



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:51 AM UTC

PDB ID : 2EUL / pdb\_00002eul  
Title : Structure of the transcription factor Gfh1.  
Authors : Symersky, J.; Perederina, A.; Vassylyeva, M.N.; Svetlov, V.; Artsimovitch, I.;  
Vassylyev, D.G.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2005-10-28  
Resolution : 2.40 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

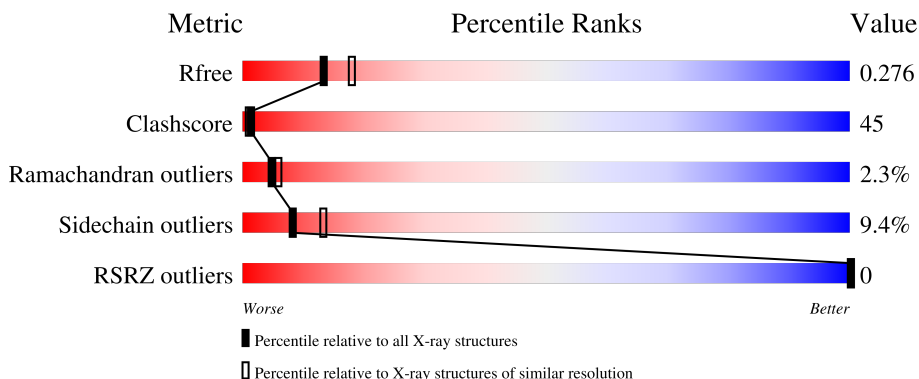
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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  $\geq 3$ , 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	156	
1	B	156	
1	C	156	
1	D	156	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5219 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 anti-cleavage anti-GreA transcription factor Gfh1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	156	1202	738	214	245	5	0	0	0
1	B	156	1202	738	214	245	5	0	0	0
1	C	156	1202	738	214	245	5	0	0	0
1	D	156	1202	738	214	245	5	0	0	0

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	9	Total	Zn	0	0
			9	9		
2	B	3	Total	Zn	0	0
			3	3		
2	C	11	Total	Zn	0	0
			11	11		
2	D	2	Total	Zn	0	0
			2	2		

- Molecule 3 is water.

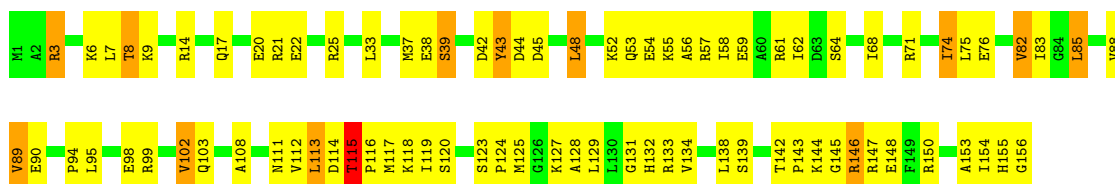
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	91	Total	O	0	0
			91	91		
3	B	105	Total	O	0	0
			105	105		
3	C	90	Total	O	0	0
			90	90		
3	D	100	Total	O	0	0
			100	100		

### 3 Residue-property plots

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.

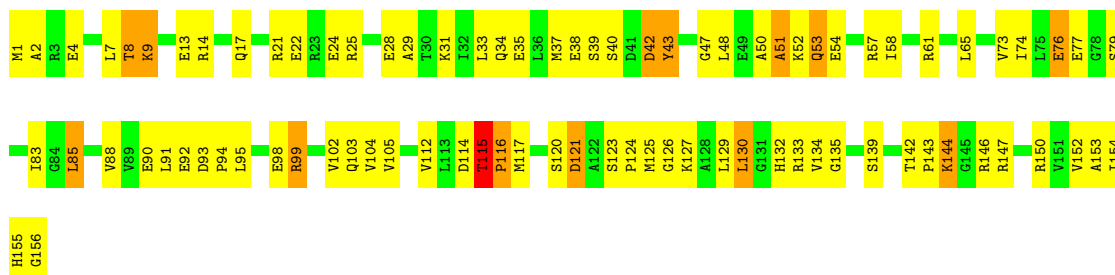
- Molecule 1: anti-cleavage anti-GreA transcription factor Gfh1

Chain A: 



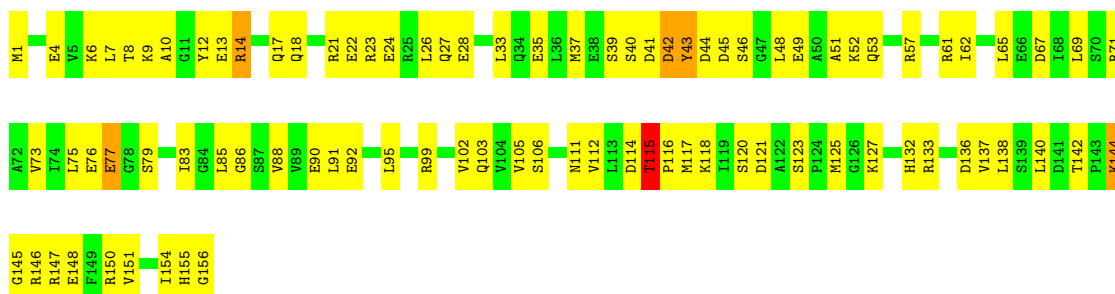
- Molecule 1: anti-cleavage anti-GreA transcription factor Gfh1

Chain B: 



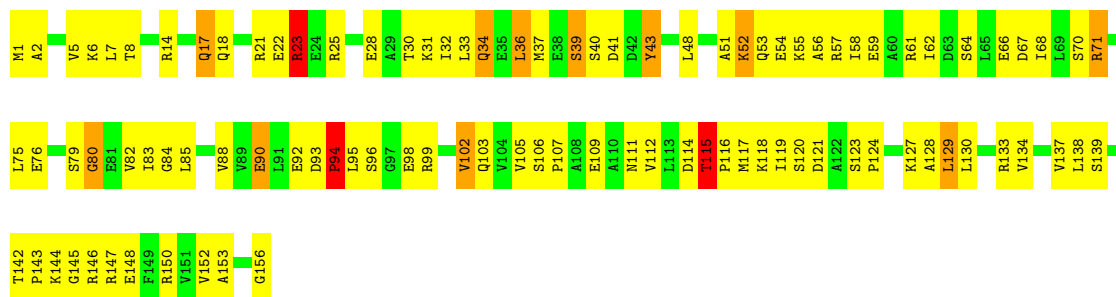
- Molecule 1: anti-cleavage anti-GreA transcription factor Gfh1

