Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:01 PM GMT

PDB ID	:	3SIQ
Title	:	Crystal Structure of autoinhibited dIAP1-BIR1 domain
Authors	:	Li, X.; Wang, J.; Shi, Y.
Deposited on	:	2011-06-20
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
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:

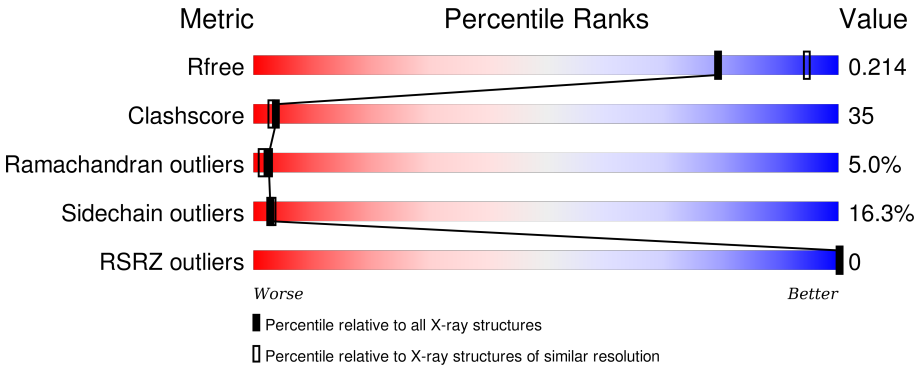
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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 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	136	40% 26% 9% 24%
1	B	136	27% 37% 5% • 30%
1	C	136	37% 29% 5% • 29%
1	D	136	27% 35% 8% • 29%
1	E	136	24% 38% 10% • 27%

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Mol	Chain	Length	Quality of chain
1	F	136	22% 32% 16% 30%

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
2	ZN	A	200	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4806 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 Apoptosis 1 inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	103	Total	C	N	O	S	0	0	0
			834	526	150	153	5			
1	B	95	Total	C	N	O	S	0	0	0
			776	491	140	141	4			
1	C	97	Total	C	N	O	S	0	0	0
			794	501	143	146	4			
1	D	97	Total	C	N	O	S	0	0	0
			796	503	143	146	4			
1	E	99	Total	C	N	O	S	0	1	0
			817	516	147	150	4			
1	F	95	Total	C	N	O	S	0	0	0
			779	494	140	141	4			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	DELETION	UNP Q24306
A	?	-	ASP	DELETION	UNP Q24306
A	?	-	LEU	DELETION	UNP Q24306
A	?	-	PRO	DELETION	UNP Q24306
A	?	-	SER	DELETION	UNP Q24306
A	?	-	TYR	DELETION	UNP Q24306
A	?	-	GLY	DELETION	UNP Q24306
A	89	SER	CYS	ENGINEERED MUTATION	UNP Q24306
A	136	LEU	-	EXPRESSION TAG	UNP Q24306
A	137	GLU	-	EXPRESSION TAG	UNP Q24306
A	138	HIS	-	EXPRESSION TAG	UNP Q24306
A	139	HIS	-	EXPRESSION TAG	UNP Q24306
A	140	HIS	-	EXPRESSION TAG	UNP Q24306
A	141	HIS	-	EXPRESSION TAG	UNP Q24306
A	142	HIS	-	EXPRESSION TAG	UNP Q24306
A	143	HIS	-	EXPRESSION TAG	UNP Q24306
B	?	-	ALA	DELETION	UNP Q24306

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASP	DELETION	UNP Q24306
B	?	-	LEU	DELETION	UNP Q24306
B	?	-	PRO	DELETION	UNP Q24306
B	?	-	SER	DELETION	UNP Q24306
B	?	-	TYR	DELETION	UNP Q24306
B	?	-	GLY	DELETION	UNP Q24306
B	89	SER	CYS	ENGINEERED MUTATION	UNP Q24306
B	136	LEU	-	EXPRESSION TAG	UNP Q24306
B	137	GLU	-	EXPRESSION TAG	UNP Q24306
B	138	HIS	-	EXPRESSION TAG	UNP Q24306
B	139	HIS	-	EXPRESSION TAG	UNP Q24306
B	140	HIS	-	EXPRESSION TAG	UNP Q24306
B	141	HIS	-	EXPRESSION TAG	UNP Q24306
B	142	HIS	-	EXPRESSION TAG	UNP Q24306
B	143	HIS	-	EXPRESSION TAG	UNP Q24306
C	?	-	ALA	DELETION	UNP Q24306
C	?	-	ASP	DELETION	UNP Q24306
C	?	-	LEU	DELETION	UNP Q24306
C	?	-	PRO	DELETION	UNP Q24306
C	?	-	SER	DELETION	UNP Q24306
C	?	-	TYR	DELETION	UNP Q24306
C	?	-	GLY	DELETION	UNP Q24306
C	89	SER	CYS	ENGINEERED MUTATION	UNP Q24306
C	136	LEU	-	EXPRESSION TAG	UNP Q24306
C	137	GLU	-	EXPRESSION TAG	UNP Q24306
C	138	HIS	-	EXPRESSION TAG	UNP Q24306
C	139	HIS	-	EXPRESSION TAG	UNP Q24306
C	140	HIS	-	EXPRESSION TAG	UNP Q24306
C	141	HIS	-	EXPRESSION TAG	UNP Q24306
C	142	HIS	-	EXPRESSION TAG	UNP Q24306
C	143	HIS	-	EXPRESSION TAG	UNP Q24306
D	?	-	ALA	DELETION	UNP Q24306
D	?	-	ASP	DELETION	UNP Q24306
D	?	-	LEU	DELETION	UNP Q24306
D	?	-	PRO	DELETION	UNP Q24306
D	?	-	SER	DELETION	UNP Q24306
D	?	-	TYR	DELETION	UNP Q24306
D	?	-	GLY	DELETION	UNP Q24306
D	89	SER	CYS	ENGINEERED MUTATION	UNP Q24306
D	136	LEU	-	EXPRESSION TAG	UNP Q24306
D	137	GLU	-	EXPRESSION TAG	UNP Q24306
D	138	HIS	-	EXPRESSION TAG	UNP Q24306

