:NE	2:B:1398:LEU:HD21	1.77	0.98
1:A:1113:GLN:OE1	1:A:1123:GLU:HA	1.66	0.94
2:B:1393:ARG:HD2	2:B:1398:LEU:HD23	1.55	0.88
1:A:491:LYS:HE2	1:A:491:LYS:HA	1.56	0.85
2:B:1145:ARG:NH2	2:B:1186:LYS:O	2.10	0.84
2:B:1393:ARG:HD2	2:B:1398:LEU:CG	2.08	0.83
1:A:111:ARG:NH1	1:A:112:ILE:HG21	1.95	0.82
1:A:496:LYS:O	6:A:1301:HOH:O	1.96	0.82
2:B:1393:ARG:CD	2:B:1398:LEU:CD2	2.14	0.81
2:B:1207:THR:HG23	2:B:1209:ASN:H	1.46	0.81
1:A:467:GLN:HG3	1:A:478:LEU:HD11	1.61	0.79
3:C:-72:ARG:NH1	3:C:-14:PHE:O	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ARG:HH11	1:A:112:ILE:HG22	1.00	0.79
3:C:-53:PHE:HB3	3:C:-50:SER:HB2	1.65	0.79
1:A:654:ASP:O	1:A:675:GLU:HG2	1.82	0.77
3:C:-75:ASP:OD1	3:C:-72:ARG:HD2	1.86	0.75
3:C:-157:ASP:OD1	3:C:-19:ARG:NH1	2.20	0.74
1:A:606:LEU:HD11	1:A:612:PHE:HE1	1.53	0.74
1:A:11:LYS:NZ	1:A:38:ARG:HH21	1.87	0.73
1:A:285:LEU:HB3	1:A:297:LEU:HD11	1.71	0.72
2:B:1259:ASN:HD21	2:B:1296:GLN:HE21	1.37	0.72
3:C:14:SER:HB3	3:C:17:VAL:HG12	1.72	0.72
2:B:1370:GLU:OE1	2:B:1385:ARG:NH1	2.23	0.71
1:A:244:LYS:HE2	1:A:246:LEU:HD11	1.73	0.71
1:A:47:GLU:OE2	1:A:47:GLU:N	2.24	0.71
3:C:-157:ASP:HB3	3:C:-22:ARG:HE	1.56	0.70
1:A:38:ARG:HH11	1:A:56:GLY:HA3	1.55	0.70
1:A:396:ILE:CG1	1:A:673:LEU:HD11	2.22	0.70
3:C:-95:ASP:O	3:C:-91:ARG:HG3	1.92	0.70
1:A:674:LYS:O	1:A:675:GLU:HG3	1.91	0.69
3:C:-50:SER:O	3:C:-46:LEU:HD12	1.94	0.68
1:A:798:THR:HG23	1:A:800:GLU:H	1.57	0.68
1:A:81:THR:HG22	1:A:83:LYS:H	1.60	0.66
1:A:419:ARG:HG3	1:A:420:GLU:N	2.09	0.66
1:A:986:ASP:OD1	1:A:989:ARG:NH1	2.27	0.66
2:B:1312:MET:HB2	2:B:1331:GLY:HA3	1.77	0.66
1:A:1061:VAL:HG13	1:A:1104:LYS:HD2	1.77	0.65
1:A:1057:ARG:HA	1:A:1060:LYS:HE3	1.78	0.64
1:A:190:VAL:HG21	1:A:231:ILE:HD13	1.79	0.64
1:A:374:GLN:OE1	1:A:391:ARG:HB2	1.98	0.64
1:A:419:ARG:HG3	1:A:420:GLU:H	1.64	0.63
3:C:-89:ILE:HG23	3:C:-83:LEU:HB3	1.78	0.63
2:B:1224:LYS:HE2	2:B:1260:MET:HG2	1.79	0.63
2:B:1226:ASN:HA	2:B:1263:SER:HB2	1.80	0.63
1:A:891:TYR:CE1	1:A:901:THR:HG22	2.33	0.63
2:B:1262:ILE:HB	2:B:1276:ASN:HB2	1.80	0.63
3:C:-75:ASP:OD1	3:C:-75:ASP:N	2.31	0.63
1:A:413:LEU:HD11	1:A:468:LEU:HD22	1.81	0.62
1:A:339:ASP:OD2	6:A:1303:HOH:O	2.16	0.62
2:B:1204:ASP:HB3	2:B:1207:THR:HG22	1.80	0.62
3:C:-23:ASN:O	3:C:-19:ARG:HG3	2.01	0.61
1:A:498:ILE:HA	1:A:512:VAL:HG12	1.82	0.61
