Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:02 PM GMT

PDB ID	:	3SJC
Title	:	Crystal structure of S.cerevisiae Get3 in the semi-open state in complex with Get1 cytosolic domain
Authors	:	Reitz, S.; Wild, K.; Sinning, I.
Deposited on	:	2011-06-21
Resolution	:	3.20 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:

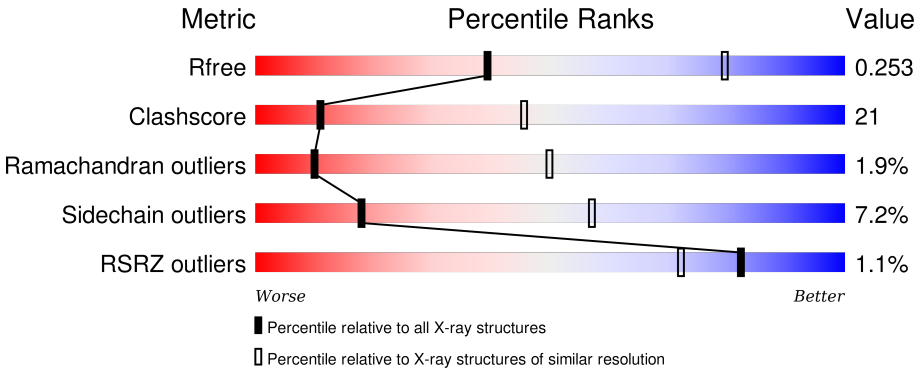
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	362	40% 33% 24%
1	B	362	44% 30% 23%
1	E	362	46% 28% 23%
1	F	362	44% 30% 24%
2	C	65	48% 34% 17%

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Mol	Chain	Length	Quality of chain
2	D	65	52% 29% 17%
2	G	65	3% 52% 29% 17%
2	H	65	58% 23% 17%

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
3	ZN	A	363	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10570 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 ATPase GET3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2180	1382	360	423	15			
1	B	277	Total	C	N	O	S	0	1	0
			2191	1389	363	424	15			
1	E	279	Total	C	N	O	S	0	0	0
			2202	1396	365	426	15			
1	F	276	Total	C	N	O	S	0	1	0
			2183	1384	362	422	15			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	355	LEU	-	EXPRESSION TAG	UNP Q12154
A	356	GLU	-	EXPRESSION TAG	UNP Q12154
A	357	HIS	-	EXPRESSION TAG	UNP Q12154
A	358	HIS	-	EXPRESSION TAG	UNP Q12154
A	359	HIS	-	EXPRESSION TAG	UNP Q12154
A	360	HIS	-	EXPRESSION TAG	UNP Q12154
A	361	HIS	-	EXPRESSION TAG	UNP Q12154
A	362	HIS	-	EXPRESSION TAG	UNP Q12154
B	355	LEU	-	EXPRESSION TAG	UNP Q12154
B	356	GLU	-	EXPRESSION TAG	UNP Q12154
B	357	HIS	-	EXPRESSION TAG	UNP Q12154
B	358	HIS	-	EXPRESSION TAG	UNP Q12154
B	359	HIS	-	EXPRESSION TAG	UNP Q12154
B	360	HIS	-	EXPRESSION TAG	UNP Q12154
B	361	HIS	-	EXPRESSION TAG	UNP Q12154
B	362	HIS	-	EXPRESSION TAG	UNP Q12154
E	355	LEU	-	EXPRESSION TAG	UNP Q12154
E	356	GLU	-	EXPRESSION TAG	UNP Q12154
E	357	HIS	-	EXPRESSION TAG	UNP Q12154
E	358	HIS	-	EXPRESSION TAG	UNP Q12154
E	359	HIS	-	EXPRESSION TAG	UNP Q12154

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Chain	Residue	Modelled	Actual	Comment	Reference
E	360	HIS	-	EXPRESSION TAG	UNP Q12154
E	361	HIS	-	EXPRESSION TAG	UNP Q12154
E	362	HIS	-	EXPRESSION TAG	UNP Q12154
F	355	LEU	-	EXPRESSION TAG	UNP Q12154
F	356	GLU	-	EXPRESSION TAG	UNP Q12154
F	357	HIS	-	EXPRESSION TAG	UNP Q12154
F	358	HIS	-	EXPRESSION TAG	UNP Q12154
F	359	HIS	-	EXPRESSION TAG	UNP Q12154
F	360	HIS	-	EXPRESSION TAG	UNP Q12154
F	361	HIS	-	EXPRESSION TAG	UNP Q12154
F	362	HIS	-	EXPRESSION TAG	UNP Q12154

- Molecule 2 is a protein called Golgi to ER traffic protein 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	54	Total	C	N	O	0	0	0
			453	282	82	89			
2	D	54	Total	C	N	O	0	0	0
			453	282	82	89			
2	G	54	Total	C	N	O	0	0	0
			453	282	82	89			
2	H	54	Total	C	N	O	0	0	0
			453	282	82	89			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	35	MET	-	EXPRESSION TAG	UNP P53192
C	94	HIS	-	EXPRESSION TAG	UNP P53192
C	95	HIS	-	EXPRESSION TAG	UNP P53192
C	96	HIS	-	EXPRESSION TAG	UNP P53192
C	97	HIS	-	EXPRESSION TAG	UNP P53192
C	98	HIS	-	EXPRESSION TAG	UNP P53192
C	99	HIS	-	EXPRESSION TAG	UNP P53192
D	35	MET	-	EXPRESSION TAG	UNP P53192
D	94	HIS	-	EXPRESSION TAG	UNP P53192
D	95	HIS	-	EXPRESSION TAG	UNP P53192
D	96	HIS	-	EXPRESSION TAG	UNP P53192
D	97	HIS	-	EXPRESSION TAG	UNP P53192
D	98	HIS	-	EXPRESSION TAG	UNP P53192
D	99	HIS	-	EXPRESSION TAG	UNP P53192
G	35	MET	-	EXPRESSION TAG	UNP P53192

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Chain	Residue	Modelled	Actual	Comment	Reference
G	94	HIS	-	EXPRESSION TAG	UNP P53192
G	95	HIS	-	EXPRESSION TAG	UNP P53192
G	96	HIS	-	EXPRESSION TAG	UNP P53192
G	97	HIS	-	EXPRESSION TAG	UNP P53192
G	98	HIS	-	EXPRESSION TAG	UNP P53192
G	99	HIS	-	EXPRESSION TAG	UNP P53192
H	35	MET	-	EXPRESSION TAG	UNP P53192
H	94	HIS	-	EXPRESSION TAG	UNP P53192
H	95	HIS	-	EXPRESSION TAG	UNP P53192
H	96	HIS	-	EXPRESSION TAG	UNP P53192
H	97	HIS	-	EXPRESSION TAG	UNP P53192
H	98	HIS	-	EXPRESSION TAG	UNP P53192
H	99	HIS	-	EXPRESSION TAG	UNP P53192