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Chain	Residue	Modelled	Actual	Comment	Reference
D	139	HIS	-	EXPRESSION TAG	UNP Q24306
D	140	HIS	-	EXPRESSION TAG	UNP Q24306
D	141	HIS	-	EXPRESSION TAG	UNP Q24306
D	142	HIS	-	EXPRESSION TAG	UNP Q24306
D	143	HIS	-	EXPRESSION TAG	UNP Q24306
E	?	-	ALA	DELETION	UNP Q24306
E	?	-	ASP	DELETION	UNP Q24306
E	?	-	LEU	DELETION	UNP Q24306
E	?	-	PRO	DELETION	UNP Q24306
E	?	-	SER	DELETION	UNP Q24306
E	?	-	TYR	DELETION	UNP Q24306
E	?	-	GLY	DELETION	UNP Q24306
E	89	SER	CYS	ENGINEERED MUTATION	UNP Q24306
E	136	LEU	-	EXPRESSION TAG	UNP Q24306
E	137	GLU	-	EXPRESSION TAG	UNP Q24306
E	138	HIS	-	EXPRESSION TAG	UNP Q24306
E	139	HIS	-	EXPRESSION TAG	UNP Q24306
E	140	HIS	-	EXPRESSION TAG	UNP Q24306
E	141	HIS	-	EXPRESSION TAG	UNP Q24306
E	142	HIS	-	EXPRESSION TAG	UNP Q24306
E	143	HIS	-	EXPRESSION TAG	UNP Q24306
F	?	-	ALA	DELETION	UNP Q24306
F	?	-	ASP	DELETION	UNP Q24306
F	?	-	LEU	DELETION	UNP Q24306
F	?	-	PRO	DELETION	UNP Q24306
F	?	-	SER	DELETION	UNP Q24306
F	?	-	TYR	DELETION	UNP Q24306
F	?	-	GLY	DELETION	UNP Q24306
F	89	SER	CYS	ENGINEERED MUTATION	UNP Q24306
F	136	LEU	-	EXPRESSION TAG	UNP Q24306
F	137	GLU	-	EXPRESSION TAG	UNP Q24306
F	138	HIS	-	EXPRESSION TAG	UNP Q24306
F	139	HIS	-	EXPRESSION TAG	UNP Q24306
F	140	HIS	-	EXPRESSION TAG	UNP Q24306
F	141	HIS	-	EXPRESSION TAG	UNP Q24306
F	142	HIS	-	EXPRESSION TAG	UNP Q24306
F	143	HIS	-	EXPRESSION TAG	UNP Q24306

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0

- Molecule 3 is water.

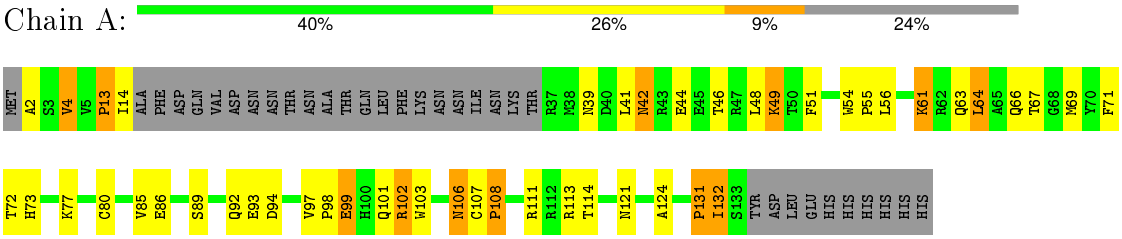
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total O 2 2	0	0
3	B	1	Total O 1 1	0	0
3	F	1	Total O 1 1	0	0

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.

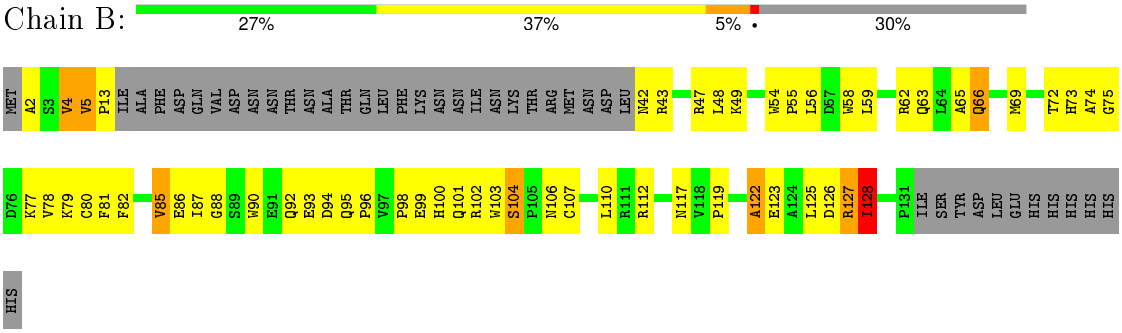
- Molecule 1: Apoptosis 1 inhibitor

Chain A:



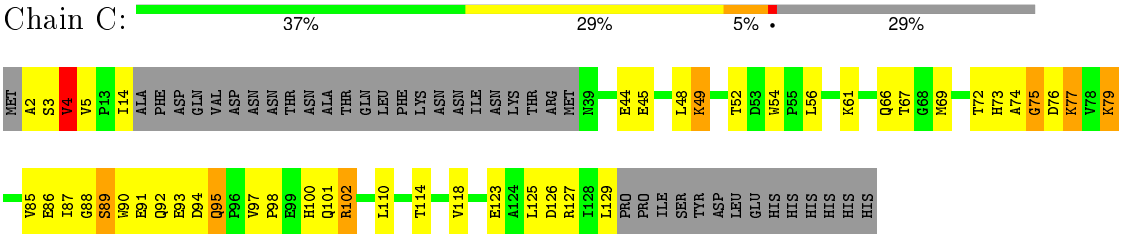
- Molecule 1: Apoptosis 1 inhibitor

Chain B:



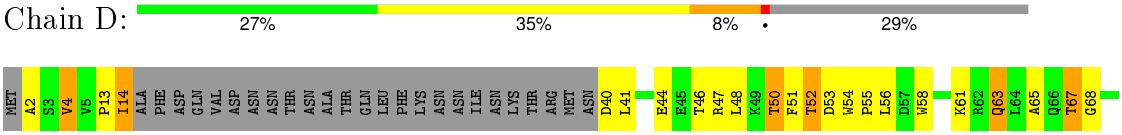
- Molecule 1: Apoptosis 1 inhibitor

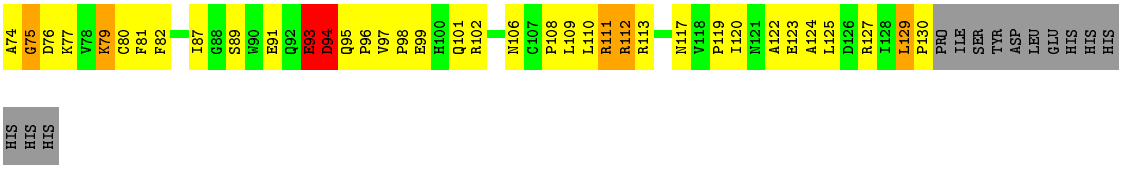
Chain C:



- Molecule 1: Apoptosis 1 inhibitor

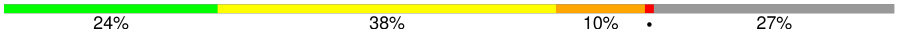
Chain D:

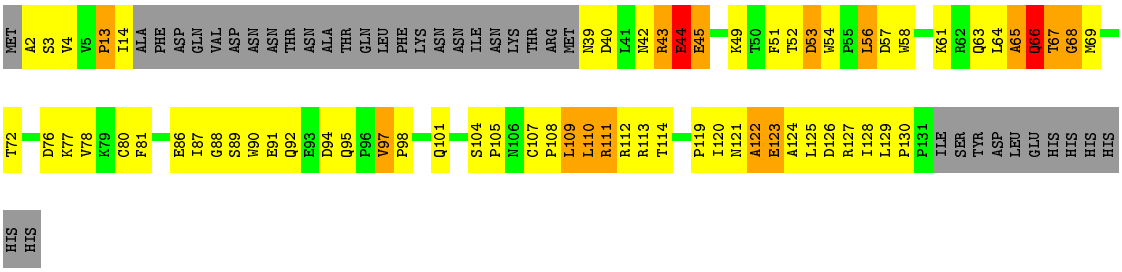




• Molecule 1: Apoptosis 1 inhibitor

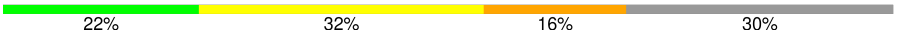
Chain E:

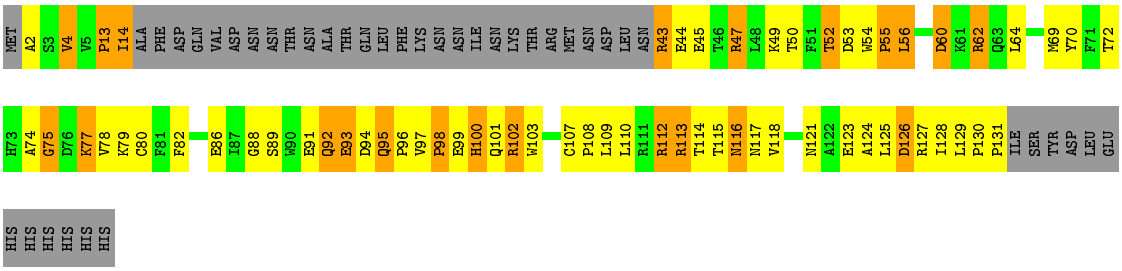




• Molecule 1: Apoptosis 1 inhibitor

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	99.78Å 99.78Å 71.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.98 – 2.40 32.97 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (32.98-2.40) 99.5 (32.97-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.146 , 0.217 0.145 , 0.214	Depositor DCC
R_{free} test set	1622 reflections (5.55%)	DCC
Wilson B-factor (Å^2)	32.8	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 11.1	EDS
Estimated twinning fraction	0.317 for H, K, L 0.182 for -H, H+K, -L 0.305 for -H, -K, L 0.197 for K, H, -L 0.467 for -h,-k,l 0.408 for h,-h-k,-l 0.416 for -k,-h,-l	Xtriage
Reported twinning fraction	0.317 for H, K, L 0.182 for -H, H+K, -L 0.305 for -H, -K, L 0.197 for K, H, -L	Depositor
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.18$	Xtriage
Outliers	0 of 30861 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4806	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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

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	0/856	0.51	0/1166
1	B	0.28	0/798	0.53	0/1087
1	C	0.29	0/814	0.54	0/1107
1	D	0.27	0/817	0.51	0/1112
1	E	0.30	0/842	0.59	0/1148
1	F	0.28	0/801	0.52	0/1091
All	All	0.29	0/4928	0.54	0/6711

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
1	B	0	2
1	C	0	2
1	D	0	1
1	E	0	4
1	F	0	1
All	All	0	11

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	B	128	ILE	Peptide
1	B	5	VAL	Peptide
1	C	127	ARG	Peptide
1	C	4	VAL	Peptide
1	D	4	VAL	Peptide
1	E	13	PRO	Peptide
1	E	44	GLU	Peptide
1	E	68	GLY	Peptide
1	E	72	THR	Mainchain
1	F	55	PRO	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	834	0	796	32	0
1	B	776	0	745	59	0
1	C	794	0	763	44	0
1	D	796	0	768	71	0
1	E	817	0	789	64	0
1	F	779	0	754	61	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	F	1	0	0	0	0
All	All	4806	0	4615	330	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 35.