1:A:578:HIS:NE2	1:A:580:GLU:HG2	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LYS:HZ1	1:A:38:ARG:HH21	1.50	0.60
1:A:672:ASN:O	1:A:673:LEU:HD12	2.02	0.60
1:A:432:GLN:HB2	1:A:453:ASP:O	2.02	0.60
3:C:-45:GLN:O	3:C:-43:LYS:HG2	2.02	0.60
1:A:231:ILE:HD12	1:A:240:HIS:CD2	2.37	0.59
1:A:727:GLN:HG2	1:A:818:SER:OG	2.02	0.59
2:B:1074:HIS:HD1	2:B:1345:ILE:HG12	1.67	0.58
1:A:389:ILE:HD13	1:A:713:ARG:HD2	1.85	0.58
2:B:1351:LYS:HD2	2:B:1351:LYS:N	2.18	0.58
3:C:-151:LYS:HG2	3:C:-110:VAL:HG22	1.84	0.58
2:B:1047:PRO:HD2	2:B:1053:ARG:HG2	1.84	0.58
2:B:1393:ARG:CZ	2:B:1398:LEU:HD21	2.31	0.57
1:A:285:LEU:HB3	1:A:297:LEU:CD1	2.32	0.57
1:A:491:LYS:HE2	1:A:491:LYS:CA	2.29	0.57
1:A:589:ARG:NH1	1:A:637:VAL:HG22	2.20	0.57
1:A:641:PHE:HB3	1:A:681:PRO:HG3	1.86	0.57
1:A:885:ASN:O	1:A:910:MET:HA	2.05	0.56
2:B:1259:ASN:HD21	2:B:1296:GLN:NE2	2.02	0.56
2:B:1357:LEU:HD13	2:B:1366:LEU:HD11	1.86	0.56
1:A:396:ILE:HG12	1:A:673:LEU:HD11	1.86	0.56
1:A:485:ALA:O	1:A:487:VAL:HG23	2.05	0.56
1:A:432:GLN:HG2	1:A:434:ARG:NH1	2.20	0.56
1:A:263:ARG:HG3	1:A:271:TYR:CE1	2.41	0.55
1:A:492:GLU:HG3	1:A:512:VAL:HG21	1.88	0.55
3:C:-45:GLN:C	3:C:-43:LYS:H	2.08	0.55
2:B:1081:ARG:HH22	2:B:1397:GLU:CD	2.09	0.55
1:A:446:THR:HG22	1:A:447:GLU:H	1.72	0.55
1:A:425:LEU:HD21	1:A:427:LEU:HD21	1.88	0.55
1:A:719:GLU:HG3	1:A:755:SER:HB2	1.87	0.54
2:B:1259:ASN:ND2	2:B:1296:GLN:HE21	2.05	0.54
2:B:1221:ASN:N	2:B:1240:ASP:OD2	2.41	0.54
1:A:676:VAL:HG11	1:A:693:LEU:HD23	1.90	0.54
1:A:993:GLN:HA	1:A:993:GLN:OE1	2.08	0.54
2:B:1185:SER:OG	2:B:1188:SER:O	2.21	0.54
1:A:448:LEU:HA	1:A:484:LYS:NZ	2.23	0.54
1:A:642:ARG:NH1	1:A:647:THR:HB	2.22	0.54
1:A:745:THR:HG23	1:A:782:PHE:HE2	1.73	0.54
3:C:-77:SER:O	3:C:-43:LYS:CE	2.56	0.54
1:A:1113:GLN:OE1	1:A:1123:GLU:CA	2.49	0.54
2:B:1225:ARG:HD2	2:B:1261:ASN:HB3	1.90	0.54
2:B:1236:LEU:HD13	2:B:1243:LEU:HD21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1128:ASP:O	1:A:1132:VAL:HG23	2.08	0.53
1:A:385:GLY:HA3	1:A:719:GLU:O	2.08	0.53
1:A:561:TRP:HB3	1:A:562:THR:HG23	1.90	0.53
1:A:81:THR:HG22	1:A:83:LYS:N	2.23	0.53
2:B:1081:ARG:NH2	2:B:1397:GLU:OE1	2.41	0.53
1:A:690:SER:OG	1:A:691:LEU:N	2.42	0.53
3:C:15:ARG:NH2	3:C:72:ASP:OD1	2.42	0.53
1:A:246:LEU:HD13	1:A:297:LEU:HD23	1.91	0.53
1:A:886:SER:O	1:A:908:ASN:HB2	2.09	0.53
3:C:-12:THR:OG1	3:C:-10:THR:HG22	2.08	0.53