Chain C: 



- Molecule 1: anti-cleavage anti-GreA transcription factor Gfh1

Chain D: 37% 54% 7% •



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.29Å 59.29Å 218.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 30.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.9 (30.00-2.40) 98.9 (30.00-2.40)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.88 (at 2.20Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.206 , 0.245 (Not available) , 0.276	Depositor DCC
$R_{free}$ test set	1641 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.0	Xtrriage
Anisotropy	0.465	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 86.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.499 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	5219	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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

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	0.54	0/1211	1.03	6/1625 (0.4%)
1	B	0.56	0/1211	1.02	7/1625 (0.4%)
1	C	0.51	0/1211	1.01	3/1625 (0.2%)
1	D	0.52	0/1211	1.02	6/1625 (0.4%)
All	All	0.53	0/4844	1.02	22/6500 (0.3%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	115	THR	CA-C-N	-10.11	107.80	120.23
1	C	115	THR	C-N-CA	-10.11	107.80	120.23
1	B	115	THR	CA-C-N	-9.06	108.52	119.84
1	B	115	THR	C-N-CA	-9.06	108.52	119.84
1	A	115	THR	CA-C-N	-9.04	108.55	119.84
1	A	115	THR	C-N-CA	-9.04	108.55	119.84
1	B	50	ALA	N-CA-C	-8.53	102.87	113.28
1	D	115	THR	CA-C-N	-8.06	109.76	119.84
1	D	115	THR	C-N-CA	-8.06	109.76	119.84
1	D	129	LEU	N-CA-C	7.03	118.74	111.14
1	D	8	THR	N-CA-C	-6.83	101.72	110.53
1	B	51	ALA	CA-C-N	-6.25	112.10	120.54
1	B	51	ALA	C-N-CA	-6.25	112.10	120.54
1	B	8	THR	N-CA-C	-5.87	101.83	110.52
1	A	89	VAL	N-CA-C	5.80	116.29	108.17
1	A	8	THR	N-CA-C	-5.75	102.25	110.59
1	D	36	LEU	N-CA-C	-5.66	106.41	113.15
1	C	8	THR	N-CA-C	-5.46	102.67	110.59
1	A	44	ASP	N-CA-C	-5.39	106.55	113.02
1	D	23	ARG	N-CA-C	-5.36	105.34	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	PRO	N-CA-C	-5.35	101.46	112.47
1	A	74	ILE	N-CA-C	5.13	115.72	109.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1202	0	1222	107	0
1	B	1202	0	1222	108	1
1	C	1202	0	1222	92	0
1	D	1202	0	1222	138	1
2	A	9	0	0	0	0
2	B	3	0	0	0	0
2	C	11	0	0	0	0
2	D	2	0	0	0	0
3	A	91	0	0	23	0
3	B	105	0	0	19	0
3	C	90	0	0	11	0
3	D	100	0	0	11	0
All	All	5219	0	4888	436	1

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 45.