All (330) 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:D:47:ARG:O	1:D:50:THR:HG22	1.08	1.25
1:C:77:LYS:HE2	1:C:86:GLU:OE2	1.35	1.23
1:C:77:LYS:CE	1:C:86:GLU:OE2	1.91	1.19
1:D:47:ARG:O	1:D:50:THR:CG2	1.92	1.17
1:E:13:PRO:O	1:E:14:ILE:HD12	1.42	1.15
1:F:101:GLN:HB3	1:F:110:LEU:HD13	1.27	1.13
1:D:125:LEU:CD1	1:D:129:LEU:HD12	1.77	1.13
1:F:97:VAL:CG1	1:F:101:GLN:HE21	1.60	1.12
1:D:125:LEU:HD11	1:D:129:LEU:HD12	1.19	1.11
1:D:125:LEU:HD11	1:D:129:LEU:CD1	1.80	1.11
1:B:2:ALA:HB3	1:B:87:ILE:CG2	1.80	1.11
1:B:2:ALA:HB3	1:B:87:ILE:HG22	1.12	1.11
1:B:5:VAL:HG12	1:B:13:PRO:HD2	1.26	1.10
1:C:97:VAL:HB	1:C:98:PRO:HD3	1.32	1.10
1:B:5:VAL:HG12	1:B:13:PRO:CD	1.81	1.08
1:F:97:VAL:HG12	1:F:101:GLN:HE21	1.05	1.07
1:F:74:ALA:HB3	1:F:77:LYS:HD2	1.36	1.06
1:C:95:GLN:HA	1:C:95:GLN:HE21	1.19	1.04
1:F:97:VAL:CG1	1:F:101:GLN:NE2	2.21	1.03
1:F:101:GLN:HB3	1:F:110:LEU:CD1	1.88	1.02
1:E:101:GLN:NE2	1:E:130:PRO:HG3	1.75	1.02
1:E:43:ARG:HG2	1:E:43:ARG:HH11	0.89	1.00
1:E:43:ARG:NH1	1:E:43:ARG:HG2	1.67	0.96
1:D:47:ARG:NH2	1:D:117:ASN:OD1	1.97	0.95
1:D:95:GLN:O	1:D:99:GLU:HB2	1.66	0.95
1:D:13:PRO:O	1:D:14:ILE:HB	1.65	0.94
1:E:44:GLU:OE2	1:E:120:ILE:HG13	1.67	0.94
1:E:44:GLU:CD	1:E:120:ILE:HG13	1.87	0.94
1:D:91:GLU:HB2	1:D:94:ASP:OD1	1.68	0.93
1:B:2:ALA:CB	1:B:87:ILE:HG22	1.98	0.93
1:D:94:ASP:HB3	1:D:99:GLU:HG3	1.48	0.93
1:D:63:GLN:O	1:D:67:THR:HG23	1.67	0.93
1:C:44:GLU:OE2	1:C:66:GLN:HG2	1.72	0.90
1:F:70:TYR:OH	1:F:79:LYS:HE2	1.73	0.89
1:A:99:GLU:OE2	1:A:102:ARG:NH1	2.04	0.89
1:C:97:VAL:HB	1:C:98:PRO:CD	2.02	0.89
1:E:43:ARG:HH11	1:E:43:ARG:CG	1.81	0.87
1:E:45:GLU:O	1:E:49:LYS:HD3	1.73	0.87
1:C:95:GLN:HE21	1:C:95:GLN:CA	1.88	0.87
1:F:43:ARG:HA	1:F:118:VAL:HB	1.57	0.87
1:B:100:HIS:CD2	1:B:110:LEU:HD11	2.09	0.86
1:B:127:ARG:O	1:B:127:ARG:HG3	1.73	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:MET:HE3	1:B:78:VAL:HG23	1.54	0.86
1:B:2:ALA:HB1	1:B:88:GLY:O	1.75	0.86
1:F:97:VAL:HG12	1:F:101:GLN:NE2	1.86	0.84
1:D:91:GLU:OE1	1:D:91:GLU:HA	1.79	0.83
1:E:78:VAL:O	1:E:86:GLU:HB2	1.79	0.83
1:D:50:THR:HG23	1:D:51:PHE:HD1	1.43	0.82
1:B:42:ASN:CB	1:B:81:PHE:CE2	2.64	0.81
1:D:50:THR:HG23	1:D:51:PHE:CD1	2.17	0.80
1:A:97:VAL:HB	1:A:98:PRO:HD3	1.63	0.80
1:E:112:ARG:HH12	1:E:126:ASP:HA	1.47	0.79
1:C:95:GLN:HA	1:C:95:GLN:NE2	1.96	0.79
1:F:70:TYR:HH	1:F:79:LYS:HE2	1.49	0.78
1:E:101:GLN:HE22	1:E:130:PRO:HG3	1.49	0.78
1:E:101:GLN:HB3	1:E:110:LEU:HD12	1.67	0.77
1:E:69:MET:HE2	1:E:80:CYS:HB2	1.66	0.77
1:B:69:MET:CE	1:B:78:VAL:HG23	2.13	0.77
1:B:79:LYS:HA	1:B:85:VAL:O	1.86	0.75
1:E:107:CYS:HB3	1:E:110:LEU:HB2	1.68	0.75
1:D:41:LEU:O	1:D:47:ARG:NH1	2.20	0.75
1:C:77:LYS:NZ	1:C:86:GLU:OE2	2.20	0.75
1:C:123:GLU:O	1:C:123:GLU:HG3	1.87	0.74
1:B:93:GLU:N	1:B:93:GLU:OE2	2.19	0.74
1:F:97:VAL:O	1:F:98:PRO:C	2.26	0.73
1:B:85:VAL:HG22	1:B:86:GLU:H	1.52	0.73
1:F:13:PRO:CA	1:F:14:ILE:HD13	2.18	0.73
1:C:94:ASP:O	1:C:95:GLN:NE2	2.22	0.73
1:B:117:ASN:ND2	1:B:119:PRO:HG3	2.03	0.72
1:D:94:ASP:HB3	1:D:99:GLU:CG	2.19	0.72
1:D:119:PRO:CG	1:D:122:ALA:HB2	2.20	0.72
1:B:117:ASN:O	1:B:119:PRO:HD3	1.90	0.71
1:B:42:ASN:CB	1:B:81:PHE:HE2	2.03	0.71
1:A:72:THR:O	1:A:73:HIS:HB2	1.91	0.70
1:B:42:ASN:CB	1:B:81:PHE:CD2	2.75	0.70
1:F:43:ARG:HH21	1:F:45:GLU:HB3	1.58	0.69
1:F:47:ARG:O	1:F:50:THR:OG1	2.11	0.68
1:B:122:ALA:O	1:B:125:LEU:HB3	1.92	0.68
1:D:48:LEU:HD12	1:D:48:LEU:O	1.93	0.68
1:D:63:GLN:HB3	1:D:96:PRO:HG2	1.75	0.68
1:D:91:GLU:CB	1:D:93:GLU:HG2	2.25	0.67
1:F:113:ARG:HG3	1:F:114:THR:N	2.07	0.67
1:B:5:VAL:CG1	1:B:13:PRO:HD2	2.14	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ILE:HG23	1:B:128:ILE:O	1.94	0.67