3:C:57:ASP:HB2	3:C:60:TRP:CD2	2.43	0.53
1:A:589:ARG:HH12	1:A:637:VAL:HG22	1.74	0.52
1:A:782:PHE:CD1	1:A:782:PHE:C	2.83	0.52
1:A:328:LEU:HD22	1:A:381:ALA:HB2	1.91	0.52
2:B:1074:HIS:NE2	2:B:1343:LYS:HE3	2.25	0.52
3:C:-77:SER:O	3:C:-43:LYS:HE2	2.09	0.51
1:A:381:ALA:O	1:A:720:SER:OG	2.22	0.51
1:A:38:ARG:HH11	1:A:56:GLY:CA	2.22	0.51
1:A:474:ALA:HB2	6:A:1315:HOH:O	2.08	0.51
1:A:492:GLU:HB3	6:A:1301:HOH:O	2.10	0.51
1:A:127:GLU:HB3	1:A:129:ARG:HD3	1.93	0.51
1:A:421:THR:OG1	1:A:423:ASP:OD1	2.28	0.51
1:A:504:ASN:HD22	1:A:545:PRO:HD3	1.75	0.51
1:A:396:ILE:HD12	1:A:396:ILE:O	2.11	0.51
1:A:148:ASP:OD1	1:A:148:ASP:N	2.38	0.50
3:C:-161:MET:HG3	3:C:-6:TYR:CE2	2.46	0.50
1:A:188:ARG:NH1	1:A:216:ALA:O	2.44	0.50
1:A:491:LYS:HD2	1:A:495:ALA:HA	1.93	0.50
1:A:467:GLN:NE2	1:A:478:LEU:HD21	2.27	0.50
1:A:907:ASN:OD1	2:B:1391:ARG:NH2	2.44	0.50
2:B:1134:HIS:CG	2:B:1154:ALA:HB2	2.47	0.50
3:C:-96:VAL:O	3:C:-92:VAL:HG12	2.12	0.50
3:C:-44:GLN:O	3:C:-42:ARG:NE	2.45	0.50
1:A:356:LEU:HD21	1:A:712:ILE:HD13	1.94	0.50
1:A:507:GLN:NE2	1:A:552:LEU:HG	2.26	0.50
1:A:538:VAL:HA	1:A:560:LEU:HD23	1.94	0.50
1:A:72:GLU:OE2	1:A:103:ARG:NH2	2.37	0.49
1:A:231:ILE:HD12	1:A:240:HIS:HD2	1.76	0.49
1:A:467:GLN:HE21	1:A:478:LEU:HD21	1.77	0.49
1:A:453:ASP:OD1	1:A:453:ASP:N	2.44	0.49
3:C:-108:THR:O	3:C:-105:GLU:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:-40:ASP:O	3:C:-36:VAL:HG23	2.12	0.49
1:A:55:VAL:HG21	1:A:1065:VAL:HG21	1.93	0.49
1:A:58:TYR:HB3	1:A:1073:TRP:HB2	1.95	0.49
2:B:1156:TRP:CD2	3:C:34:GLU:HG2	2.48	0.49
1:A:944:GLU:OE2	1:A:947:ARG:HD2	2.13	0.49
3:C:-21:ALA:O	3:C:-17:ILE:HG13	2.13	0.49
1:A:318:ASP:OD1	4:A:1204:GOL:H31	2.12	0.49
1:A:492:GLU:CB	6:A:1301:HOH:O	2.60	0.49
2:B:1245:ASP:HB2	2:B:1252:ILE:HD11	1.93	0.49
3:C:-162:GLU:O	3:C:-158:ILE:HD12	2.13	0.49
1:A:695:ASN:OD1	1:A:698:THR:N	2.27	0.48
1:A:828:TYR:CD1	1:A:852:GLN:HB3	2.48	0.48
1:A:36:ASN:O	1:A:60:LYS:HA	2.14	0.48
2:B:1192:VAL:HG23	2:B:1205:ILE:HG22	1.94	0.48
1:A:749:THR:HG21	1:A:786:VAL:HG11	1.96	0.48
3:C:-62:GLN:HB2	3:C:-22:ARG:NH1	2.28	0.48
1:A:607:GLY:HA2	1:A:635:PRO:HB3	1.95	0.48
1:A:480:SER:O	1:A:484:LYS:HA	2.14	0.48
3:C:76:ARG:NE	6:C:202:HOH:O	2.42	0.48
1:A:1056:ASN:O	1:A:1060:LYS:HG3	2.14	0.47
1:A:674:LYS:O	1:A:675:GLU:CG	2.59	0.47