All (436) 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:C:77:GLU:OE1	3:C:507:HOH:O	1.53	1.21
1:D:90:GLU:HG2	1:D:99:ARG:HH11	1.22	1.04
1:D:76:GLU:HG2	1:D:79:SER:HB2	1.38	1.00
1:B:104:VAL:HG11	1:B:130:LEU:HD11	1.40	0.98
1:C:57:ARG:HH11	1:C:61:ARG:HG3	1.26	0.97
1:B:33:LEU:HD11	1:B:52:LYS:HG3	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:ARG:HD2	1:C:95:LEU:HD13	1.49	0.94
1:D:5:VAL:HG23	1:D:71:ARG:HD2	1.47	0.93
1:D:43:TYR:HB2	1:D:48:LEU:HD22	1.50	0.92
1:B:143:PRO:HG3	3:B:421:HOH:O	1.71	0.91
1:C:14:ARG:HH11	1:C:14:ARG:HB2	1.37	0.89
1:A:57:ARG:NH1	1:A:61:ARG:HH21	1.71	0.88
1:C:76:GLU:HG2	1:C:79:SER:HB3	1.56	0.87
1:A:88:VAL:H	1:A:156:GLY:HA3	1.40	0.87
1:B:88:VAL:H	1:B:156:GLY:HA3	1.40	0.86
1:A:57:ARG:HH11	1:A:61:ARG:HH21	1.22	0.86
1:D:103:GLN:HE21	1:D:105:VAL:CG1	1.89	0.86
1:D:127:LYS:HD3	1:D:128:ALA:N	1.90	0.86
1:D:61:ARG:HD3	1:D:95:LEU:HD13	1.56	0.86
1:D:33:LEU:HD13	1:D:51:ALA:HB3	1.58	0.85
3:A:499:HOH:O	1:D:2:ALA:HB3	1.77	0.84
1:B:9:LYS:HE2	1:B:9:LYS:H	1.40	0.84
1:B:115:THR:HB	1:B:116:PRO:HD3	1.58	0.84
1:B:33:LEU:CD1	1:B:52:LYS:HG3	2.07	0.84
1:D:5:VAL:CG2	1:D:71:ARG:HD2	2.06	0.84
1:D:33:LEU:O	1:D:37:MET:HG3	1.77	0.84
1:C:53:GLN:HB2	3:C:499:HOH:O	1.76	0.84
1:D:90:GLU:HG2	1:D:99:ARG:NH1	1.93	0.84
1:D:31:LYS:O	1:D:34:GLN:HG3	1.79	0.83
1:B:9:LYS:HG2	3:B:499:HOH:O	1.79	0.82
1:C:142:THR:HG21	3:C:508:HOH:O	1.79	0.82
1:A:43:TYR:HB2	1:A:48:LEU:HD22	1.62	0.81
1:B:61:ARG:CZ	1:B:95:LEU:HD13	2.10	0.81
1:B:120:SER:HB3	1:B:123:SER:HB3	1.62	0.81
1:C:9:LYS:O	1:C:13:GLU:HG3	1.79	0.81
1:A:94:PRO:HA	3:A:501:HOH:O	1.80	0.81
1:D:103:GLN:HE21	1:D:105:VAL:HG11	1.45	0.81
1:A:57:ARG:HH11	1:A:61:ARG:NH2	1.78	0.81
1:B:43:TYR:HB3	1:B:48:LEU:HD13	1.64	0.80
1:B:48:LEU:HD22	3:B:449:HOH:O	1.81	0.80
1:A:52:LYS:HB2	3:A:433:HOH:O	1.81	0.80
1:D:23:ARG:HD3	3:D:470:HOH:O	1.81	0.80
1:C:4:GLU:HB3	1:C:73:VAL:HG21	1.65	0.79
1:A:21:ARG:HD2	1:C:24:GLU:OE2	1.84	0.78
1:D:6:LYS:HB3	1:D:75:LEU:HD11	1.64	0.78
1:B:94:PRO:HG3	3:B:519:HOH:O	1.83	0.78
1:B:99:ARG:HH22	1:B:152:VAL:HG11	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:O	1:D:23:ARG:HD2	1.84	0.77
1:D:143:PRO:HA	3:D:495:HOH:O	1.84	0.76
1:D:120:SER:HB3	1:D:123:SER:HB3	1.66	0.76
1:D:76:GLU:CG	1:D:79:SER:HB2	2.16	0.76
1:D:129:LEU:HA	1:D:138:LEU:HD11	1.66	0.75
1:C:61:ARG:O	1:C:65:LEU:HG	1.85	0.75
1:A:115:THR:HG23	3:A:478:HOH:O	1.85	0.75
1:B:142:THR:HG22	1:B:144:LYS:HG2	1.68	0.74
1:D:22:GLU:OE2	1:D:58:ILE:HG23	1.87	0.74
1:D:33:LEU:HD13	1:D:51:ALA:CB	2.18	0.74
1:B:31:LYS:O	1:B:35:GLU:HG3	1.87	0.74
1:B:90:GLU:OE2	1:B:153:ALA:HB3	1.87	0.74
1:D:96:SER:HB3	1:D:147:ARG:HH22	1.52	0.74
1:C:43:TYR:HA	1:C:48:LEU:HD13	1.70	0.74
1:B:115:THR:HB	1:B:116:PRO:CD	2.19	0.73
1:A:68:ILE:HD13	1:A:94:PRO:HB3	1.71	0.73
1:D:7:LEU:HD21	1:D:150:ARG:HD2	1.71	0.73
1:A:83:ILE:HG12	1:A:154:ILE:HG12	1.71	0.72
1:C:120:SER:HB3	1:C:123:SER:HB3	1.71	0.72
1:C:57:ARG:NH1	1:C:61:ARG:HG3	2.02	0.72
1:C:33:LEU:O	1:C:37:MET:HG3	1.90	0.71
1:A:7:LEU:HD21	1:A:150:ARG:HD2	1.70	0.71
1:D:14:ARG:HG3	1:D:14:ARG:HH11	1.55	0.71
1:A:120:SER:HB3	1:A:123:SER:HB3	1.71	0.70
1:D:90:GLU:CG	1:D:99:ARG:HH11	2.02	0.70
1:B:42:ASP:HB2	3:B:501:HOH:O	1.91	0.70
1:D:56:ALA:HA	1:D:59:GLU:OE2	1.92	0.70
1:A:57:ARG:NH1	1:A:61:ARG:HE	1.89	0.70
1:A:57:ARG:HH11	1:A:61:ARG:HE	1.39	0.70
1:D:103:GLN:HE22	1:D:118:LYS:HE2	1.56	0.70
1:D:143:PRO:HD2	3:D:507:HOH:O	1.91	0.70
1:A:127:LYS:HD3	1:A:127:LYS:C	2.17	0.69
1:D:57:ARG:HD3	1:D:61:ARG:CZ	2.23	0.69
1:A:115:THR:HB	1:A:116:PRO:HD3	1.73	0.69
1:C:52:LYS:HE2	3:C:454:HOH:O	1.92	0.69
1:B:57:ARG:HB2	3:B:428:HOH:O	1.91	0.69
1:B:99:ARG:NH1	1:B:152:VAL:HG21	2.07	0.69
1:A:42:ASP:HB3	3:A:429:HOH:O	1.91	0.68
1:C:142:THR:HB	1:C:145:GLY:O	1.93	0.68
1:D:90:GLU:HG3	1:D:99:ARG:HD2	1.75	0.68
1:B:79:SER:H	1:B:133:ARG:HH11	1.38	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:PRO:HD2	1:B:144:LYS:HE3	1.74	0.68
1:D:43:TYR:HB3	1:D:48:LEU:HD13	1.75	0.68
1:C:6:LYS:HB3	1:C:75:LEU:HD21	1.77	0.67
1:A:6:LYS:HB3	1:A:75:LEU:HD21	1.76	0.67
1:A:57:ARG:HH11	1:A:61:ARG:NE	1.93	0.67
1:C:77:GLU:O	1:C:133:ARG:NH1	2.28	0.66
1:A:125:MET:O	1:A:129:LEU:HG	1.95	0.66
1:C:14:ARG:HB2	1:C:14:ARG:NH1	2.08	0.66
1:C:45:ASP:HB3	3:C:475:HOH:O	1.95	0.66
1:B:33:LEU:HD23	1:B:33:LEU:O	1.94	0.66
1:A:3:ARG:HG3	1:A:3:ARG:HH11	1.61	0.66
1:D:82:VAL:HA	1:D:133:ARG:HG2	1.78	0.65
1:D:115:THR:HB	1:D:116:PRO:HD3	1.78	0.65
1:A:42:ASP:HB2	3:A:494:HOH:O	1.95	0.65
1:D:57:ARG:HH11	1:D:61:ARG:CD	2.09	0.65
1:B:34:GLN:OE1	1:B:34:GLN:HA	1.96	0.65
1:D:85:LEU:HD21	1:D:121:ASP:CG	2.21	0.65
1:A:108:ALA:HA	3:A:448:HOH:O	1.95	0.65
1:A:57:ARG:HH11	1:A:61:ARG:CZ	2.10	0.65