1:E:119:PRO:HB3	1:E:125:LEU:HD22	1.76	0.67
1:E:69:MET:CE	1:E:80:CYS:HB2	2.25	0.66
1:F:13:PRO:C	1:F:14:ILE:HD13	2.15	0.66
1:F:72:THR:OG1	1:F:77:LYS:HD3	1.96	0.66
1:B:63:GLN:HG2	1:B:96:PRO:HG2	1.76	0.66
1:D:54:TRP:CZ2	1:D:56:LEU:HD12	2.31	0.66
1:F:125:LEU:O	1:F:125:LEU:HD12	1.96	0.66
1:A:67:THR:HG21	1:A:97:VAL:HG22	1.77	0.66
1:E:39:ASN:O	1:E:40:ASP:HB2	1.96	0.66
1:B:95:GLN:O	1:B:99:GLU:HB2	1.97	0.65
1:E:91:GLU:O	1:E:94:ASP:HB2	1.96	0.65
1:B:5:VAL:HG12	1:B:13:PRO:HD3	1.78	0.65
1:D:124:ALA:HB2	1:D:127:ARG:HH21	1.61	0.65
1:E:42:ASN:HB3	1:E:81:PHE:HE2	1.62	0.65
1:F:13:PRO:HA	1:F:14:ILE:HD13	1.78	0.64
1:E:52:THR:O	1:E:53:ASP:HB2	1.98	0.64
1:D:125:LEU:CD1	1:D:129:LEU:CD1	2.54	0.64
1:E:45:GLU:O	1:E:49:LYS:CD	2.46	0.64
1:D:119:PRO:HG3	1:D:122:ALA:HB2	1.82	0.62
1:D:125:LEU:HD12	1:D:129:LEU:HD12	1.74	0.62
1:F:101:GLN:CB	1:F:110:LEU:HD13	2.18	0.62
1:B:69:MET:HA	1:B:79:LYS:O	1.99	0.62
1:E:63:GLN:O	1:E:67:THR:OG1	2.17	0.62
1:C:97:VAL:CB	1:C:98:PRO:HD3	2.20	0.62
1:D:91:GLU:OE1	1:D:91:GLU:CA	2.48	0.62
1:D:52:THR:O	1:D:53:ASP:HB2	2.00	0.62
1:D:94:ASP:N	1:D:94:ASP:OD1	2.32	0.61
1:E:121:ASN:OD1	1:E:123:GLU:HB3	2.01	0.61
1:E:42:ASN:HB3	1:E:81:PHE:CE2	2.36	0.60
1:B:72:THR:O	1:B:73:HIS:HB2	2.01	0.60
1:B:95:GLN:O	1:B:98:PRO:HD2	2.00	0.60
1:B:79:LYS:HD2	1:B:86:GLU:OE1	2.02	0.59
1:E:44:GLU:OE2	1:E:120:ILE:CG1	2.46	0.59
1:A:108:PRO:HA	1:A:113:ARG:HH11	1.66	0.59
1:D:91:GLU:HB3	1:D:93:GLU:HG2	1.84	0.59
1:C:69:MET:HA	1:C:79:LYS:O	2.02	0.58
1:E:51:PHE:HB3	1:E:61:LYS:HD2	1.84	0.58
1:D:101:GLN:HG3	1:D:110:LEU:HD13	1.84	0.58
1:A:4:VAL:HG22	1:A:86:GLU:O	2.03	0.58
1:D:56:LEU:HD22	1:D:58:TRP:CZ2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2:ALA:HB3	1:F:99:GLU:HG3	1.84	0.57
1:C:102:ARG:NH2	1:D:101:GLN:OE1	2.37	0.57
1:F:2:ALA:HA	1:F:89:SER:O	2.04	0.57
1:F:54:TRP:CE3	1:F:55:PRO:HD2	2.38	0.57
1:F:101:GLN:HB3	1:F:110:LEU:HD12	1.83	0.57
1:A:39:ASN:HB3	1:A:41:LEU:HG	1.87	0.57
1:B:117:ASN:HD21	1:B:119:PRO:HG3	1.67	0.57
1:A:131:PRO:O	1:A:132:ILE:CB	2.53	0.57
1:C:72:THR:HG21	1:C:77:LYS:HD3	1.86	0.57
1:F:70:TYR:OH	1:F:79:LYS:CE	2.49	0.56
1:A:72:THR:O	1:A:73:HIS:CB	2.53	0.56
1:E:95[B]:GLN:HB2	1:E:98:PRO:HD2	1.85	0.56
1:F:74:ALA:CB	1:F:77:LYS:HD2	2.25	0.56
1:A:2:ALA:N	1:A:94:ASP:OD2	2.39	0.56
1:F:69:MET:HA	1:F:79:LYS:O	2.06	0.56
1:C:98:PRO:O	1:C:102:ARG:HB2	2.06	0.55
1:B:112:ARG:NH2	1:B:126:ASP:O	2.40	0.55
1:E:101:GLN:HE22	1:E:130:PRO:CG	2.18	0.55
1:D:2:ALA:N	1:D:94:ASP:OD2	2.40	0.55
1:F:44:GLU:HA	1:F:47:ARG:HG3	1.87	0.55
1:E:2:ALA:HB3	1:E:87:ILE:CG2	2.37	0.55
1:D:94:ASP:CB	1:D:99:GLU:HG3	2.31	0.55
1:C:69:MET:CE	1:C:87:ILE:HD12	2.37	0.55
1:B:93:GLU:CD	1:B:93:GLU:H	2.09	0.55
1:B:63:GLN:CG	1:B:96:PRO:HG2	2.36	0.54
1:F:102:ARG:HG3	1:F:103:TRP:N	2.22	0.54
1:D:54:TRP:NE1	1:D:56:LEU:O	2.40	0.54
1:D:40:ASP:HB3	1:D:46:THR:HG21	1.90	0.54
1:F:80:CYS:SG	1:F:100:HIS:HE1	2.29	0.54
1:B:69:MET:CE	1:B:78:VAL:CG2	2.84	0.54
1:E:78:VAL:O	1:E:86:GLU:CB	2.55	0.54
1:E:122:ALA:O	1:E:123:GLU:C	2.46	0.54
1:B:56:LEU:HD23	1:B:58:TRP:CZ2	2.43	0.53
1:D:63:GLN:O	1:D:67:THR:CG2	2.48	0.53
1:D:119:PRO:HG2	1:D:122:ALA:HB2	1.90	0.53
1:D:54:TRP:CH2	1:D:56:LEU:HD12	2.43	0.53
1:C:54:TRP:HD1	1:C:61:LYS:HZ2	1.55	0.53
1:B:104:SER:C	1:B:106:ASN:H	2.11	0.53
1:B:78:VAL:O	1:B:86:GLU:HA	2.08	0.53
1:A:71:PHE:CE2	1:A:73:HIS:HA	2.43	0.53
1:F:92:GLN:O	1:F:93:GLU:C	2.46	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:128:ILE:O	1:E:128:ILE:HG13	2.08	0.53
1:C:88:GLY:O	1:C:89:SER:HB2	2.08	0.53
1:D:47:ARG:HB3	1:D:65:ALA:HB1	1.90	0.53