1:A:181:VAL:HG22	1:A:190:VAL:HG22	1.97	0.47
1:A:332:GLN:HB3	1:A:334:VAL:HG23	1.95	0.47
1:A:1011:SER:OG	1:A:1013:VAL:HG22	2.14	0.47
2:B:1224:LYS:HG3	2:B:1260:MET:O	2.14	0.47
1:A:578:HIS:CD2	1:A:580:GLU:HG2	2.49	0.47
1:A:143:ILE:HG12	1:A:154:ALA:HB2	1.97	0.47
1:A:777:PRO:HG3	1:A:837:TYR:CD1	2.50	0.47
2:B:1120:TYR:CZ	2:B:1127:GLU:HG3	2.50	0.47
2:B:1352:ARG:HB3	2:B:1371:ASN:O	2.15	0.47
1:A:368:GLU:OE1	1:A:368:GLU:HA	2.14	0.47
1:A:1097:PHE:O	1:A:1100:ILE:HG12	2.15	0.47
2:B:1046:ALA:HB1	2:B:1071:PHE:HE2	1.80	0.47
2:B:1074:HIS:ND1	2:B:1345:ILE:HG12	2.28	0.47
2:B:1259:ASN:HD22	2:B:1276:ASN:ND2	2.12	0.47
3:C:-84:LYS:HB3	3:C:-84:LYS:HE3	1.65	0.47
1:A:474:ALA:O	1:A:475:SER:HB2	2.16	0.46
1:A:1131:LYS:HD3	6:A:1302:HOH:O	2.13	0.46
1:A:468:LEU:HD21	1:A:481:GLN:NE2	2.31	0.46
1:A:168:LYS:HE3	6:A:1399:HOH:O	2.14	0.46
1:A:440:GLY:O	1:A:686:GLY:HA3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:727:GLN:HG3	1:A:829:PHE:CZ	2.51	0.46
1:A:828:TYR:HD1	1:A:852:GLN:HB3	1.79	0.46
1:A:906:TYR:CZ	2:B:1396:GLU:OE1	2.62	0.46
3:C:-102:LYS:O	3:C:-98:GLN:HG3	2.15	0.46
1:A:40:GLU:HB3	1:A:42:TYR:CE1	2.51	0.46
1:A:190:VAL:HG21	1:A:231:ILE:CD1	2.45	0.46
1:A:490:TRP:CG	1:A:519:LEU:HD21	2.50	0.46
1:A:770:LEU:HG	1:A:865:GLU:HG3	1.98	0.46
1:A:1136:LEU:O	1:A:1139:ILE:HG12	2.15	0.46
1:A:417:PRO:HG3	1:A:481:GLN:OE1	2.16	0.46
1:A:560:LEU:HD12	1:A:567:ARG:HH11	1.81	0.46
3:C:-30:ARG:HH21	3:C:-26:GLN:HG2	1.81	0.46
1:A:131:ILE:HG13	1:A:145:LEU:HD11	1.98	0.45
1:A:255:GLN:HB3	1:A:279:ARG:NH2	2.30	0.45
3:C:-75:ASP:O	3:C:-71:ARG:HG2	2.17	0.45
1:A:777:PRO:HG3	1:A:837:TYR:CE1	2.51	0.45
2:B:1224:LYS:HB2	2:B:1261:ASN:HA	1.98	0.45
1:A:208:LYS:HA	1:A:208:LYS:HD3	1.79	0.45
1:A:334:VAL:HG11	1:A:347:VAL:HG13	1.98	0.45
1:A:491:LYS:CD	1:A:495:ALA:HA	2.47	0.45
2:B:1074:HIS:HA	2:B:1345:ILE:HG23	1.98	0.45
3:C:-51:ASN:O	3:C:-47:MET:CG	2.65	0.45
1:A:124:ILE:HG12	1:A:131:ILE:HG12	1.98	0.45
1:A:921:ILE:HB	1:A:933:LEU:HB2	1.99	0.45
2:B:1341:ASP:OD2	2:B:1343:LYS:HE2	2.17	0.45
2:B:1105:GLU:OE1	2:B:1360:ASP:HB2	2.17	0.45
3:C:-12:THR:HG22	6:C:213:HOH:O	2.17	0.45
1:A:560:LEU:CD1	1:A:567:ARG:HH11	2.30	0.45
1:A:637:VAL:HB	1:A:652:CYS:HB2	1.99	0.45
1:A:857:LYS:NZ	6:A:1304:HOH:O	2.33	0.44
2:B:1119:LEU:CD2	3:C:4:VAL:HG21	2.47	0.44
1:A:1125:THR:HG23	1:A:1128:ASP:H	1.81	0.44