1:A:9:LYS:HD3	1:A:74:ILE:HD13	1.80	0.64
1:D:84:GLY:HA2	1:D:130:LEU:CD1	2.28	0.64
1:B:48:LEU:HD23	1:B:48:LEU:O	1.97	0.64
1:C:147:ARG:HD2	3:C:473:HOH:O	1.97	0.64
1:B:38:GLU:HB2	3:B:439:HOH:O	1.97	0.64
1:C:83:ILE:HG13	1:C:154:ILE:HD11	1.80	0.64
1:D:64:SER:O	1:D:67:ASP:HB3	1.98	0.63
1:A:83:ILE:N	3:A:467:HOH:O	2.30	0.63
1:A:55:LYS:O	1:A:59:GLU:HG3	1.98	0.63
1:B:54:GLU:O	1:B:58:ILE:HG13	1.99	0.63
1:B:40:SER:HA	3:B:462:HOH:O	1.99	0.63
1:D:96:SER:HB3	1:D:147:ARG:NH2	2.13	0.63
1:D:103:GLN:NE2	1:D:118:LYS:HE2	2.14	0.62
1:D:115:THR:CB	1:D:116:PRO:HD3	2.29	0.62
1:D:14:ARG:HD2	1:D:137:VAL:HG12	1.80	0.62
1:A:33:LEU:O	1:A:37:MET:HG3	2.00	0.61
1:B:33:LEU:HD11	1:B:52:LYS:CG	2.28	0.61
1:C:65:LEU:HD21	1:C:95:LEU:HD21	1.82	0.61
1:A:17:GLN:O	1:A:21:ARG:HG3	2.01	0.61
1:A:82:VAL:HG22	3:A:467:HOH:O	2.00	0.61
1:A:114:ASP:OD2	1:A:118:LYS:HE3	2.01	0.61
1:A:143:PRO:HD2	3:A:427:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:ASP:CB	1:B:147:ARG:HH21	2.13	0.61
1:D:92:GLU:O	1:D:94:PRO:HD3	2.01	0.61
1:C:67:ASP:O	1:C:71:ARG:HG3	2.01	0.61
1:D:142:THR:HB	1:D:145:GLY:O	2.01	0.60
1:A:71:ARG:HG2	1:A:71:ARG:HH11	1.67	0.60
1:C:112:VAL:O	1:C:117:MET:HE2	2.00	0.60
1:B:9:LYS:H	1:B:9:LYS:CE	2.11	0.60
1:B:13:GLU:O	1:B:17:GLN:HG3	2.01	0.60
1:D:85:LEU:HD21	1:D:121:ASP:OD1	2.01	0.60
1:B:14:ARG:HA	1:B:17:GLN:OE1	2.01	0.60
1:C:57:ARG:HD3	1:C:61:ARG:CZ	2.32	0.59
1:D:18:GLN:HG2	1:D:148:GLU:OE1	2.02	0.59
1:C:144:LYS:HE2	3:C:461:HOH:O	2.02	0.59
1:B:115:THR:CB	1:B:116:PRO:HD3	2.31	0.59
1:D:14:ARG:HD2	1:D:137:VAL:CG1	2.32	0.59
1:B:142:THR:CG2	1:B:144:LYS:HG2	2.32	0.59
1:C:83:ILE:HG13	1:C:154:ILE:CD1	2.32	0.59
1:D:54:GLU:O	1:D:58:ILE:HG13	2.03	0.59
1:A:90:GLU:OE1	1:A:155:HIS:NE2	2.36	0.59
1:B:150:ARG:NH1	3:B:519:HOH:O	2.36	0.58
1:A:129:LEU:HD23	1:A:138:LEU:HD12	1.83	0.58
1:C:57:ARG:HD2	1:C:57:ARG:C	2.29	0.58
1:D:14:ARG:HG3	1:D:14:ARG:NH1	2.18	0.58
1:B:33:LEU:CD1	1:B:52:LYS:N	2.67	0.58
1:C:114:ASP:O	1:C:115:THR:O	2.21	0.58
1:A:145:GLY:O	1:A:147:ARG:HG3	2.02	0.58
1:D:80:GLY:O	1:D:133:ARG:NH2	2.23	0.58
1:D:106:SER:HB3	1:D:109:GLU:OE2	2.04	0.58
1:A:131:GLY:HA3	3:A:491:HOH:O	2.04	0.57
1:A:3:ARG:HG3	1:A:3:ARG:NH1	2.20	0.57
1:B:117:MET:HG3	3:B:515:HOH:O	2.03	0.57
1:D:52:LYS:HG3	1:D:53:GLN:N	2.18	0.57
1:D:43:TYR:HB2	1:D:48:LEU:CD2	2.30	0.57
1:D:102:VAL:HG22	1:D:119:ILE:HD11	1.87	0.57
1:D:111:ASN:HB3	1:D:114:ASP:OD1	2.05	0.57
1:B:57:ARG:CZ	1:B:61:ARG:HD2	2.35	0.57
1:B:83:ILE:HG13	1:B:154:ILE:CD1	2.34	0.57
1:D:83:ILE:O	1:D:130:LEU:HD12	2.05	0.57
1:D:18:GLN:HE22	1:D:21:ARG:CZ	2.18	0.56
1:D:30:THR:OG1	1:D:55:LYS:HE3	2.05	0.56
1:B:139:SER:OG	1:B:146:ARG:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:TYR:CB	1:D:48:LEU:HD13	2.35	0.56
1:B:92:GLU:O	1:B:94:PRO:HD3	2.06	0.56
1:C:37:MET:HE2	1:C:43:TYR:CD1	2.41	0.56
1:C:115:THR:HB	1:C:116:PRO:HD3	1.87	0.56
1:A:43:TYR:CB	1:A:48:LEU:HD13	2.35	0.56
1:B:4:GLU:HB2	1:B:73:VAL:HG21	1.87	0.56
1:B:51:ALA:O	1:B:52:LYS:C	2.43	0.56
1:B:61:ARG:NH1	1:B:95:LEU:HD13	2.21	0.56
1:D:90:GLU:CG	1:D:99:ARG:HD2	2.35	0.56
1:A:56:ALA:HA	1:A:59:GLU:CD	2.31	0.56
1:D:34:GLN:O	1:D:37:MET:HB2	2.06	0.56
1:D:127:LYS:HA	3:D:439:HOH:O	2.06	0.56
1:A:127:LYS:HD3	1:A:128:ALA:N	2.22	0.55
1:C:43:TYR:CA	1:C:48:LEU:HD13	2.37	0.55
1:D:18:GLN:HE22	1:D:21:ARG:NE	2.05	0.55
1:B:33:LEU:HD11	1:B:52:LYS:N	2.21	0.55
1:C:48:LEU:C	1:C:48:LEU:HD23	2.31	0.55
1:C:88:VAL:H	1:C:156:GLY:HA3	1.71	0.55
1:A:111:ASN:OD1	1:A:113:LEU:HD12	2.07	0.55
1:B:142:THR:HG21	3:B:423:HOH:O	2.05	0.55
1:C:14:ARG:HH11	1:C:14:ARG:CB	2.17	0.55
1:D:62:ILE:O	1:D:66:GLU:HG3	2.07	0.55
1:D:88:VAL:H	1:D:156:GLY:HA3	1.72	0.55
1:B:28:GLU:O	1:B:31:LYS:HG2	2.06	0.55
1:B:79:SER:H	1:B:133:ARG:NH1	2.05	0.55
1:B:93:ASP:OD2	1:B:147:ARG:NH2	2.40	0.54
1:A:142:THR:HB	1:A:145:GLY:O	2.07	0.54
1:A:25:ARG:HB3	1:C:28:GLU:OE1	2.07	0.54
1:C:4:GLU:HB3	1:C:73:VAL:CG2	2.36	0.54
1:D:6:LYS:H	1:D:6:LYS:HD2	1.73	0.54
1:D:57:ARG:HD3	1:D:61:ARG:NE	2.22	0.54
1:A:71:ARG:HG2	1:A:71:ARG:NH1	2.22	0.54
1:A:119:ILE:HG13	1:A:125:MET:HE3	1.89	0.54
1:C:102:VAL:HG21	1:C:125:MET:HE1	1.88	0.53
1:D:61:ARG:HD3	1:D:95:LEU:CD1	2.34	0.53
1:B:48:LEU:HB3	3:B:449:HOH:O	2.06	0.53
1:B:29:ALA:HB2	3:B:497:HOH:O	2.07	0.53
1:D:7:LEU:CD2	1:D:150:ARG:HD2	2.37	0.53
1:B:21:ARG:HG2	1:B:25:ARG:CZ	2.39	0.53
1:A:68:ILE:CD1	1:A:94:PRO:HB3	2.36	0.53
1:C:76:GLU:CG	1:C:79:SER:HB3	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:VAL:HG22	1:D:153:ALA:HA	1.89	0.53
1:A:39:SER:HB2	1:C:46:SER:HB3	1.91	0.53
1:B:93:ASP:CG	1:B:147:ARG:HH21	2.17	0.53
3:A:434:HOH:O	1:B:2:ALA:HB2	2.08	0.53
1:D:127:LYS:HD3	1:D:127:LYS:C	2.34	0.53
1:B:112:VAL:O	1:B:117:MET:HE2	2.09	0.53
1:A:7:LEU:CD2	1:A:150:ARG:HD2	2.39	0.52