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

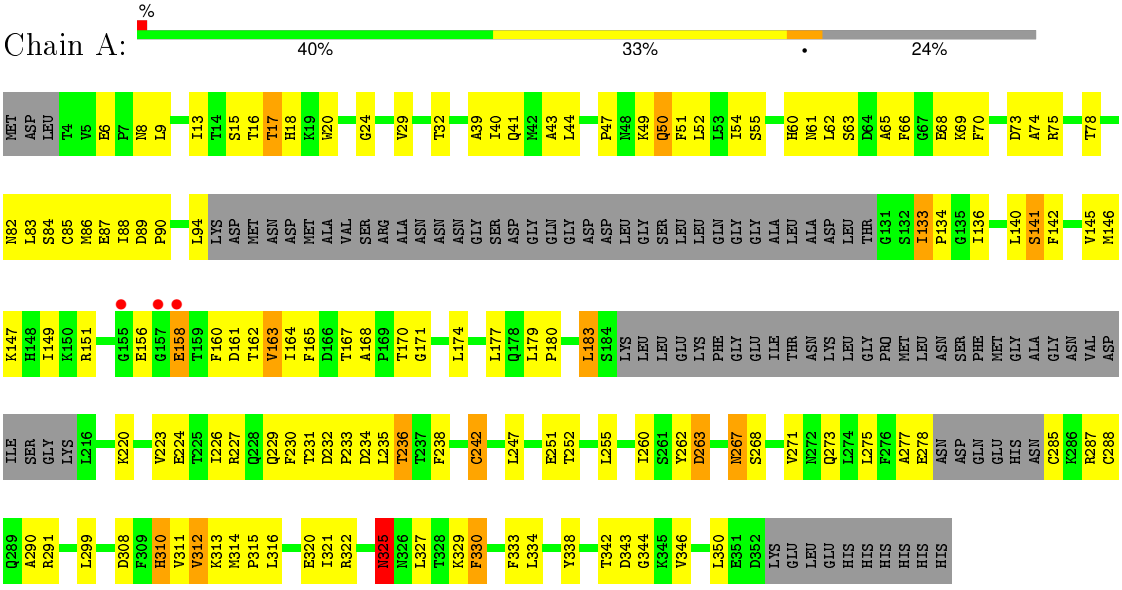
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	E	1	Total Zn 1 1	0	0

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.

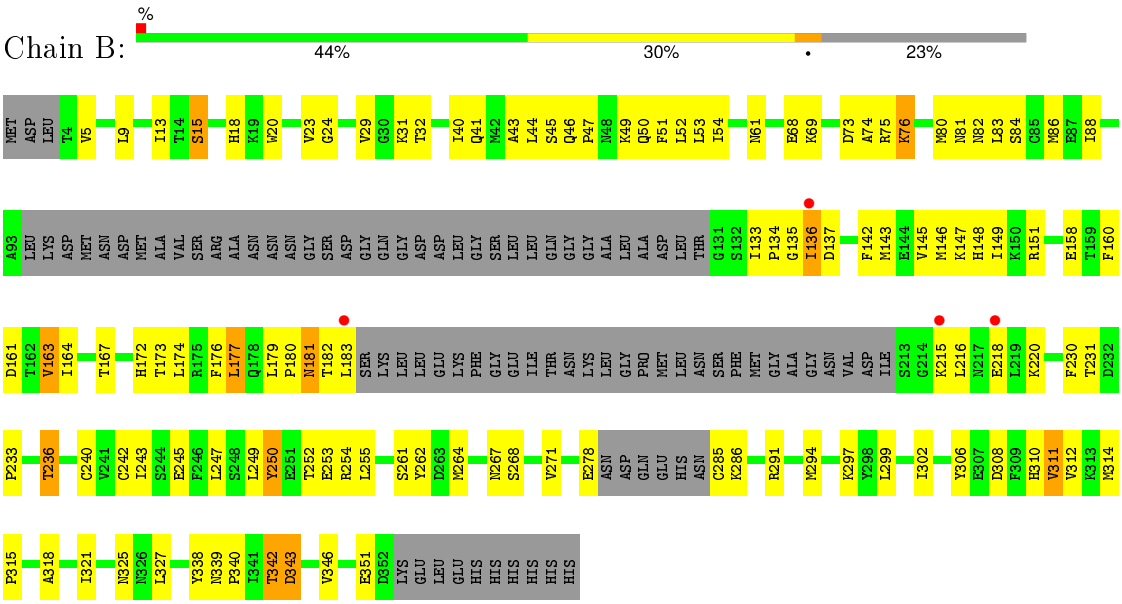
- Molecule 1: ATPase GET3

Chain A:



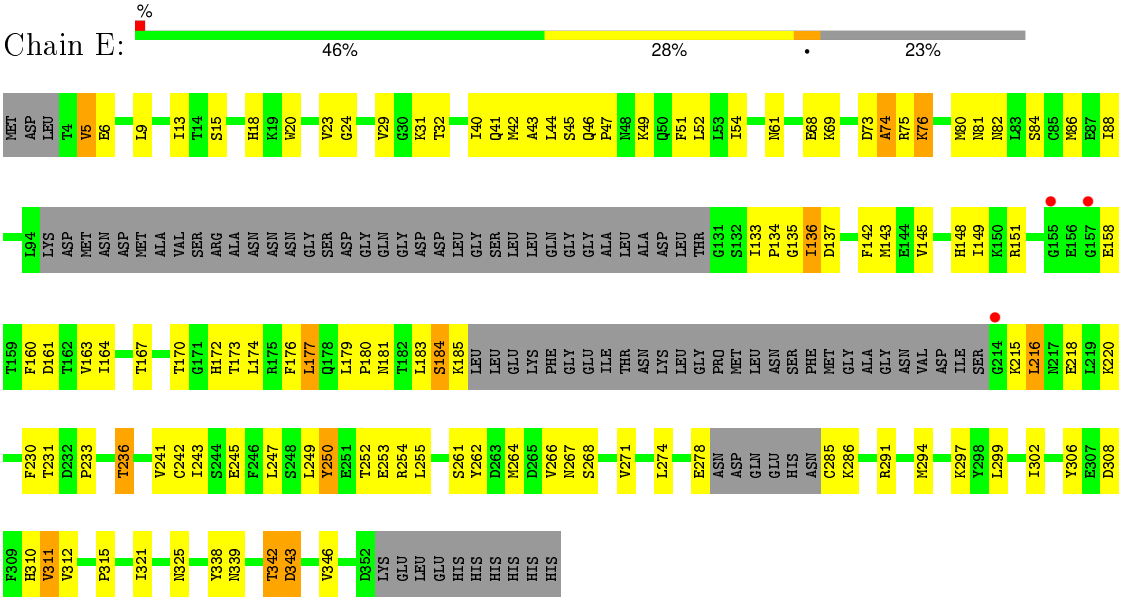
- Molecule 1: ATPase GET3

Chain B:



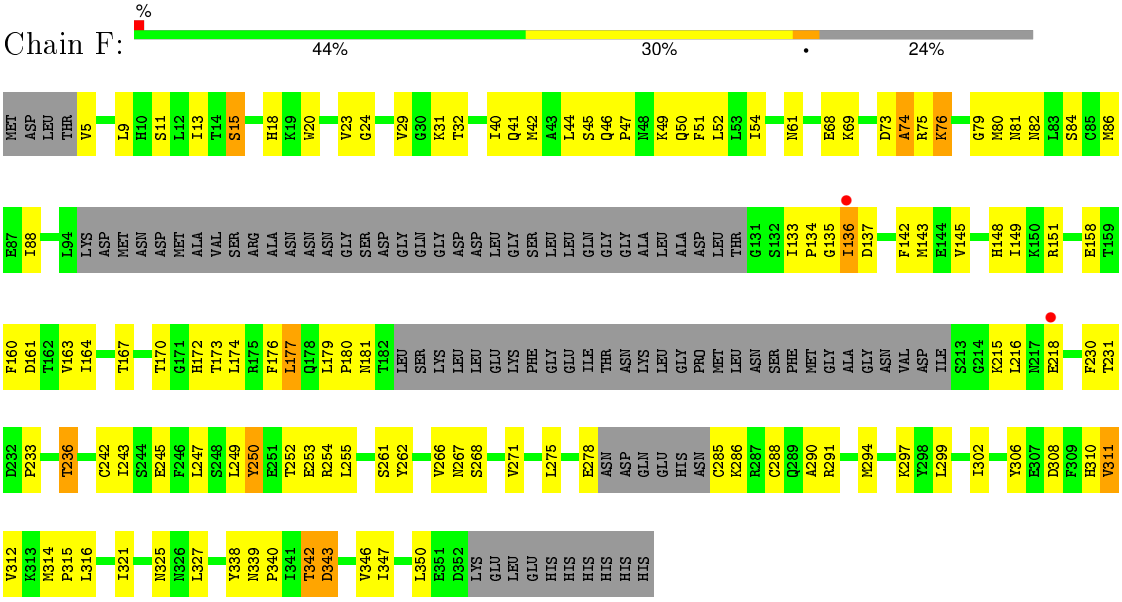
- Molecule 1: ATPase GET3

Chain E:



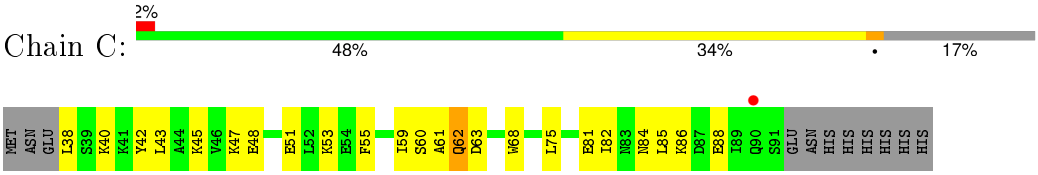
• Molecule 1: ATPase GET3

Chain F:



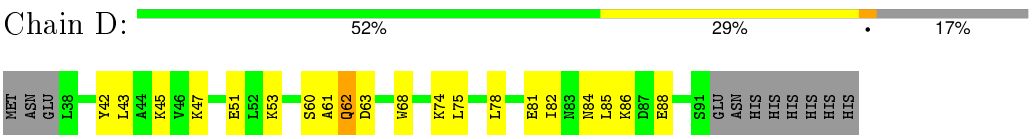
• Molecule 2: Golgi to ER traffic protein 1

Chain C:



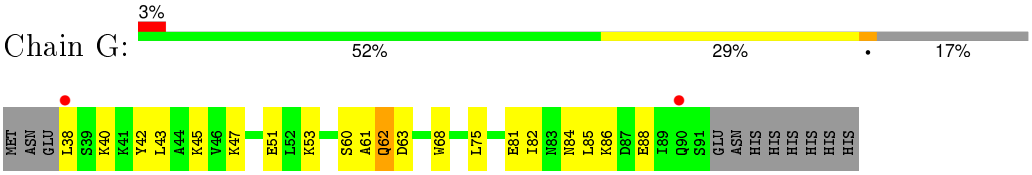
• Molecule 2: Golgi to ER traffic protein 1

Chain D:



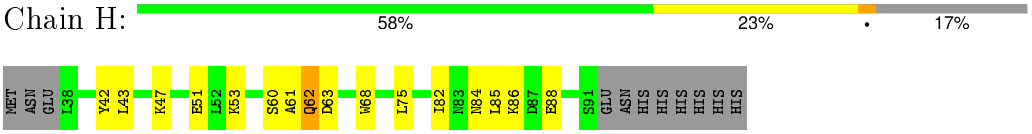
• Molecule 2: Golgi to ER traffic protein 1

Chain G:



• Molecule 2: Golgi to ER traffic protein 1

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.07Å 112.24Å 135.98Å 90.00° 103.82° 90.00°	Depositor
Resolution (Å)	47.44 – 3.20 47.43 – 3.20	Depositor EDS
% Data completeness (in resolution range)	90.8 (47.44-3.20) 90.5 (47.43-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.209 , 0.259 0.201 , 0.253	Depositor DCC
R_{free} test set	1439 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	55.7	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 69.7	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	11 of 31466 reflections (0.035%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10570	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 75.36 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.2821e-06.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.47	0/2217	0.64	0/2992
1	B	0.43	0/2231	0.59	0/3008
1	E	0.45	0/2239	0.58	0/3019
1	F	0.45	0/2224	0.58	0/2998
2	C	0.40	0/458	0.54	0/610
2	D	0.44	0/458	0.53	0/610
2	G	0.50	0/458	0.54	0/610
2	H	0.45	0/458	0.55	0/610
All	All	0.45	0/10743	0.59	0/14457

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2180	0	2161	106	0
1	B	2191	0	2179	101	0
1	E	2202	0	2190	92	0
1	F	2183	0	2169	93	0
2	C	453	0	458	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	453	0	458	17	0
2	G	453	0	458	15	0
2	H	453	0	458	13	0
3	A	1	0	0	0	0
3	E	1	0	0	0	0
All	All	10570	0	10531	442	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 21.