1:A:439:ASN:OD1	1:A:439:ASN:N	2.51	0.44
1:A:520:GLN:HG3	1:A:529:ILE:HG13	1.99	0.44
1:A:891:TYR:HE1	1:A:901:THR:HG22	1.79	0.44
2:B:1298:ARG:O	2:B:1310:GLY:HA2	2.17	0.44
1:A:155:PHE:CD1	1:A:155:PHE:C	2.91	0.44
1:A:597:GLU:OE2	1:A:661:SER:OG	2.28	0.44
1:A:606:LEU:HD11	1:A:612:PHE:CE1	2.43	0.44
3:C:-45:GLN:C	3:C:-43:LYS:N	2.69	0.44
1:A:112:ILE:HD12	2:B:1232:PRO:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:TYR:OH	1:A:209:GLN:OE1	2.25	0.44
1:A:448:LEU:HA	1:A:484:LYS:HZ1	1.82	0.44
2:B:1388:GLU:HG2	2:B:1391:ARG:HG3	1.99	0.44
3:C:-30:ARG:HH21	3:C:-26:GLN:CG	2.30	0.44
1:A:851:PHE:HB3	1:A:858:LEU:HD11	2.00	0.44
1:A:586:ILE:HD12	1:A:587:ILE:H	1.82	0.43
2:B:1076:ILE:O	2:B:1390:GLY:HA2	2.17	0.43
2:B:1146:ASP:OD1	2:B:1146:ASP:N	2.49	0.43
2:B:1332:SER:HB3	2:B:1375:MET:SD	2.58	0.43
1:A:23:PHE:CE2	1:A:91:TYR:HB2	2.53	0.43
1:A:477:ARG:NH2	1:A:486:LEU:HD22	2.32	0.43
1:A:1030:PHE:CD1	1:A:1030:PHE:C	2.92	0.43
1:A:158:ARG:HD3	2:B:1283:ARG:HG2	1.99	0.43
1:A:1106:GLN:O	1:A:1109:VAL:HG12	2.18	0.43
3:C:-140:ILE:HG13	3:C:-139:GLY:N	2.33	0.43
3:C:-140:ILE:HG21	3:C:-121:LEU:HD13	2.00	0.43
2:B:1236:LEU:HB3	2:B:1243:LEU:HD21	2.00	0.43
3:C:-117:ILE:HD13	3:C:-105:GLU:HB3	2.00	0.43
1:A:334:VAL:CG1	1:A:347:VAL:HG13	2.48	0.43
1:A:432:GLN:HG2	1:A:434:ARG:HH12	1.84	0.43
1:A:605:ALA:HB2	1:A:611:LEU:HD23	2.01	0.43
1:A:811:GLU:OE2	1:A:847:ARG:HD3	2.18	0.43
2:B:1109:MET:HG2	2:B:1119:LEU:HG	2.01	0.43
3:C:-162:GLU:OE1	3:C:-159:ARG:NE	2.48	0.43
1:A:610:ALA:HB1	1:A:628:LYS:HE3	2.00	0.43
2:B:1190:ASP:O	2:B:1205:ILE:HG12	2.19	0.43
2:B:1231:ASN:ND2	2:B:1233:THR:OG1	2.49	0.43
1:A:353:PHE:CG	4:A:1203:GOL:H11	2.54	0.43
1:A:414:ARG:NH2	1:A:419:ARG:O	2.49	0.43
3:C:4:VAL:HG22	3:C:5:PRO:HD2	2.01	0.43
1:A:554:PRO:O	1:A:570:LYS:HD2	2.19	0.42
2:B:1081:ARG:HH21	2:B:1391:ARG:NH1	2.18	0.42
2:B:1291:VAL:HG23	2:B:1291:VAL:O	2.19	0.42
1:A:261:HIS:HA	1:A:272:LEU:O	2.20	0.42
1:A:745:THR:HG23	1:A:782:PHE:CE2	2.54	0.42
1:A:969:GLU:OE2	1:A:973:ASN:HB2	2.19	0.42
2:B:1151:LEU:HB3	2:B:1182:VAL:HG13	2.01	0.42
1:A:358:PRO:O	1:A:379:SER:HA	2.20	0.42
1:A:359:ILE:HG21	1:A:362:MET:CE	2.49	0.42
3:C:-42:ARG:HA	3:C:-42:ARG:HD3	1.82	0.42
1:A:425:LEU:HD12	1:A:682:LEU:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:LEU:HD12	1:A:479:VAL:H	1.84	0.42
2:B:1214:LEU:HD22	2:B:1244:TRP:CE3	2.54	0.42