1:B:134:VAL:CG2	1:B:153:ALA:HA	2.39	0.52
1:D:18:GLN:OE1	1:D:21:ARG:CZ	2.57	0.52
1:D:127:LYS:HD3	1:D:128:ALA:CA	2.39	0.52
1:C:26:LEU:HD23	1:D:1:MET:CE	2.38	0.52
1:D:142:THR:HG22	1:D:144:LYS:H	1.73	0.52
1:A:112:VAL:HG13	1:A:117:MET:CE	2.39	0.52
1:A:57:ARG:HD3	1:A:61:ARG:NH2	2.25	0.52
1:B:90:GLU:OE1	1:B:152:VAL:HB	2.10	0.52
1:D:133:ARG:HB3	3:D:521:HOH:O	2.09	0.52
1:C:14:ARG:HD2	1:C:148:GLU:OE2	2.09	0.52
1:C:111:ASN:H	1:C:118:LYS:HB2	1.74	0.52
1:C:137:VAL:HG12	1:C:148:GLU:HG2	1.91	0.52
1:B:37:MET:HB3	3:B:517:HOH:O	2.10	0.51
1:A:114:ASP:O	1:A:115:THR:O	2.27	0.51
1:D:84:GLY:HA2	1:D:130:LEU:HD11	1.92	0.51
1:A:64:SER:O	1:A:68:ILE:HG13	2.10	0.51
1:C:91:LEU:HD23	1:C:151:VAL:HA	1.93	0.51
1:D:93:ASP:HB3	1:D:98:GLU:HB3	1.93	0.51
1:B:9:LYS:O	1:B:13:GLU:HG3	2.10	0.51
1:B:76:GLU:CD	1:B:76:GLU:H	2.18	0.51
1:C:127:LYS:O	1:C:127:LYS:HD3	2.11	0.51
3:C:489:HOH:O	1:D:70:SER:HA	2.10	0.51
1:D:5:VAL:HG23	1:D:71:ARG:CD	2.31	0.51
1:A:25:ARG:O	1:C:28:GLU:HG2	2.10	0.51
1:D:103:GLN:NE2	1:D:105:VAL:HG11	2.18	0.51
1:C:65:LEU:O	1:C:69:LEU:HD12	2.10	0.51
1:A:139:SER:HA	1:A:148:GLU:HG3	1.92	0.51
1:B:61:ARG:O	1:B:65:LEU:HG	2.10	0.51
1:C:26:LEU:HD23	1:D:1:MET:HE1	1.93	0.51
1:D:6:LYS:HD2	1:D:6:LYS:N	2.26	0.51
1:B:8:THR:HG23	1:B:135:GLY:C	2.35	0.51
1:D:57:ARG:HH11	1:D:61:ARG:NE	2.09	0.50
1:D:144:LYS:HA	3:D:437:HOH:O	2.11	0.50
1:D:36:LEU:HD23	1:D:48:LEU:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:TYR:CB	1:A:48:LEU:HD22	2.39	0.50
1:B:126:GLY:O	1:B:130:LEU:HD22	2.12	0.50
1:C:6:LYS:HD3	1:C:75:LEU:HD21	1.94	0.50
1:C:76:GLU:HG2	1:C:79:SER:CB	2.37	0.50
1:D:115:THR:CB	1:D:116:PRO:CD	2.90	0.50
1:B:7:LEU:CD2	1:B:150:ARG:HD2	2.42	0.50
1:B:99:ARG:HH12	1:B:152:VAL:HG21	1.77	0.50
1:A:88:VAL:N	1:A:156:GLY:HA3	2.19	0.50
1:B:134:VAL:HG22	1:B:153:ALA:HA	1.93	0.50
1:C:127:LYS:HD3	1:C:127:LYS:C	2.37	0.50
1:A:146:ARG:O	1:A:146:ARG:HG2	2.11	0.49
1:B:129:LEU:O	1:B:132:HIS:HD2	1.95	0.49
1:C:23:ARG:HD3	1:D:1:MET:O	2.12	0.49
1:B:76:GLU:CD	1:B:76:GLU:N	2.68	0.49
1:B:92:GLU:HA	1:B:98:GLU:O	2.12	0.49
1:D:18:GLN:HE22	1:D:21:ARG:NH2	2.10	0.49
1:A:112:VAL:HG13	1:A:117:MET:HE3	1.95	0.49
1:B:83:ILE:HG13	1:B:154:ILE:HD13	1.95	0.49
1:A:14:ARG:NH2	1:A:139:SER:HB2	2.27	0.49
1:B:43:TYR:HD2	3:B:506:HOH:O	1.94	0.48
1:C:112:VAL:HG13	1:C:117:MET:HE2	1.95	0.48
1:C:90:GLU:OE2	1:C:155:HIS:ND1	2.45	0.48
1:C:132:HIS:HD1	1:C:136:ASP:CG	2.21	0.48
1:D:102:VAL:HG13	1:D:119:ILE:HG12	1.94	0.48
1:C:42:ASP:HB3	1:C:44:ASP:OD1	2.12	0.48
1:D:58:ILE:O	1:D:62:ILE:HG13	2.14	0.48
1:B:21:ARG:O	1:B:25:ARG:HD2	2.14	0.48
1:C:7:LEU:HD23	1:C:150:ARG:HD2	1.96	0.48
1:A:56:ALA:HA	1:A:59:GLU:OE2	2.14	0.48
1:A:102:VAL:HG13	1:A:119:ILE:HG12	1.96	0.48
1:C:43:TYR:H	1:C:43:TYR:HD2	1.62	0.48
1:D:21:ARG:NH1	1:D:146:ARG:NH2	2.62	0.48
1:B:114:ASP:O	1:B:115:THR:O	2.32	0.47
1:B:115:THR:CB	1:B:116:PRO:CD	2.91	0.47
1:A:132:HIS:HE1	3:A:452:HOH:O	1.96	0.47
1:D:96:SER:OG	1:D:98:GLU:HB2	2.14	0.47
1:A:115:THR:CB	1:A:116:PRO:HD3	2.42	0.47
1:D:67:ASP:OD2	1:D:71:ARG:NH2	2.47	0.47
1:A:128:ALA:O	1:A:132:HIS:CD2	2.66	0.47
1:C:33:LEU:HD13	1:C:51:ALA:HB3	1.97	0.47
1:A:8:THR:HG22	3:A:435:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:LEU:HD12	1:B:52:LYS:N	2.29	0.47
1:D:103:GLN:HE21	1:D:105:VAL:HG13	1.72	0.47
1:D:153:ALA:HB2	3:D:433:HOH:O	2.13	0.47
1:C:23:ARG:HD3	1:D:1:MET:HG2	1.96	0.47
1:D:55:LYS:O	1:D:59:GLU:HG3	2.14	0.47
1:A:119:ILE:HG22	1:A:123:SER:OG	2.15	0.47
1:A:115:THR:CB	1:A:116:PRO:CD	2.93	0.46
1:D:127:LYS:HB2	3:D:439:HOH:O	2.15	0.46
1:C:43:TYR:CB	1:C:48:LEU:HD13	2.45	0.46
1:C:85:LEU:HD23	1:C:86:GLY:N	2.30	0.46
1:D:52:LYS:HD2	1:D:52:LYS:C	2.40	0.46
1:C:10:ALA:HA	1:C:13:GLU:OE1	2.15	0.46
1:C:125:MET:HG2	1:C:140:LEU:HD13	1.96	0.46
1:B:91:LEU:HD11	1:B:129:LEU:HD21	1.97	0.46
1:B:144:LYS:H	1:B:144:LYS:HD3	1.81	0.46
1:A:61:ARG:HG2	1:A:95:LEU:HD13	1.97	0.46
1:B:9:LYS:HZ3	1:B:74:ILE:CG2	2.29	0.46
1:B:115:THR:O	1:B:117:MET:N	2.48	0.46
1:B:144:LYS:H	1:B:144:LYS:CD	2.29	0.46
1:D:61:ARG:HH11	1:D:61:ARG:HG2	1.81	0.46
1:B:33:LEU:CD1	1:B:52:LYS:CA	2.93	0.46
1:A:102:VAL:HG22	1:A:119:ILE:HD11	1.97	0.46
1:A:129:LEU:CD2	1:A:138:LEU:HD12	2.46	0.46
1:C:77:GLU:CD	3:C:507:HOH:O	2.31	0.45
1:C:102:VAL:HG12	1:C:103:GLN:N	2.31	0.45
1:D:34:GLN:HA	1:D:37:MET:SD	2.56	0.45
1:C:12:TYR:CE1	1:C:69:LEU:HD23	2.51	0.45
1:C:142:THR:HG22	1:C:144:LYS:N	2.32	0.45
1:B:33:LEU:HD11	1:B:52:LYS:CA	2.46	0.45
1:B:33:LEU:CD1	1:B:52:LYS:HA	2.46	0.45
1:D:6:LYS:O	1:D:7:LEU:HD23	2.17	0.45
1:D:21:ARG:CZ	1:D:146:ARG:NH2	2.80	0.45
1:A:83:ILE:HG13	1:A:132:HIS:O	2.17	0.45
1:B:48:LEU:O	1:B:51:ALA:HB3	2.17	0.45
1:C:52:LYS:HD2	1:C:52:LYS:HA	1.77	0.45