All (442) 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:A:230:PHE:HA	1:A:236:THR:HG21	1.33	1.04
1:E:184:SER:O	1:E:185:LYS:HB2	1.72	0.90
1:E:183:LEU:HD22	1:E:220:LYS:HD2	1.53	0.89
1:A:315:PRO:HG3	1:A:338:TYR:CD1	2.09	0.87
1:B:183:LEU:HD22	1:B:220:LYS:HD2	1.58	0.85
1:A:40:ILE:O	1:A:44:LEU:HD13	1.79	0.83
1:A:70:PHE:CD1	1:A:85:CYS:HB2	2.15	0.81
1:A:285:CYS:N	1:B:285:CYS:HB3	1.96	0.81
1:A:52:LEU:HD12	1:A:84:SER:O	1.80	0.81
1:E:230:PHE:HA	1:E:236:THR:HG21	1.64	0.80
1:F:9:LEU:O	1:F:13:ILE:HG13	1.82	0.80
1:E:9:LEU:O	1:E:13:ILE:HG13	1.82	0.80
1:F:15:SER:OG	1:F:18:HIS:HD2	1.65	0.79
1:F:230:PHE:HA	1:F:236:THR:HG21	1.64	0.78
1:E:15:SER:OG	1:E:18:HIS:HD2	1.66	0.78
1:A:183:LEU:HG	1:A:220:LYS:HD2	1.66	0.77
1:B:230:PHE:HA	1:B:236:THR:HG21	1.66	0.76
1:E:285:CYS:N	1:F:285:CYS:HB3	2.01	0.76
1:E:285:CYS:HB3	1:F:285:CYS:N	2.01	0.76
1:B:29:VAL:HG11	1:B:242:CYS:HA	1.67	0.76
1:B:15:SER:OG	1:B:18:HIS:HD2	1.68	0.76
1:E:231:THR:O	1:E:233:PRO:HD3	1.85	0.75
2:G:62:GLN:H	2:G:62:GLN:NE2	1.85	0.75
1:A:315:PRO:HG3	1:A:338:TYR:CG	2.22	0.73
1:A:88:ILE:HD11	1:A:145:VAL:HG22	1.68	0.73
1:B:9:LEU:O	1:B:13:ILE:HG13	1.90	0.72
1:F:29:VAL:HG11	1:F:242:CYS:HA	1.71	0.72
1:B:231:THR:O	1:B:233:PRO:HD3	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:62:GLN:H	2:C:62:GLN:NE2	1.87	0.71
1:A:262:TYR:O	1:A:263:ASP:HB2	1.90	0.71
1:A:242:CYS:SG	1:A:271:VAL:HG22	2.31	0.70
1:E:145:VAL:O	1:E:149:ILE:HG13	1.91	0.70
2:D:62:GLN:NE2	2:D:62:GLN:H	1.89	0.70
2:D:62:GLN:HE21	2:D:62:GLN:H	1.38	0.70
2:G:62:GLN:H	2:G:62:GLN:HE21	1.40	0.69
1:F:231:THR:O	1:F:233:PRO:HD3	1.91	0.69
1:E:29:VAL:HG11	1:E:242:CYS:HA	1.74	0.69
1:B:145:VAL:O	1:B:149:ILE:HG13	1.91	0.69
1:A:179:LEU:HB3	1:A:180:PRO:HD3	1.74	0.69
1:A:70:PHE:CE1	1:A:85:CYS:HB2	2.29	0.68
1:F:20:TRP:HB2	1:F:236:THR:HB	1.76	0.68
1:E:311:VAL:CG2	1:E:311:VAL:O	2.42	0.68
1:B:315:PRO:HG3	1:B:338:TYR:CD1	2.29	0.68
1:F:135:GLY:HA3	1:F:179:LEU:HD13	1.75	0.68
1:E:20:TRP:HB2	1:E:236:THR:HB	1.75	0.67
1:B:20:TRP:HB2	1:B:236:THR:HB	1.76	0.67
1:B:135:GLY:HA3	1:B:179:LEU:HD13	1.75	0.67
1:E:135:GLY:HA3	1:E:179:LEU:HD13	1.77	0.67
1:E:29:VAL:HG12	1:E:29:VAL:O	1.96	0.66
1:A:52:LEU:HD21	1:A:86:MET:CE	2.25	0.66
1:F:145:VAL:O	1:F:149:ILE:HG13	1.95	0.66
1:A:8:ASN:HA	1:A:312:VAL:HG13	1.77	0.65
1:F:29:VAL:O	1:F:29:VAL:HG12	1.97	0.65
2:C:62:GLN:H	2:C:62:GLN:HE21	1.44	0.65
2:H:62:GLN:H	2:H:62:GLN:NE2	1.95	0.65
2:D:47:LYS:O	2:D:51:GLU:HG3	1.96	0.64
2:G:82:ILE:O	2:G:85:LEU:HB2	1.97	0.64
1:A:163:VAL:HG22	1:A:165:PHE:CE2	2.33	0.64
1:A:164:ILE:HD12	1:A:164:ILE:N	2.13	0.64
1:F:311:VAL:O	1:F:311:VAL:CG2	2.45	0.63
2:H:82:ILE:O	2:H:85:LEU:HB2	1.98	0.63
1:B:29:VAL:HG11	1:B:242:CYS:CA	2.27	0.63
1:F:29:VAL:HG11	1:F:242:CYS:CA	2.28	0.62
1:B:164:ILE:HD12	1:B:164:ILE:N	2.13	0.62
2:D:82:ILE:O	2:D:85:LEU:HB2	1.99	0.62
1:B:311:VAL:O	1:B:311:VAL:CG2	2.46	0.62
2:C:47:LYS:O	2:C:51:GLU:HG3	1.98	0.62
1:E:291:ARG:NH1	1:F:291:ARG:NH1	2.47	0.62
1:F:164:ILE:HD12	1:F:164:ILE:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:LEU:HB2	1:A:87:GLU:OE1	2.00	0.62
1:B:52:LEU:HD22	1:B:160:PHE:CE2	2.35	0.61
1:A:230:PHE:CA	1:A:236:THR:HG21	2.21	0.61
2:C:82:ILE:O	2:C:85:LEU:HB2	2.00	0.61
1:E:29:VAL:HG11	1:E:242:CYS:CA	2.31	0.61
1:E:315:PRO:HG3	1:E:338:TYR:CD1	2.35	0.61
1:E:183:LEU:CD2	1:E:220:LYS:HD2	2.28	0.60
1:F:230:PHE:HA	1:F:236:THR:CG2	2.31	0.60
1:B:29:VAL:O	1:B:29:VAL:HG12	2.02	0.60
2:H:47:LYS:O	2:H:51:GLU:HG3	2.00	0.60
1:E:230:PHE:HA	1:E:236:THR:CG2	2.30	0.60
1:A:24:GLY:HA3	1:A:238:PHE:HZ	1.67	0.60
2:H:62:GLN:H	2:H:62:GLN:HE21	1.48	0.60
1:B:52:LEU:HD21	1:B:86:MET:CE	2.31	0.60
1:E:164:ILE:N	1:E:164:ILE:HD12	2.16	0.59
1:E:52:LEU:HD21	1:E:86:MET:CE	2.32	0.59
1:A:299:LEU:HD22	1:A:313:LYS:HE3	1.84	0.59
2:G:47:LYS:O	2:G:51:GLU:HG3	2.01	0.59
1:F:315:PRO:HG3	1:F:338:TYR:CD1	2.37	0.59
1:F:133:ILE:HG23	1:F:134:PRO:HD2	1.85	0.59