3:C:-161:MET:HE2	3:C:-6:TYR:OH	2.20	0.42
1:A:147:ARG:O	1:A:150:LYS:NZ	2.53	0.42
1:A:654:ASP:OD1	1:A:654:ASP:N	2.53	0.42
1:A:996:GLY:O	1:A:997:LEU:HD23	2.20	0.42
1:A:609:GLY:HA3	1:A:632:GLY:O	2.20	0.42
2:B:1109:MET:HE1	2:B:1150:LEU:HD22	2.01	0.42
2:B:1204:ASP:HB3	2:B:1207:THR:CG2	2.48	0.42
2:B:1396:GLU:HG2	6:B:1626:HOH:O	2.20	0.42
3:C:-140:ILE:HB	3:C:-134:LEU:HD11	2.01	0.42
1:A:133:LEU:HB2	1:A:141:LYS:HB3	2.01	0.42
1:A:181:VAL:HA	1:A:189:HIS:O	2.20	0.42
1:A:413:LEU:HD13	1:A:461:GLY:HA2	2.02	0.41
1:A:491:LYS:HD3	1:A:492:GLU:N	2.35	0.41
3:C:14:SER:CB	3:C:17:VAL:HG12	2.45	0.41
1:A:396:ILE:HG12	1:A:673:LEU:HD21	2.02	0.41
1:A:650:PHE:HD1	1:A:651:ALA:N	2.19	0.41
1:A:288:GLU:HG3	1:A:298:LYS:HB2	2.02	0.41
1:A:446:THR:HG22	1:A:447:GLU:N	2.35	0.41
1:A:654:ASP:HA	1:A:675:GLU:HG2	2.01	0.41
1:A:719:GLU:HG2	1:A:739:ARG:HB3	2.01	0.41
1:A:719:GLU:OE2	1:A:757:SER:OG	2.26	0.41
1:A:394:ILE:HG12	1:A:708:GLN:HA	2.02	0.41
2:B:1067:ASP:OD1	2:B:1067:ASP:N	2.54	0.41
1:A:14:ALA:HB1	1:A:327:ARG:HB2	2.03	0.41
1:A:40:GLU:HB3	1:A:42:TYR:HE1	1.85	0.41
1:A:451:PHE:HA	1:A:470:GLN:OE1	2.21	0.41
1:A:512:VAL:O	1:A:512:VAL:HG23	2.21	0.41
3:C:14:SER:HB3	3:C:17:VAL:CG1	2.46	0.41
1:A:10:GLN:HB3	1:A:1037:ILE:HB	2.03	0.41
1:A:112:ILE:HG23	1:A:112:ILE:O	2.21	0.41
1:A:743:GLN:HG2	1:A:782:PHE:HA	2.03	0.41
1:A:889:ARG:HD2	1:A:891:TYR:OH	2.21	0.41
2:B:1109:MET:HE3	2:B:1117:LEU:HD21	2.02	0.41
2:B:1178:GLU:OE1	2:B:1196:LYS:NZ	2.54	0.41
2:B:1333:SER:OG	2:B:1349:ASP:HA	2.21	0.41
1:A:650:PHE:CD2	1:A:679:MET:HG3	2.56	0.41
1:A:927:MET:HG3	1:A:953:TRP:CE2	2.56	0.41
3:C:-45:GLN:O	3:C:-43:LYS:N	2.53	0.41
3:C:31:LEU:HD21	3:C:77:THR:HB	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:TYR:HB3	1:A:1073:TRP:CB	2.50	0.40
1:A:284:LEU:HD13	1:A:301[A]:ARG:NH2	2.36	0.40
2:B:1104:ARG:C	2:B:1105:GLU:HG2	2.41	0.40
1:A:983:ALA:HB1	1:A:988:GLU:HB3	2.04	0.40
2:B:1104:ARG:HD3	3:C:2:GLU:HB2	2.02	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	1117/1142 (98%)	1061 (95%)	56 (5%)	0	100	100
2	B	329/360 (91%)	309 (94%)	20 (6%)	0	100	100
3	C	255/258 (99%)	247 (97%)	7 (3%)	1 (0%)	34	53
All	All	1701/1760 (97%)	1617 (95%)	83 (5%)	1 (0%)	51	71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	-44	GLN