1:D:17:GLN:HE21	1:D:17:GLN:HB2	1.59	0.45
1:D:68:ILE:O	1:D:71:ARG:HG3	2.16	0.45
1:B:93:ASP:HB2	1:B:147:ARG:HH21	1.80	0.45
1:D:28:GLU:O	1:D:32:ILE:HG13	2.17	0.45
1:A:144:LYS:HE3	1:A:144:LYS:HB2	1.85	0.45
1:C:92:GLU:HB2	1:C:99:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:GLU:OE2	1:A:25:ARG:NH1	2.50	0.45
1:C:115:THR:CB	1:C:116:PRO:CD	2.95	0.45
1:D:144:LYS:HE2	3:D:512:HOH:O	2.17	0.45
1:A:43:TYR:HB3	1:A:48:LEU:HD13	1.98	0.44
1:A:118:LYS:NZ	3:A:488:HOH:O	2.50	0.44
1:C:57:ARG:HD3	1:C:61:ARG:NE	2.32	0.44
1:D:114:ASP:O	1:D:115:THR:O	2.35	0.44
1:A:142:THR:HB	1:A:145:GLY:C	2.43	0.44
1:B:9:LYS:NZ	1:B:74:ILE:CG2	2.81	0.44
1:D:57:ARG:HD3	1:D:61:ARG:NH2	2.32	0.44
1:B:99:ARG:HG3	1:B:99:ARG:HH11	1.83	0.44
1:A:88:VAL:HG22	1:A:103:GLN:HG3	2.00	0.44
1:C:41:ASP:O	1:C:43:TYR:CD2	2.71	0.44
1:D:76:GLU:HG2	1:D:79:SER:CB	2.28	0.44
1:D:115:THR:OG1	1:D:116:PRO:CD	2.65	0.44
1:B:22:GLU:HA	1:B:25:ARG:HD2	1.99	0.44
1:C:142:THR:HG22	1:C:144:LYS:H	1.82	0.44
1:D:5:VAL:HG21	1:D:71:ARG:HD2	1.95	0.44
1:D:57:ARG:C	1:D:57:ARG:HD2	2.43	0.44
1:A:52:LYS:HG2	3:A:426:HOH:O	2.18	0.44
1:C:18:GLN:OE1	1:C:21:ARG:NH2	2.51	0.44
1:D:6:LYS:HB3	1:D:75:LEU:CD1	2.41	0.43
1:A:139:SER:OG	1:A:146:ARG:HG3	2.18	0.43
1:B:57:ARG:NH1	1:B:61:ARG:HD2	2.34	0.43
1:B:114:ASP:O	1:B:115:THR:C	2.61	0.43
1:A:22:GLU:OE1	1:A:58:ILE:HG23	2.19	0.43
1:B:7:LEU:HD23	1:B:150:ARG:HD2	1.99	0.43
1:B:142:THR:HG22	1:B:144:LYS:HE3	2.01	0.43
1:C:115:THR:CB	1:C:116:PRO:HD3	2.46	0.43
1:A:90:GLU:CD	1:A:155:HIS:NE2	2.77	0.43
1:D:112:VAL:HG12	1:D:117:MET:HE2	2.01	0.43
1:A:21:ARG:HG2	3:C:487:HOH:O	2.19	0.43
1:A:85:LEU:HD23	1:A:85:LEU:HA	1.73	0.43
1:B:127:LYS:HD3	1:B:127:LYS:C	2.44	0.43
1:D:56:ALA:HA	1:D:59:GLU:CD	2.44	0.43
1:D:79:SER:O	1:D:133:ARG:NE	2.52	0.43
1:C:17:GLN:O	1:C:21:ARG:HG3	2.18	0.43
1:A:21:ARG:HD3	3:A:472:HOH:O	2.19	0.42
1:D:18:GLN:NE2	1:D:21:ARG:NH2	2.67	0.42
1:D:133:ARG:NH2	3:D:486:HOH:O	2.52	0.42
1:B:90:GLU:HG2	1:B:153:ALA:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:ARG:NH1	1:D:152:VAL:HG22	2.35	0.42
1:C:26:LEU:HD22	1:C:62:ILE:HD12	2.02	0.42
1:B:121:ASP:OD1	1:B:121:ASP:C	2.62	0.42
1:B:144:LYS:HB2	3:B:454:HOH:O	2.18	0.42
1:C:114:ASP:HB3	3:C:428:HOH:O	2.19	0.42
1:D:88:VAL:HG23	1:D:156:GLY:HA3	2.01	0.42
1:A:115:THR:HB	1:A:116:PRO:CD	2.44	0.42
1:A:128:ALA:O	1:A:138:LEU:HD13	2.19	0.42
1:B:85:LEU:CD2	1:B:105:VAL:HA	2.50	0.42
1:D:68:ILE:HD12	1:D:94:PRO:HB3	2.02	0.42
1:D:34:GLN:C	1:D:34:GLN:OE1	2.63	0.42
1:A:112:VAL:HG22	1:A:117:MET:HE2	2.02	0.42
1:D:115:THR:OG1	1:D:116:PRO:HD3	2.19	0.42
1:A:22:GLU:HB3	1:A:62:ILE:CG1	2.50	0.42
1:C:43:TYR:HB3	1:C:48:LEU:HD13	2.01	0.42
1:B:95:LEU:HB3	3:B:509:HOH:O	2.19	0.41
1:C:92:GLU:CD	1:C:150:ARG:HH12	2.28	0.41
1:A:102:VAL:HG13	1:A:119:ILE:CG1	2.50	0.41
1:C:132:HIS:CD2	1:C:138:LEU:HD21	2.55	0.41
1:D:82:VAL:HG22	1:D:133:ARG:CD	2.50	0.41
1:D:116:PRO:O	1:D:117:MET:C	2.63	0.41
1:A:21:ARG:NH1	3:A:499:HOH:O	2.53	0.41
1:A:54:GLU:O	1:A:58:ILE:HG13	2.20	0.41
1:A:111:ASN:H	1:A:118:LYS:HB2	1.85	0.41
1:A:134:VAL:CG2	1:A:153:ALA:HA	2.50	0.41
1:B:90:GLU:O	1:B:90:GLU:HG3	2.19	0.41
1:A:61:ARG:HG2	1:A:61:ARG:HH11	1.85	0.41
1:A:83:ILE:HD13	1:A:89:VAL:HG21	2.00	0.41
1:C:37:MET:HE2	1:C:43:TYR:HD1	1.84	0.41
1:D:22:GLU:OE1	1:D:25:ARG:NH1	2.52	0.41
1:A:21:ARG:NH2	1:A:25:ARG:HH22	2.19	0.41
1:C:105:VAL:HG21	1:C:118:LYS:HB3	2.02	0.41
1:C:115:THR:O	1:C:117:MET:N	2.53	0.41
1:A:124:PRO:HB2	3:A:493:HOH:O	2.21	0.41
1:B:52:LYS:O	1:B:53:GLN:C	2.63	0.41
1:D:48:LEU:HD23	1:D:48:LEU:C	2.44	0.41
1:A:83:ILE:CG1	1:A:154:ILE:HG12	2.46	0.41
1:B:2:ALA:HB3	3:B:443:HOH:O	2.20	0.41
1:B:102:VAL:CG1	1:B:103:GLN:N	2.83	0.41
1:C:33:LEU:HD13	1:C:51:ALA:CB	2.51	0.41
1:D:39:SER:OG	1:D:40:SER:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:SER:OG	1:D:107:PRO:HD2	2.20	0.41
1:D:39:SER:O	1:D:41:ASP:N	2.54	0.41
1:D:18:GLN:NE2	1:D:21:ARG:CZ	2.84	0.40
1:D:53:GLN:HB2	3:D:428:HOH:O	2.20	0.40
1:D:57:ARG:NH1	1:D:61:ARG:HD2	2.35	0.40
1:A:43:TYR:C	1:A:45:ASP:H	2.30	0.40
1:A:138:LEU:O	1:A:148:GLU:HA	2.20	0.40
1:B:33:LEU:HD13	1:B:52:LYS:HG3	1.93	0.40
1:D:18:GLN:OE1	1:D:21:ARG:NH2	2.55	0.40
1:A:111:ASN:ND2	3:A:468:HOH:O	2.53	0.40
1:A:131:GLY:CA	3:A:467:HOH:O	2.69	0.40
1:A:132:HIS:CE1	3:A:452:HOH:O	2.72	0.40
1:C:18:GLN:HE21	1:C:22:GLU:HG2	1.86	0.40
1:A:82:VAL:HG13	3:A:467:HOH:O	2.21	0.40
1:A:127:LYS:O	1:A:128:ALA:C	2.64	0.40
1:B:125:MET:HG2	1:B:129:LEU:HD11	2.03	0.40
1:B:144:LYS:HD3	1:B:144:LYS:N	2.36	0.40
1:C:92:GLU:OE2	1:C:150:ARG:NH2	2.54	0.40
1:D:142:THR:HG22	1:D:144:LYS:N	2.36	0.40
1:B:47:GLY:HA3	3:B:434:HOH:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LYS:NZ	1:D:76:GLU:OE2[1_455]	2.03	0.17