1:C:101:GLN:HG3	1:C:101:GLN:O	2.10	0.52
1:E:87:ILE:O	1:E:90:TRP:NE1	2.42	0.52
1:F:123:GLU:O	1:F:126:ASP:N	2.42	0.52
1:E:122:ALA:O	1:E:124:ALA:N	2.42	0.52
1:C:54:TRP:NE1	1:C:56:LEU:O	2.43	0.52
1:D:129:LEU:N	1:D:130:PRO:CD	2.72	0.51
1:E:112:ARG:NH1	1:E:126:ASP:HA	2.22	0.51
1:B:107:CYS:HB3	1:B:110:LEU:HD12	1.92	0.51
1:A:4:VAL:O	1:A:13:PRO:HD3	2.10	0.51
1:D:2:ALA:HB1	1:D:87:ILE:CG2	2.41	0.51
1:A:14:ILE:HG22	1:A:14:ILE:O	2.10	0.51
1:E:109:LEU:O	1:E:112:ARG:N	2.29	0.51
1:D:109:LEU:O	1:D:129:LEU:HD21	2.12	0.50
1:A:54:TRP:CE3	1:A:55:PRO:HD2	2.46	0.50
1:B:55:PRO:HG2	1:B:56:LEU:HD12	1.93	0.50
1:C:118:VAL:HG12	1:C:118:VAL:O	2.11	0.50
1:D:79:LYS:HG3	1:D:80:CYS:N	2.26	0.50
1:F:52:THR:O	1:F:53:ASP:HB2	2.12	0.50
1:D:129:LEU:N	1:D:130:PRO:HD2	2.26	0.49
1:B:80:CYS:SG	1:B:100:HIS:HE1	2.34	0.49
1:A:71:PHE:CZ	1:A:73:HIS:HA	2.46	0.49
1:B:82:PHE:CZ	1:B:117:ASN:HB2	2.47	0.49
1:B:48:LEU:HD13	1:B:62:ARG:HA	1.93	0.49
1:B:65:ALA:O	1:B:66:GLN:C	2.51	0.49
1:B:4:VAL:HG21	1:B:103:TRP:HB3	1.93	0.49
1:F:97:VAL:N	1:F:98:PRO:HD2	2.27	0.49
1:F:43:ARG:NH2	1:F:45:GLU:HB3	2.26	0.49
1:E:109:LEU:O	1:E:111:ARG:N	2.46	0.49
1:E:76:ASP:OD2	1:E:89:SER:N	2.46	0.49
1:C:48:LEU:HD23	1:C:49:LYS:NZ	2.28	0.49
1:E:112:ARG:NH1	1:E:126:ASP:OD1	2.46	0.49
1:C:45:GLU:O	1:C:49:LYS:HE2	2.13	0.49
1:C:90:TRP:O	1:C:91:GLU:HG2	2.13	0.49
1:E:86:GLU:C	1:E:87:ILE:HG13	2.33	0.48
1:B:5:VAL:CG1	1:B:13:PRO:CD	2.73	0.48
1:D:41:LEU:O	1:D:47:ARG:HG3	2.13	0.48
1:C:5:VAL:HB	1:C:86:GLU:HB3	1.94	0.48
1:D:125:LEU:HD11	1:D:129:LEU:HD11	1.86	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ALA:O	1:B:75:GLY:C	2.51	0.48
1:C:69:MET:HE1	1:C:87:ILE:HD12	1.95	0.48
1:F:112:ARG:NH1	1:F:126:ASP:OD1	2.47	0.48
1:F:100:HIS:CG	1:F:110:LEU:HD11	2.49	0.48
1:A:80:CYS:HB3	1:A:85:VAL:HG12	1.95	0.48
1:B:63:GLN:HG2	1:B:96:PRO:CG	2.43	0.48
1:E:65:ALA:O	1:E:66:GLN:C	2.52	0.48
1:C:74:ALA:O	1:C:75:GLY:C	2.52	0.48
1:D:76:ASP:OD2	1:D:89:SER:HA	2.14	0.47
1:C:98:PRO:HA	1:C:101:GLN:HB3	1.95	0.47
1:B:63:GLN:OE1	1:B:96:PRO:HG2	2.14	0.47
1:F:82:PHE:CE2	1:F:109:LEU:HD22	2.49	0.47
1:F:13:PRO:HB2	1:F:14:ILE:H	1.56	0.47
1:D:110:LEU:C	1:D:112:ARG:H	2.17	0.47
1:D:54:TRP:CE3	1:D:55:PRO:HD2	2.50	0.47
1:F:125:LEU:C	1:F:125:LEU:HD12	2.34	0.47
1:A:108:PRO:HA	1:A:113:ARG:NH1	2.29	0.47
1:F:97:VAL:HG13	1:F:101:GLN:NE2	2.22	0.47
1:E:68:GLY:O	1:E:80:CYS:HA	2.15	0.47
1:E:64:LEU:O	1:E:67:THR:N	2.48	0.47
1:B:4:VAL:HG13	1:B:5:VAL:O	2.15	0.46
1:B:42:ASN:CB	1:B:81:PHE:HD2	2.25	0.46
1:F:92:GLN:HA	1:F:92:GLN:HE21	1.80	0.46
1:F:77:LYS:HE2	1:F:86:GLU:OE2	2.15	0.46
1:D:106:ASN:OD1	1:D:113:ARG:NH1	2.45	0.46
1:A:121:ASN:OD1	1:A:121:ASN:C	2.53	0.46
1:C:72:THR:O	1:C:73:HIS:HB2	2.15	0.46
1:E:67:THR:HG21	1:E:97:VAL:HG22	1.97	0.46
1:E:52:THR:O	1:E:53:ASP:CB	2.63	0.46
1:C:5:VAL:O	1:C:5:VAL:HG12	2.15	0.46
1:E:108:PRO:HA	1:E:113:ARG:HB2	1.98	0.46
1:E:95[B]:GLN:CB	1:E:98:PRO:HD2	2.46	0.46
1:C:79:LYS:HD2	1:C:86:GLU:CG	2.46	0.45
1:C:72:THR:HG21	1:C:77:LYS:CD	2.47	0.45
1:C:72:THR:CG2	1:C:77:LYS:HD3	2.46	0.45
1:D:110:LEU:C	1:D:112:ARG:N	2.70	0.45
1:E:64:LEU:O	1:E:65:ALA:C	2.55	0.45
1:F:97:VAL:HG21	1:F:128:ILE:HG22	1.98	0.45
1:D:2:ALA:HB1	1:D:87:ILE:HG23	1.99	0.45
1:C:3:SER:O	1:C:4:VAL:C	2.54	0.45
1:D:41:LEU:HB2	1:D:81:PHE:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:87:ILE:O	1:E:87:ILE:HG22	2.17	0.45
1:F:92:GLN:CA	1:F:92:GLN:HE21	2.30	0.45
1:D:74:ALA:O	1:D:75:GLY:C	2.53	0.45
1:F:107:CYS:HA	1:F:108:PRO:HD2	1.76	0.45
1:E:43:ARG:NH1	1:E:43:ARG:CG	2.51	0.45
1:E:121:ASN:O	1:E:122:ALA:O	2.35	0.45
1:A:46:THR:O	1:A:49:LYS:HB2	2.16	0.45