1:A:310:HIS:CD2	1:A:310:HIS:H	2.20	0.59
1:B:230:PHE:HA	1:B:236:THR:CG2	2.33	0.59
1:F:13:ILE:HG21	1:F:41:GLN:HB3	1.84	0.59
1:F:52:LEU:HD21	1:F:86:MET:CE	2.32	0.59
1:A:24:GLY:HA2	1:A:167:THR:OG1	2.03	0.59
1:F:24:GLY:HA2	1:F:31:LYS:NZ	2.18	0.58
1:E:294:MET:O	1:E:297:LYS:HB3	2.03	0.58
1:A:24:GLY:HA3	1:A:238:PHE:CZ	2.38	0.58
1:A:15:SER:OG	1:A:18:HIS:CD2	2.56	0.58
1:B:133:ILE:HG23	1:B:134:PRO:HD2	1.86	0.57
1:B:315:PRO:HG3	1:B:338:TYR:CG	2.39	0.57
1:E:133:ILE:HG23	1:E:134:PRO:HD2	1.86	0.57
1:F:15:SER:OG	1:F:18:HIS:CD2	2.53	0.57
1:A:180:PRO:O	1:A:183:LEU:HB3	2.05	0.57
1:B:13:ILE:HG21	1:B:41:GLN:HB3	1.86	0.57
1:B:183:LEU:HD23	1:B:183:LEU:C	2.26	0.56
1:B:181:ASN:O	1:B:183:LEU:N	2.38	0.56
1:E:13:ILE:HG21	1:E:41:GLN:HB3	1.87	0.56
1:B:24:GLY:HA2	1:B:31:LYS:NZ	2.21	0.56
1:A:321:ILE:O	1:A:321:ILE:HG23	2.06	0.56
1:F:29:VAL:HG13	1:F:243:ILE:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:24:GLY:HA2	1:E:31:LYS:NZ	2.21	0.56
1:B:177:LEU:CD1	1:B:262:TYR:HB3	2.36	0.56
1:A:273:GLN:HA	1:A:316:LEU:HB2	1.87	0.56
1:F:177:LEU:CD1	1:F:262:TYR:HB3	2.36	0.55
1:F:315:PRO:HG3	1:F:338:TYR:CG	2.41	0.55
1:E:15:SER:OG	1:E:18:HIS:CD2	2.55	0.55
1:F:88:ILE:HD11	1:F:145:VAL:HG22	1.88	0.55
1:B:294:MET:O	1:B:297:LYS:HB3	2.07	0.54
1:F:253:GLU:HB2	1:F:306:TYR:OH	2.07	0.54
1:A:142:PHE:O	1:A:145:VAL:HB	2.07	0.54
1:B:69:LYS:O	1:B:75:ARG:NH2	2.41	0.54
1:A:44:LEU:HD12	1:A:44:LEU:N	2.21	0.54
1:A:55:SER:HB2	1:A:62:LEU:HD11	1.89	0.54
1:F:252:THR:O	1:F:255:LEU:HB3	2.06	0.54
1:E:88:ILE:HD11	1:E:145:VAL:HG22	1.90	0.54
1:B:15:SER:OG	1:B:18:HIS:CD2	2.57	0.54
1:A:9:LEU:HG	1:A:312:VAL:HG21	1.90	0.54
1:F:76:LYS:HE3	1:F:81:ASN:O	2.08	0.54
1:B:32:THR:CG2	1:B:61:ASN:HD22	2.22	0.53
1:A:333:PHE:HZ	1:A:346:VAL:HG11	1.73	0.53
1:A:231:THR:O	1:A:233:PRO:HD3	2.07	0.53
1:B:242:CYS:SG	1:B:271:VAL:HG22	2.49	0.53
1:B:88:ILE:HD11	1:B:145:VAL:HG22	1.90	0.53
1:E:315:PRO:HG3	1:E:338:TYR:CG	2.42	0.53
1:E:52:LEU:HD22	1:E:160:PHE:CE2	2.44	0.53
1:B:52:LEU:HD12	1:B:84:SER:O	2.08	0.53
1:A:15:SER:CB	1:A:18:HIS:HD2	2.21	0.53
1:B:76:LYS:HE3	1:B:81:ASN:O	2.09	0.53
1:F:69:LYS:O	1:F:75:ARG:NH2	2.42	0.53
1:B:249:LEU:HD21	1:B:302:ILE:HD11	1.90	0.53
1:F:52:LEU:HD12	1:F:84:SER:O	2.08	0.53
1:E:177:LEU:CD1	1:E:262:TYR:HB3	2.38	0.53
1:B:181:ASN:C	1:B:183:LEU:N	2.62	0.52
1:E:311:VAL:HG23	1:E:311:VAL:O	2.08	0.52
1:F:242:CYS:SG	1:F:271:VAL:HG22	2.49	0.52
1:A:325:ASN:OD1	1:A:329:LYS:HE3	2.08	0.52
1:E:242:CYS:SG	1:E:271:VAL:HG22	2.49	0.52
1:E:249:LEU:HD21	1:E:302:ILE:HD11	1.90	0.52
1:A:32:THR:CG2	1:A:61:ASN:HD22	2.22	0.52
1:A:32:THR:HG23	1:A:61:ASN:HD22	1.75	0.52
1:A:55:SER:HB2	1:A:62:LEU:CD1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:62:GLN:NE2	2:G:62:GLN:N	2.57	0.52
1:F:40:ILE:O	1:F:44:LEU:HD13	2.10	0.52
1:B:54:ILE:CG2	1:B:86:MET:HE3	2.41	0.51
1:F:294:MET:O	1:F:297:LYS:HB3	2.10	0.51
1:A:43:ALA:HA	1:A:51:PHE:CE2	2.45	0.51
1:E:45:SER:O	1:E:46:GLN:HG3	2.10	0.51
1:A:333:PHE:CZ	1:A:346:VAL:HG11	2.45	0.51
2:G:42:TYR:CD2	2:G:43:LEU:HD23	2.45	0.51
1:F:52:LEU:HD22	1:F:160:PHE:CE2	2.45	0.51
1:B:252:THR:O	1:B:255:LEU:HB3	2.09	0.51
1:B:311:VAL:HG23	1:B:311:VAL:O	2.10	0.51
1:B:47:PRO:C	1:B:49:LYS:H	2.13	0.51
1:F:54:ILE:CG2	1:F:86:MET:HE3	2.41	0.51
1:F:172:HIS:CD2	1:F:174:LEU:HB3	2.45	0.51
1:F:311:VAL:O	1:F:311:VAL:HG23	2.10	0.51
1:A:15:SER:OG	1:A:18:HIS:HD2	1.94	0.51
1:A:47:PRO:HA	1:A:82:ASN:ND2	2.26	0.51
1:B:342:THR:OG1	1:B:343:ASP:N	2.41	0.51
1:E:291:ARG:NH1	1:F:291:ARG:HH12	2.09	0.51
1:F:24:GLY:HA2	1:F:31:LYS:HZ2	1.76	0.51
2:D:42:TYR:CD2	2:D:43:LEU:HD23	2.46	0.50
1:E:52:LEU:HD12	1:E:84:SER:O	2.11	0.50
1:B:172:HIS:CD2	1:B:174:LEU:HB3	2.46	0.50
1:B:23:VAL:O	1:B:167:THR:HG23	2.12	0.50
1:A:226:ILE:O	1:A:229:GLN:N	2.42	0.50
1:F:179:LEU:N	1:F:180:PRO:HD2	2.27	0.50
2:C:42:TYR:CD2	2:C:43:LEU:HD23	2.46	0.50