## 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	154/156 (99%)	137 (89%)	15 (10%)	2 (1%)	<b>9</b> <b>14</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	154/156 (99%)	133 (86%)	17 (11%)	4 (3%)	4	4
1	C	154/156 (99%)	138 (90%)	12 (8%)	4 (3%)	4	4
1	D	154/156 (99%)	135 (88%)	15 (10%)	4 (3%)	4	4
All	All	616/624 (99%)	543 (88%)	59 (10%)	14 (2%)	5	6

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	THR
1	B	115	THR
1	C	39	SER
1	C	115	THR
1	D	39	SER
1	D	115	THR
1	A	39	SER
1	C	42	ASP
1	C	77	GLU
1	B	77	GLU
1	B	39	SER
1	B	124	PRO
1	D	94	PRO
1	D	80	GLY

### 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	131/131 (100%)	116 (88%)	15 (12%)	5	8
1	B	131/131 (100%)	118 (90%)	13 (10%)	7	11
1	C	131/131 (100%)	121 (92%)	10 (8%)	12	21
1	D	131/131 (100%)	120 (92%)	11 (8%)	10	17
All	All	524/524 (100%)	475 (91%)	49 (9%)	8	13

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	20	GLU
1	A	38	GLU
1	A	43	TYR
1	A	48	LEU
1	A	53	GLN
1	A	76	GLU
1	A	82	VAL
1	A	85	LEU
1	A	98	GLU
1	A	99	ARG
1	A	102	VAL
1	A	113	LEU
1	A	133	ARG
1	A	146	ARG
1	B	1	MET
1	B	9	LYS
1	B	24	GLU
1	B	42	ASP
1	B	43	TYR
1	B	53	GLN
1	B	76	GLU
1	B	85	LEU
1	B	99	ARG
1	B	121	ASP
1	B	130	LEU
1	B	144	LYS
1	B	155	HIS
1	C	14	ARG
1	C	27	GLN
1	C	35	GLU
1	C	40	SER
1	C	43	TYR
1	C	49	GLU
1	C	106	SER
1	C	121	ASP
1	C	144	LYS
1	C	146	ARG
1	D	17	GLN
1	D	23	ARG
1	D	34	GLN
1	D	43	TYR