1:D:44:GLU:HA	1:D:47:ARG:HB2	1.98	0.45
1:D:91:GLU:HB2	1:D:93:GLU:HG2	1.95	0.45
1:F:95:GLN:O	1:F:98:PRO:HG2	2.17	0.44
1:E:2:ALA:N	1:E:94:ASP:OD2	2.51	0.44
1:A:97:VAL:HB	1:A:98:PRO:CD	2.41	0.44
1:D:67:THR:HG21	1:D:96:PRO:HB2	1.99	0.44
1:B:90:TRP:HA	1:B:94:ASP:OD2	2.18	0.44
1:D:82:PHE:CZ	1:D:117:ASN:HB2	2.53	0.44
1:B:95:GLN:HB2	1:B:98:PRO:CG	2.48	0.44
1:F:91:GLU:O	1:F:92:GLN:C	2.54	0.44
1:B:43:ARG:O	1:B:47:ARG:HG3	2.18	0.44
1:E:58:TRP:CZ3	1:E:92:GLN:HA	2.52	0.44
1:D:93:GLU:HB2	1:D:94:ASP:H	1.52	0.44
1:B:85:VAL:HG22	1:B:86:GLU:N	2.26	0.44
1:B:95:GLN:HB2	1:B:98:PRO:HG2	2.00	0.44
1:E:76:ASP:CG	1:E:89:SER:H	2.21	0.44
1:C:101:GLN:O	1:C:101:GLN:CG	2.65	0.43
1:F:74:ALA:O	1:F:75:GLY:C	2.56	0.43
1:D:44:GLU:HG3	1:D:47:ARG:HH21	1.83	0.43
1:F:60:ASP:OD1	1:F:62:ARG:HB2	2.18	0.43
1:C:49:LYS:N	1:C:49:LYS:HD3	2.33	0.43
1:B:69:MET:HE3	1:B:78:VAL:CG2	2.38	0.43
1:E:78:VAL:O	1:E:86:GLU:HA	2.17	0.43
1:A:72:THR:HG23	1:A:77:LYS:O	2.18	0.43
1:D:106:ASN:HA	1:D:111:ARG:HG3	2.00	0.43
1:E:104:SER:HA	1:E:105:PRO:HD2	1.77	0.43
1:A:107:CYS:HA	1:A:108:PRO:HD2	1.76	0.43
1:C:2:ALA:HB1	1:C:88:GLY:O	2.18	0.43
1:F:123:GLU:CG	1:F:127:ARG:HH21	2.32	0.43
1:A:54:TRP:HD1	1:A:61:LYS:HZ2	1.67	0.43
1:E:54:TRP:CE2	1:E:56:LEU:HB2	2.53	0.43
1:E:78:VAL:O	1:E:86:GLU:CA	2.67	0.42
1:A:4:VAL:HG21	1:A:103:TRP:HB3	2.00	0.42
1:A:51:PHE:CD2	1:A:61:LYS:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:TRP:HZ2	1:B:59:LEU:HD23	1.84	0.42
1:C:95:GLN:NE2	1:C:95:GLN:CA	2.60	0.42
1:F:69:MET:HB3	1:F:78:VAL:HB	2.01	0.42
1:C:56:LEU:HD21	1:C:90:TRP:HB2	2.01	0.42
1:D:106:ASN:CG	1:D:113:ARG:HH12	2.22	0.42
1:F:97:VAL:HG11	1:F:101:GLN:NE2	2.22	0.42
1:E:112:ARG:NH2	1:E:129:LEU:HB2	2.34	0.42
1:F:121:ASN:OD1	1:F:124:ALA:N	2.26	0.42
1:F:130:PRO:HA	1:F:131:PRO:HD3	1.90	0.42
1:C:125:LEU:O	1:C:129:LEU:HG	2.19	0.42
1:D:97:VAL:HB	1:D:98:PRO:HD3	2.00	0.42
1:E:121:ASN:O	1:E:122:ALA:C	2.58	0.42
1:A:106:ASN:HA	1:A:111:ARG:HD2	2.02	0.42
1:C:123:GLU:HA	1:C:126:ASP:HB2	2.02	0.41
1:E:54:TRP:CZ2	1:E:56:LEU:HB2	2.54	0.41
1:B:77:LYS:HE2	1:B:77:LYS:HB2	1.81	0.41
1:E:43:ARG:O	1:E:44:GLU:C	2.58	0.41
1:D:108:PRO:HA	1:D:113:ARG:CG	2.50	0.41
1:A:64:LEU:HD23	1:A:69:MET:HG3	2.01	0.41
1:D:93:GLU:CD	1:D:93:GLU:N	2.72	0.41
1:B:63:GLN:O	1:B:66:GLN:HB3	2.20	0.41
1:F:116:ASN:N	1:F:116:ASN:HD22	2.19	0.41
1:B:69:MET:HE2	1:B:78:VAL:CG2	2.50	0.41
1:E:51:PHE:CG	1:E:61:LYS:HB2	2.55	0.41
1:A:48:LEU:O	1:A:51:PHE:HB2	2.21	0.41
1:F:115:THR:C	1:F:117:ASN:H	2.23	0.41
1:E:2:ALA:HB1	1:E:88:GLY:O	2.21	0.41
1:A:107:CYS:O	1:A:108:PRO:C	2.58	0.41
1:C:48:LEU:HD23	1:C:49:LYS:HZ2	1.85	0.41
1:D:76:ASP:CG	1:D:89:SER:H	2.25	0.41
1:D:91:GLU:CB	1:D:94:ASP:OD1	2.55	0.41
1:A:42:ASN:H	1:A:42:ASN:HD22	1.69	0.41
1:A:44:GLU:HG3	1:A:66:GLN:HA	2.03	0.41
1:D:68:GLY:O	1:D:80:CYS:HA	2.21	0.40
1:F:64:LEU:HD13	1:F:78:VAL:HG11	2.02	0.40
1:A:66:GLN:HE22	1:A:124:ALA:HB1	1.86	0.40
1:F:110:LEU:HA	1:F:129:LEU:HD22	2.03	0.40
1:F:88:GLY:O	1:F:89:SER:HB2	2.20	0.40
1:D:81:PHE:O	1:D:81:PHE:CD2	2.74	0.40
1:D:124:ALA:HA	1:D:127:ARG:HE	1.86	0.40
1:F:55:PRO:HG2	1:F:56:LEU:HD13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:THR:O	1:C:100:HIS:CE1	2.75	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	99/136 (73%)	85 (86%)	11 (11%)	3 (3%)	5	4
1	B	91/136 (67%)	75 (82%)	12 (13%)	4 (4%)	3	2
1	C	93/136 (68%)	85 (91%)	6 (6%)	2 (2%)	8	9
1	D	93/136 (68%)	76 (82%)	14 (15%)	3 (3%)	5	4
1	E	96/136 (71%)	69 (72%)	19 (20%)	8 (8%)	1	0
1	F	91/136 (67%)	72 (79%)	11 (12%)	8 (9%)	1	0
All	All	563/816 (69%)	462 (82%)	73 (13%)	28 (5%)	3	1