1:B:172:HIS:C	1:B:174:LEU:H	2.15	0.50
1:F:45:SER:O	1:F:46:GLN:HG3	2.11	0.50
1:E:291:ARG:HH12	1:F:291:ARG:NH1	2.09	0.50
1:B:54:ILE:HG21	1:B:86:MET:HE3	1.94	0.50
1:E:76:LYS:HE3	1:E:81:ASN:O	2.12	0.50
1:A:311:VAL:CG2	1:A:311:VAL:O	2.59	0.50
1:E:254:ARG:HH12	1:F:170:THR:HG21	1.77	0.50
1:B:29:VAL:HG13	1:B:243:ILE:HG23	1.93	0.50
1:E:29:VAL:HG13	1:E:243:ILE:HG23	1.94	0.50
1:E:54:ILE:CG2	1:E:86:MET:HE3	2.41	0.50
1:A:60:HIS:HB3	1:A:87:GLU:OE2	2.12	0.50
1:A:156:GLU:HG3	1:A:158:GLU:H	1.76	0.50
2:G:42:TYR:HD2	2:G:43:LEU:HD23	1.76	0.50
1:A:260:ILE:C	1:A:262:TYR:H	2.14	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:THR:O	1:E:255:LEU:HB3	2.11	0.49
1:A:267:ASN:N	1:A:267:ASN:HD22	2.09	0.49
1:A:314:MET:SD	1:A:334:LEU:HD23	2.52	0.49
2:H:42:TYR:CD2	2:H:43:LEU:HD23	2.48	0.49
1:E:54:ILE:HG21	1:E:86:MET:HE3	1.94	0.49
1:F:82:ASN:N	1:F:82:ASN:OD1	2.45	0.49
1:A:82:ASN:N	1:A:82:ASN:OD1	2.45	0.49
2:G:84:ASN:O	2:G:88:GLU:HG3	2.12	0.49
1:B:253:GLU:HB2	1:B:306:TYR:OH	2.13	0.49
1:F:172:HIS:C	1:F:174:LEU:H	2.17	0.49
1:B:82:ASN:N	1:B:82:ASN:OD1	2.46	0.49
1:B:179:LEU:N	1:B:180:PRO:HD2	2.28	0.49
1:E:172:HIS:CD2	1:E:174:LEU:HB3	2.48	0.48
1:F:172:HIS:CD2	1:F:174:LEU:CB	2.96	0.48
1:E:82:ASN:N	1:E:82:ASN:OD1	2.46	0.48
1:A:223:VAL:HG12	1:A:224:GLU:N	2.28	0.48
1:A:52:LEU:HD22	1:A:160:PHE:CE2	2.48	0.48
1:F:47:PRO:C	1:F:49:LYS:H	2.16	0.48
1:B:45:SER:O	1:B:46:GLN:HG3	2.12	0.48
1:B:9:LEU:HG	1:B:312:VAL:HG21	1.96	0.48
1:F:172:HIS:O	1:F:172:HIS:CD2	2.67	0.48
1:E:68:GLU:OE2	1:E:75:ARG:NH1	2.47	0.48
1:F:249:LEU:HD21	1:F:302:ILE:HD11	1.95	0.48
2:C:42:TYR:HD2	2:C:43:LEU:HD23	1.78	0.48
1:A:69:LYS:O	1:A:75:ARG:NH2	2.47	0.48
2:D:42:TYR:HD2	2:D:43:LEU:HD23	1.79	0.48
1:F:54:ILE:HG21	1:F:86:MET:HE3	1.96	0.48
1:F:49:LYS:HA	1:F:161:ASP:OD2	2.14	0.48
2:C:84:ASN:O	2:C:88:GLU:HG3	2.14	0.47
1:A:180:PRO:HB3	1:A:220:LYS:HE2	1.96	0.47
1:E:172:HIS:O	1:E:172:HIS:CD2	2.66	0.47
1:A:65:ALA:O	1:A:322:ARG:HB2	2.14	0.47
1:F:327:LEU:HA	1:F:327:LEU:HD23	1.67	0.47
1:F:9:LEU:HG	1:F:312:VAL:HG21	1.96	0.47
1:E:172:HIS:CD2	1:E:174:LEU:CB	2.98	0.47
1:A:133:ILE:HG23	1:A:134:PRO:HD2	1.96	0.47
1:A:260:ILE:C	1:A:262:TYR:N	2.68	0.47
1:A:320:GLU:HA	1:A:320:GLU:OE1	2.14	0.47
1:A:89:ASP:HA	1:A:90:PRO:HD3	1.75	0.47
1:E:47:PRO:C	1:E:49:LYS:H	2.16	0.47
1:E:179:LEU:N	1:E:180:PRO:HD2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:342:THR:OG1	1:F:343:ASP:N	2.46	0.47
1:B:68:GLU:OE2	1:B:75:ARG:NH1	2.47	0.47
1:B:285:CYS:O	1:B:286:LYS:HD3	2.15	0.47
1:F:68:GLU:OE2	1:F:75:ARG:NH1	2.48	0.47
1:B:172:HIS:O	1:B:172:HIS:CD2	2.67	0.47
1:A:311:VAL:HG22	1:A:311:VAL:O	2.14	0.47
2:G:60:SER:HB3	2:G:63:ASP:HB2	1.97	0.47
1:F:299:LEU:HD23	1:F:299:LEU:HA	1.66	0.47
1:B:142:PHE:O	1:B:143:MET:C	2.53	0.47
1:B:181:ASN:C	1:B:183:LEU:H	2.17	0.47
1:A:32:THR:HG23	1:A:61:ASN:ND2	2.30	0.47
2:D:84:ASN:O	2:D:88:GLU:HG3	2.15	0.47
2:H:84:ASN:O	2:H:88:GLU:HG3	2.15	0.47
1:B:183:LEU:CD2	1:B:220:LYS:HD2	2.36	0.47
1:A:146:MET:O	1:A:147:LYS:C	2.53	0.47
2:D:53:LYS:HA	2:D:75:LEU:HD11	1.97	0.47
1:F:285:CYS:O	1:F:286:LYS:HD3	2.15	0.47
2:H:42:TYR:HD2	2:H:43:LEU:HD23	1.80	0.46
2:H:42:TYR:HA	2:H:85:LEU:HD13	1.98	0.46
1:A:6:GLU:CD	1:A:8:ASN:HD21	2.18	0.46
1:B:172:HIS:CD2	1:B:174:LEU:CB	2.98	0.46
1:E:183:LEU:C	1:E:183:LEU:HD23	2.36	0.46
1:B:31:LYS:NZ	1:B:167:THR:OG1	2.48	0.46
1:B:32:THR:HG23	1:B:61:ASN:ND2	2.31	0.46
1:E:253:GLU:HB2	1:E:306:TYR:OH	2.15	0.46
1:B:321:ILE:HG23	1:B:321:ILE:O	2.16	0.46
1:B:177:LEU:HD11	1:B:262:TYR:HB3	1.98	0.46
1:E:172:HIS:C	1:E:174:LEU:H	2.18	0.46
1:F:142:PHE:O	1:F:143:MET:C	2.54	0.46
1:E:285:CYS:O	1:E:286:LYS:HD3	2.14	0.46
2:D:62:GLN:N	2:D:62:GLN:NE2	2.60	0.46
1:F:31:LYS:NZ	1:F:167:THR:OG1	2.49	0.46
1:E:31:LYS:NZ	1:E:167:THR:OG1	2.48	0.46
1:F:177:LEU:HD11	1:F:262:TYR:HB3	1.98	0.46
1:E:69:LYS:O	1:E:75:ARG:NH2	2.47	0.46
1:E:23:VAL:O	1:E:167:THR:HG23	2.16	0.46