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	987/1000 (99%)	970 (98%)	17 (2%)	60 81
2	B	294/315 (93%)	289 (98%)	5 (2%)	60 81
3	C	217/218 (100%)	207 (95%)	10 (5%)	27 47
All	All	1498/1533 (98%)	1466 (98%)	32 (2%)	53 76

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	TYR
1	A	111	ARG
1	A	155	PHE
1	A	204	LYS
1	A	287	LYS
1	A	335	LYS
1	A	366	ASP
1	A	423	ASP
1	A	491	LYS
1	A	650	PHE
1	A	680	CYS
1	A	699	LEU
1	A	713	ARG
1	A	782	PHE
1	A	857	LYS
1	A	1030	PHE
1	A	1123	GLU
2	B	1070	CYS
2	B	1167	LYS
2	B	1212	LEU
2	B	1283	ARG
2	B	1327	LYS
3	C	-119	LYS
3	C	-48	ARG
3	C	-47	MET
3	C	-46	LEU
3	C	-43	LYS
3	C	-32	LYS
3	C	9	ARG
3	C	41	ARG
3	C	57	ASP
3	C	89	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	467	GLN
2	B	1296	GLN
3	C	-45	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	A	1202	-	5,5,5	0.95	0	5,5,5	0.90	0
4	GOL	A	1206	-	5,5,5	0.92	0	5,5,5	0.97	0
4	GOL	B	1501	-	5,5,5	0.90	0	5,5,5	1.00	0
4	GOL	A	1205	-	5,5,5	0.93	0	5,5,5	0.97	0
4	GOL	C	102	-	5,5,5	0.92	0	5,5,5	1.00	0
4	GOL	A	1201	-	5,5,5	0.90	0	5,5,5	1.01	0
4	GOL	A	1203	-	5,5,5	0.89	0	5,5,5	1.03	0
4	GOL	A	1204	-	5,5,5	1.00	0	5,5,5	0.82	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	GOL	A	1202	-	-	4/4/4/4	-
4	GOL	A	1206	-	-	3/4/4/4	-
4	GOL	B	1501	-	-	2/4/4/4	-
4	GOL	A	1205	-	-	2/4/4/4	-
4	GOL	C	102	-	-	0/4/4/4	-
4	GOL	A	1201	-	-	0/4/4/4	-
4	GOL	A	1203	-	-	4/4/4/4	-
4	GOL	A	1204	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1202	GOL	O1-C1-C2-C3
4	A	1202	GOL	C1-C2-C3-O3
4	A	1203	GOL	C1-C2-C3-O3
4	A	1203	GOL	O2-C2-C3-O3
4	B	1501	GOL	O1-C1-C2-C3
4	A	1204	GOL	O2-C2-C3-O3
4	A	1203	GOL	O1-C1-C2-C3
4	A	1204	GOL	O1-C1-C2-C3
4	A	1204	GOL	C1-C2-C3-O3
4	A	1205	GOL	O1-C1-C2-C3
4	A	1202	GOL	O1-C1-C2-O2
4	A	1202	GOL	O2-C2-C3-O3
4	A	1205	GOL	O1-C1-C2-O2
4	B	1501	GOL	O1-C1-C2-O2
4	A	1206	GOL	O2-C2-C3-O3
4	A	1206	GOL	O1-C1-C2-C3
4	A	1203	GOL	O1-C1-C2-O2
4	A	1206	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1203	GOL	1	0
4	A	1204	GOL	1	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	1124/1142 (98%)	0.28	34 (3%) 50 54	29, 61, 121, 175	0
2	B	335/360 (93%)	0.24	7 (2%) 63 67	39, 67, 99, 132	0
3	C	257/258 (99%)	0.45	14 (5%) 25 28	47, 86, 126, 149	0
All	All	1716/1760 (97%)	0.30	55 (3%) 47 52	29, 67, 121, 175	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	16	VAL	7.7