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Mol	Chain	Res	Type
1	D	52	LYS
1	D	71	ARG
1	D	90	GLU
1	D	94	PRO
1	D	102	VAL
1	D	124	PRO
1	D	139	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	27	GLN
1	A	132	HIS
1	B	132	HIS
1	C	17	GLN
1	C	34	GLN
1	D	17	GLN
1	D	103	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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 25 are monoatomic - leaving 0 for Mogul analysis.

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	156/156 (100%)	-1.49	0 100 100	28, 54, 85, 97	0
1	B	156/156 (100%)	-1.32	0 100 100	33, 58, 99, 107	0
1	C	156/156 (100%)	-1.43	0 100 100	22, 56, 83, 98	0
1	D	156/156 (100%)	-1.33	0 100 100	30, 60, 97, 107	0
All	All	624/624 (100%)	-1.39	0 100 100	22, 57, 93, 107	0

There are no RSRZ outliers to report.

### 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 oligosaccharides 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(Å <sup>2</sup> )	Q<0.9
2	ZN	C	415	1/1	0.98	0.05	119,119,119,119	0
2	ZN	A	417	1/1	0.99	0.02	95,95,95,95	0
2	ZN	A	419	1/1	0.99	0.03	71,71,71,71	0
2	ZN	C	409	1/1	0.99	0.03	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	C	412	1/1	0.99	0.04	81,81,81,81	0
2	ZN	A	403	1/1	0.99	0.02	75,75,75,75	0
2	ZN	C	425	1/1	0.99	0.02	88,88,88,88	0
2	ZN	D	418	1/1	0.99	0.02	85,85,85,85	0
2	ZN	A	424	1/1	1.00	0.01	76,76,76,76	0
2	ZN	B	405	1/1	1.00	0.02	49,49,49,49	0
2	ZN	B	414	1/1	1.00	0.01	54,54,54,54	0
2	ZN	B	420	1/1	1.00	0.01	63,63,63,63	0
2	ZN	C	406	1/1	1.00	0.01	68,68,68,68	0
2	ZN	C	407	1/1	1.00	0.01	61,61,61,61	0
2	ZN	C	408	1/1	1.00	0.01	30,30,30,30	0
2	ZN	A	404	1/1	1.00	0.01	48,48,48,48	0
2	ZN	C	400	1/1	1.00	0.02	76,76,76,76	0
2	ZN	C	411	1/1	1.00	0.01	39,39,39,39	0
2	ZN	A	413	1/1	1.00	0.01	38,38,38,38	0
2	ZN	A	416	1/1	1.00	0.01	68,68,68,68	0
2	ZN	C	421	1/1	1.00	0.01	45,45,45,45	0
2	ZN	C	423	1/1	1.00	0.04	68,68,68,68	0
2	ZN	A	402	1/1	1.00	0.01	49,49,49,49	0
2	ZN	A	401	1/1	1.00	0.01	40,40,40,40	0
2	ZN	D	422	1/1	1.00	0.01	54,54,54,54	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.