1:A:310:HIS:CD2	1:A:310:HIS:N	2.84	0.46
1:B:32:THR:HG23	1:B:61:ASN:HD22	1.81	0.46
1:E:32:THR:CG2	1:E:61:ASN:HD22	2.28	0.46
1:B:243:ILE:HD12	1:B:245:GLU:CD	2.37	0.46
2:H:53:LYS:HA	2:H:75:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:253:GLU:HB2	1:F:306:TYR:HH	1.81	0.45
1:A:43:ALA:HA	1:A:51:PHE:HE2	1.79	0.45
1:E:142:PHE:O	1:E:143:MET:C	2.54	0.45
2:C:60:SER:HB3	2:C:63:ASP:HB2	1.98	0.45
2:G:42:TYR:HA	2:G:85:LEU:HD13	1.98	0.45
1:E:49:LYS:HA	1:E:161:ASP:OD2	2.16	0.45
1:A:327:LEU:HA	1:A:327:LEU:HD23	1.62	0.45
1:A:44:LEU:CD1	1:A:44:LEU:N	2.79	0.45
1:A:63:SER:N	1:A:87:GLU:OE1	2.47	0.45
1:F:44:LEU:CD1	1:F:80:MET:HE1	2.46	0.45
1:A:350:LEU:HD12	1:A:350:LEU:N	2.31	0.45
1:E:342:THR:OG1	1:E:343:ASP:N	2.49	0.45
2:G:45:LYS:HE3	2:G:81:GLU:OE1	2.15	0.45
1:F:73:ASP:O	1:F:74:ALA:C	2.54	0.45
2:C:42:TYR:HA	2:C:85:LEU:HD13	1.98	0.45
2:H:61:ALA:HB1	2:H:68:TRP:CD2	2.52	0.45
1:B:40:ILE:O	1:B:44:LEU:HD13	2.17	0.45
1:B:148:HIS:HA	1:B:151:ARG:HG3	1.99	0.45
1:E:40:ILE:O	1:E:44:LEU:HD13	2.17	0.45
2:H:60:SER:HB3	2:H:63:ASP:HB2	1.99	0.45
1:E:9:LEU:HG	1:E:312:VAL:HG21	1.99	0.45
2:D:42:TYR:HA	2:D:85:LEU:HD13	1.99	0.45
1:F:32:THR:CG2	1:F:61:ASN:HD22	2.30	0.45
1:B:80:MET:HB3	1:B:80:MET:HE2	1.71	0.45
1:F:243:ILE:HD12	1:F:245:GLU:CD	2.38	0.45
2:G:53:LYS:HA	2:G:75:LEU:HD11	1.98	0.45
1:F:80:MET:HB3	1:F:80:MET:HE2	1.89	0.45
1:E:321:ILE:HG23	1:E:321:ILE:O	2.16	0.44
1:E:170:THR:HG21	1:F:254:ARG:HH12	1.82	0.44
1:A:52:LEU:HD22	1:A:160:PHE:CD2	2.52	0.44
1:B:164:ILE:CD1	1:B:164:ILE:N	2.81	0.44
1:A:47:PRO:C	1:A:49:LYS:H	2.19	0.44
1:E:230:PHE:HD1	1:E:236:THR:HG21	1.83	0.44
1:F:23:VAL:O	1:F:167:THR:HG23	2.18	0.44
1:A:232:ASP:HA	1:A:233:PRO:HD3	1.79	0.44
1:B:215:LYS:O	1:B:218:GLU:HB3	2.17	0.44
1:E:80:MET:HE2	1:E:80:MET:HB3	1.88	0.44
1:A:342:THR:C	1:A:344:GLY:H	2.21	0.44
1:B:49:LYS:HA	1:B:161:ASP:OD2	2.18	0.44
1:A:50:GLN:OE1	1:A:82:ASN:HB3	2.17	0.44
1:E:274:LEU:HD13	1:E:299:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LEU:HA	1:B:174:LEU:HD12	1.56	0.44
1:B:73:ASP:O	1:B:74:ALA:C	2.55	0.44
1:B:24:GLY:HA2	1:B:31:LYS:HZ1	1.82	0.44
1:A:13:ILE:O	1:A:13:ILE:HG22	2.17	0.44
1:E:216:LEU:HA	1:E:216:LEU:HD23	1.82	0.44
2:D:61:ALA:HB1	2:D:68:TRP:CD2	2.53	0.44
1:E:44:LEU:CD1	1:E:80:MET:HE1	2.47	0.44
1:E:250:TYR:C	1:E:250:TYR:CD2	2.89	0.44
1:B:327:LEU:HA	1:B:327:LEU:HD23	1.67	0.44
1:B:299:LEU:HA	1:B:299:LEU:HD23	1.71	0.44
1:A:94:LEU:HD11	1:A:140:LEU:HB3	2.00	0.44
1:E:73:ASP:O	1:E:74:ALA:C	2.56	0.44
1:F:215:LYS:O	1:F:218:GLU:HB3	2.18	0.44
2:C:53:LYS:HA	2:C:75:LEU:HD11	1.98	0.44
1:F:148:HIS:HA	1:F:151:ARG:HG3	2.00	0.44
1:A:17:THR:HB	1:A:234:ASP:O	2.18	0.44
1:B:339:ASN:CG	1:B:342:THR:HG23	2.39	0.43
1:E:44:LEU:HD12	1:E:80:MET:HE1	2.00	0.43
2:D:74:LYS:NZ	2:D:78:LEU:HD21	2.33	0.43
1:E:215:LYS:O	1:E:218:GLU:HB3	2.17	0.43
1:F:250:TYR:C	1:F:250:TYR:CD2	2.91	0.43
1:F:79:GLY:O	1:F:80:MET:HG2	2.19	0.43
1:E:310:HIS:N	1:E:310:HIS:CD2	2.86	0.43
1:A:73:ASP:O	1:A:74:ALA:C	2.55	0.43
1:E:243:ILE:HD12	1:E:245:GLU:CD	2.39	0.43
1:B:53:LEU:HD12	1:B:164:ILE:O	2.19	0.43
1:A:29:VAL:HG12	1:A:29:VAL:O	2.18	0.43
1:A:66:PHE:CE2	1:A:85:CYS:SG	3.11	0.43
1:B:173:THR:O	1:B:176:PHE:HD2	2.02	0.43
2:D:60:SER:HB3	2:D:63:ASP:HB2	2.01	0.43
1:F:339:ASN:CG	1:F:342:THR:HG23	2.39	0.43
1:A:51:PHE:CD1	1:A:162:THR:HB	2.54	0.43
1:F:50:GLN:OE1	1:F:82:ASN:HA	2.19	0.43
1:E:311:VAL:HG22	1:E:311:VAL:O	2.17	0.43
2:C:61:ALA:HB1	2:C:68:TRP:CD2	2.54	0.43
1:E:338:TYR:CG	1:E:339:ASN:N	2.87	0.42
1:A:52:LEU:HD13	1:A:160:PHE:CZ	2.53	0.42
1:F:179:LEU:N	1:F:180:PRO:CD	2.82	0.42
1:B:50:GLN:OE1	1:B:82:ASN:HA	2.19	0.42
1:A:291:ARG:NH1	1:B:291:ARG:NH1	2.67	0.42
1:B:136:ILE:O	1:B:137:ASP:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:MET:HB3	1:E:51:PHE:CZ	2.55	0.42
1:E:148:HIS:HA	1:E:151:ARG:HG3	2.00	0.42
1:A:252:THR:O	1:A:255:LEU:HB3	2.19	0.42