1	A	111	ARG	5.7
1	A	448	LEU	5.3
2	B	1398	LEU	5.0
1	A	644	LEU	4.9
1	A	419	ARG	4.0
1	A	438	LEU	3.9
2	B	1376	ASP	3.8
1	A	775	THR	3.7
1	A	549	SER	3.6
1	A	685	ASP	3.6
1	A	1124	ALA	3.5
2	B	1399	ALA	3.5
1	A	295	VAL	3.5
1	A	773	SER	3.3
1	A	699	LEU	3.3
1	A	435	VAL	3.1
3	C	-36	VAL	3.0
1	A	402	ILE	2.9
1	A	381	ALA	2.9
3	C	-163	PHE	2.9
1	A	427	LEU	2.9
1	A	686	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	413	LEU	2.9
1	A	439	ASN	2.7
3	C	-83	LEU	2.7
3	C	-48	ARG	2.7
1	A	691	LEU	2.7
3	C	-13	ARG	2.7
1	A	548	ASP	2.7
1	A	444	GLU	2.6
1	A	410	LEU	2.6
1	A	112	ILE	2.6
1	A	437	MET	2.6
1	A	441	GLU	2.6
1	A	526	LEU	2.6
1	A	1014	MET	2.5
3	C	-30	ARG	2.4
2	B	1375	MET	2.3
3	C	-42	ARG	2.3
1	A	301[A]	ARG	2.3
3	C	-8	ASP	2.3
1	A	403	ASP	2.2
3	C	18	PRO	2.2
3	C	-74	ALA	2.2
1	A	655	ARG	2.2
1	A	774	SER	2.2
1	A	687	TYR	2.2
3	C	-76	LEU	2.2
1	A	404	LEU	2.1
2	B	1288	LEU	2.1
2	B	1214	LEU	2.1
3	C	-89	ILE	2.1
3	C	-9	TRP	2.0
2	B	1247	ARG	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 monosaccharides in this entry.

6.4 Ligands (i)

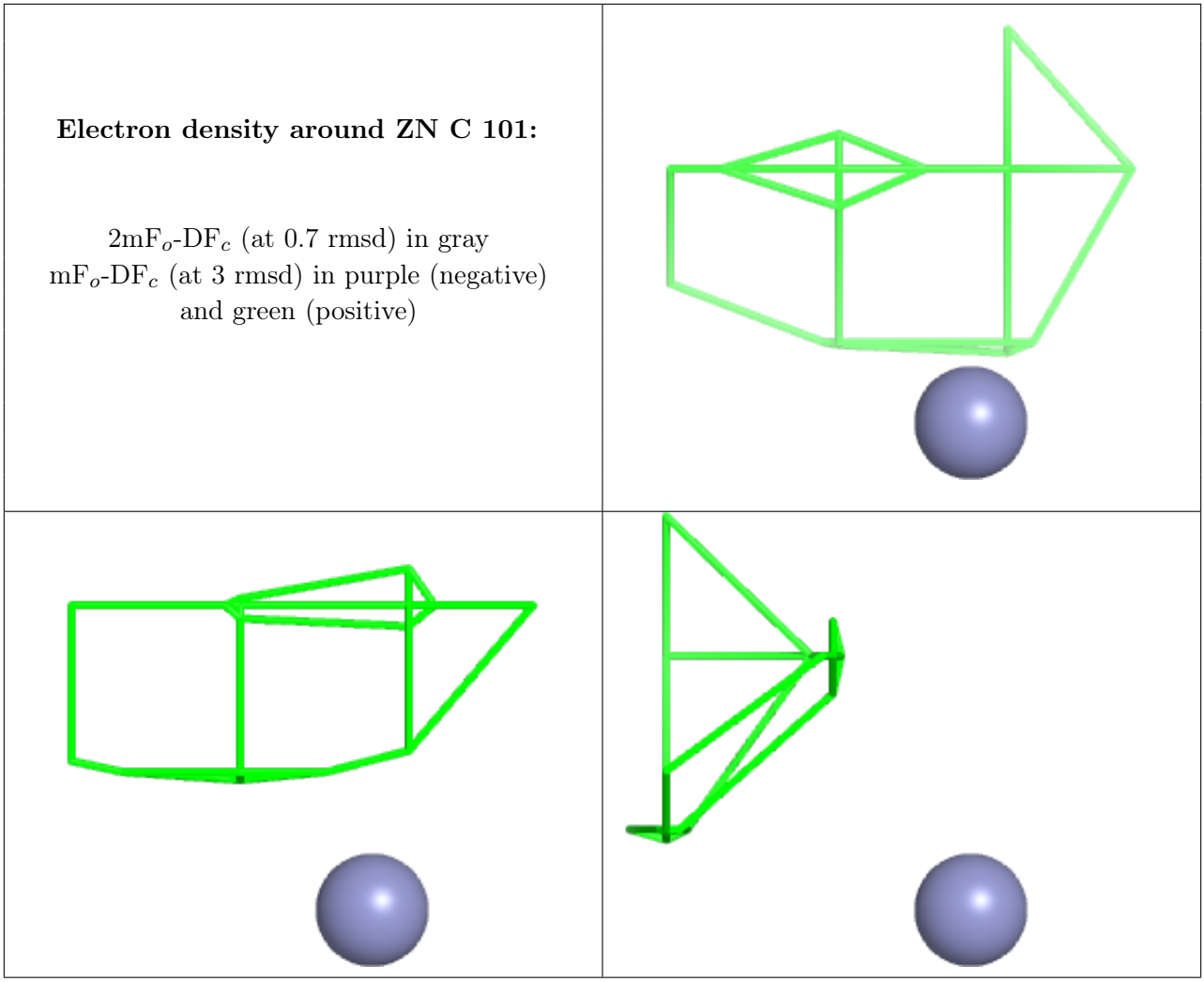
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	B	1501	6/6	0.75	0.18	73,89,90,90	0
4	GOL	A	1204	6/6	0.77	0.24	69,73,79,81	0
4	GOL	A	1206	6/6	0.87	0.20	80,89,91,92	0
4	GOL	A	1205	6/6	0.92	0.17	69,73,74,76	0
4	GOL	C	102	6/6	0.92	0.11	88,89,89,89	0
4	GOL	A	1203	6/6	0.93	0.18	61,65,74,75	0
4	GOL	A	1201	6/6	0.94	0.25	44,58,66,77	0
4	GOL	A	1202	6/6	0.96	0.11	51,57,58,62	0
5	ZN	C	101	1/1	0.97	0.17	79,79,79,79	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ZN C 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.