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	PRO
1	B	123	GLU
1	C	4	VAL
1	D	93	GLU
1	D	94	ASP
1	E	44	GLU
1	E	45	GLU
1	E	65	ALA
1	E	66	GLN
1	E	110	LEU
1	E	122	ALA

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Mol	Chain	Res	Type
1	F	13	PRO
1	F	96	PRO
1	A	132	ILE
1	B	122	ALA
1	B	128	ILE
1	C	75	GLY
1	D	75	GLY
1	E	123	GLU
1	F	100	HIS
1	B	66	GLN
1	E	109	LEU
1	F	93	GLU
1	F	112	ARG
1	F	75	GLY
1	A	108	PRO
1	F	4	VAL
1	F	98	PRO

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	91/125 (73%)	76 (84%)	15 (16%)	3 3
1	B	85/125 (68%)	76 (89%)	9 (11%)	8 12
1	C	87/125 (70%)	72 (83%)	15 (17%)	2 3
1	D	88/125 (70%)	71 (81%)	17 (19%)	2 2
1	E	91/125 (73%)	78 (86%)	13 (14%)	4 4
1	F	86/125 (69%)	69 (80%)	17 (20%)	1 2
All	All	528/750 (70%)	442 (84%)	86 (16%)	3 3

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	VAL

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Mol	Chain	Res	Type
1	A	42	ASN
1	A	49	LYS
1	A	56	LEU
1	A	61	LYS
1	A	63	GLN
1	A	64	LEU
1	A	89	SER
1	A	92	GLN
1	A	93	GLU
1	A	99	GLU
1	A	101	GLN
1	A	102	ARG
1	A	106	ASN
1	A	114	THR
1	B	4	VAL
1	B	49	LYS
1	B	85	VAL
1	B	92	GLN
1	B	101	GLN
1	B	102	ARG
1	B	104	SER
1	B	127	ARG
1	B	128	ILE
1	C	4	VAL
1	C	14	ILE
1	C	49	LYS
1	C	52	THR
1	C	76	ASP
1	C	77	LYS
1	C	79	LYS
1	C	85	VAL
1	C	89	SER
1	C	92	GLN
1	C	93	GLU
1	C	95	GLN
1	C	102	ARG
1	C	110	LEU
1	C	114	THR
1	D	4	VAL
1	D	14	ILE
1	D	50	THR
1	D	52	THR

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Mol	Chain	Res	Type
1	D	61	LYS
1	D	63	GLN
1	D	67	THR
1	D	77	LYS
1	D	79	LYS
1	D	93	GLU
1	D	94	ASP
1	D	102	ARG
1	D	111	ARG
1	D	112	ARG
1	D	120	ILE
1	D	123	GLU
1	D	129	LEU
1	E	3	SER
1	E	4	VAL
1	E	43	ARG
1	E	53	ASP
1	E	56	LEU
1	E	57	ASP
1	E	66	GLN
1	E	67	THR
1	E	77	LYS
1	E	97	VAL
1	E	111	ARG
1	E	114	THR
1	E	127	ARG
1	F	4	VAL
1	F	14	ILE
1	F	43	ARG
1	F	47	ARG
1	F	49	LYS
1	F	52	THR
1	F	56	LEU
1	F	60	ASP
1	F	62	ARG
1	F	77	LYS
1	F	92	GLN
1	F	94	ASP
1	F	95	GLN
1	F	102	ARG
1	F	113	ARG
1	F	116	ASN

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Mol	Chain	Res	Type
1	F	126	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	66	GLN
1	B	73	HIS
1	B	92	GLN
1	B	95	GLN
1	B	100	HIS
1	C	95	GLN
1	D	63	GLN
1	D	121	ASN
1	E	101	GLN
1	F	92	GLN
1	F	101	GLN
1	F	116	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 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

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	103/136 (75%)	-0.57	0	100	100	12, 25, 41, 52	0
1	B	95/136 (69%)	-0.58	0	100	100	19, 31, 42, 50	0
1	C	97/136 (71%)	-0.57	0	100	100	14, 26, 38, 44	0
1	D	97/136 (71%)	-0.61	0	100	100	21, 31, 41, 48	0
1	E	99/136 (72%)	-0.56	0	100	100	11, 27, 42, 53	0
1	F	95/136 (69%)	-0.56	0	100	100	21, 33, 43, 48	0
All	All	586/816 (71%)	-0.57	0	100	100	11, 30, 42, 53	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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
2	ZN	A	200	1/1	1.00	0.14	3.02	28,28,28,28	0
2	ZN	C	200	1/1	1.00	0.13	1.40	29,29,29,29	0
2	ZN	E	200	1/1	1.00	0.13	0.84	28,28,28,28	0
2	ZN	D	200	1/1	1.00	0.12	0.69	40,40,40,40	0
2	ZN	F	200	1/1	1.00	0.11	0.42	35,35,35,35	0
2	ZN	B	200	1/1	0.99	0.12	0.22	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.