1:F:314:MET:HA	1:F:315:PRO:HD3	1.72	0.42
1:F:338:TYR:CG	1:F:339:ASN:N	2.87	0.42
1:A:50:GLN:OE1	1:A:82:ASN:CB	2.67	0.42
1:F:310:HIS:N	1:F:310:HIS:CD2	2.88	0.42
2:G:61:ALA:HB1	2:G:68:TRP:CD2	2.54	0.42
1:B:240:CYS:SG	1:B:255:LEU:HD23	2.59	0.42
1:E:69:LYS:HG3	1:E:69:LYS:O	2.19	0.42
1:B:43:ALA:HA	1:B:51:PHE:CE2	2.55	0.42
1:F:173:THR:O	1:F:176:PHE:HD2	2.03	0.42
1:A:20:TRP:HB2	1:A:236:THR:HB	2.01	0.42
2:H:85:LEU:O	2:H:86:LYS:C	2.58	0.42
1:F:44:LEU:N	1:F:44:LEU:HD12	2.35	0.42
1:A:229:GLN:HG2	1:A:235:LEU:HD13	2.01	0.42
1:E:179:LEU:HB3	1:E:180:PRO:HD3	2.02	0.42
1:E:24:GLY:HA2	1:E:31:LYS:HZ1	1.82	0.42
1:A:330:PHE:HB2	1:A:350:LEU:CD2	2.50	0.42
1:B:339:ASN:HA	1:B:340:PRO:HD3	1.74	0.42
1:B:338:TYR:CG	1:B:339:ASN:N	2.87	0.42
2:C:85:LEU:O	2:C:86:LYS:C	2.58	0.42
1:A:299:LEU:HD23	1:A:299:LEU:HA	1.74	0.42
1:E:177:LEU:HD11	1:E:262:TYR:HB3	2.02	0.42
1:B:310:HIS:CD2	1:B:310:HIS:N	2.88	0.42
1:B:250:TYR:C	1:B:250:TYR:CD2	2.91	0.42
1:B:314:MET:HA	1:B:315:PRO:HD3	1.69	0.41
1:F:339:ASN:HA	1:F:340:PRO:HD3	1.73	0.41
1:A:226:ILE:HD13	1:A:226:ILE:HA	1.82	0.41
1:E:299:LEU:HA	1:E:299:LEU:HD23	1.69	0.41
1:A:140:LEU:HD22	1:A:140:LEU:H	1.85	0.41
1:F:42:MET:HB3	1:F:51:PHE:CZ	2.55	0.41
1:A:145:VAL:O	1:A:149:ILE:HG13	2.21	0.41
1:B:179:LEU:HB3	1:B:180:PRO:HD3	2.02	0.41
2:G:85:LEU:O	2:G:86:LYS:C	2.58	0.41
1:E:32:THR:HG23	1:E:61:ASN:ND2	2.35	0.41
1:F:136:ILE:O	1:F:137:ASP:C	2.59	0.41
1:A:49:LYS:HA	1:A:161:ASP:OD2	2.21	0.41
1:A:170:THR:HG21	1:B:254:ARG:HH12	1.85	0.41
2:D:45:LYS:HE3	2:D:81:GLU:OE1	2.19	0.41
1:E:29:VAL:HG12	1:E:241:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ASN:OD1	1:B:81:ASN:N	2.53	0.41
1:F:288:CYS:C	1:F:290:ALA:H	2.23	0.41
1:B:146:MET:O	1:B:147:LYS:C	2.59	0.41
1:F:179:LEU:HB3	1:F:180:PRO:HD3	2.02	0.41
1:E:5:VAL:O	1:E:6:GLU:C	2.58	0.41
1:F:347:ILE:HA	1:F:347:ILE:HD13	1.80	0.41
2:C:45:LYS:O	2:C:48:GLU:N	2.54	0.41
1:A:68:GLU:OE2	1:A:75:ARG:NH1	2.53	0.41
1:F:275:LEU:HD11	1:F:316:LEU:HD22	2.02	0.41
2:D:85:LEU:O	2:D:86:LYS:C	2.58	0.41
1:A:50:GLN:OE1	1:A:50:GLN:HA	2.20	0.41
1:F:321:ILE:HG23	1:F:321:ILE:O	2.21	0.41
1:B:242:CYS:O	1:B:271:VAL:HA	2.21	0.41
1:F:311:VAL:O	1:F:311:VAL:HG22	2.20	0.41
1:F:81:ASN:OD1	1:F:81:ASN:N	2.54	0.41
1:B:50:GLN:OE1	1:B:82:ASN:CB	2.69	0.41
1:A:147:LYS:O	1:A:151:ARG:HG3	2.19	0.41
1:A:330:PHE:CD2	1:A:330:PHE:C	2.94	0.41
1:E:43:ALA:HA	1:E:51:PHE:CE2	2.56	0.41
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.68	0.41
1:A:39:ALA:HB1	1:A:83:LEU:HD11	2.02	0.41
1:B:230:PHE:HD1	1:B:236:THR:HG21	1.86	0.41
2:H:62:GLN:N	2:H:62:GLN:NE2	2.66	0.41
1:B:69:LYS:HG3	1:B:69:LYS:O	2.21	0.41
1:F:44:LEU:HD12	1:F:80:MET:HE1	2.03	0.41
2:D:53:LYS:HD2	2:D:75:LEU:CD1	2.51	0.41
2:C:45:LYS:HE3	2:C:81:GLU:OE1	2.20	0.41
2:C:38:LEU:C	2:C:40:LYS:N	2.74	0.41
1:B:179:LEU:N	1:B:180:PRO:CD	2.83	0.40
1:F:350:LEU:HD12	1:F:350:LEU:N	2.37	0.40
2:C:55:PHE:O	2:C:59:ILE:HD13	2.20	0.40
1:E:310:HIS:CD2	1:E:310:HIS:H	2.38	0.40
2:G:38:LEU:C	2:G:40:LYS:N	2.75	0.40
1:E:136:ILE:O	1:E:137:ASP:C	2.59	0.40
1:A:288:CYS:C	1:A:290:ALA:H	2.25	0.40
1:E:173:THR:O	1:E:176:PHE:HD2	2.05	0.40
1:B:318:ALA:H	1:B:351:GLU:HG2	1.85	0.40
1:B:40:ILE:HA	1:B:83:LEU:HD22	2.03	0.40
1:A:333:PHE:HB3	1:A:338:TYR:HB2	2.01	0.40
2:D:62:GLN:N	2:D:62:GLN:HE21	2.12	0.40
1:B:163:VAL:C	1:B:164:ILE:HD12	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LEU:HB2	1:B:160:PHE:CD1	2.57	0.40
1:A:285:CYS:HB3	1:B:285:CYS:N	2.36	0.40
1:A:235:LEU:HA	1:A:235:LEU:HD23	1.87	0.40
1:A:168:ALA:HB3	1:A:171:GLY:O	2.22	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	268/362 (74%)	222 (83%)	39 (15%)	7 (3%)	7	40
1	B	270/362 (75%)	221 (82%)	43 (16%)	6 (2%)	8	45
1	E	271/362 (75%)	224 (83%)	41 (15%)	6 (2%)	8	45
1	F	269/362 (74%)	223 (83%)	40 (15%)	6 (2%)	8	45
2	C	52/65 (80%)	46 (88%)	6 (12%)	0	100	100
2	D	52/65 (80%)	47 (90%)	5 (10%)	0	100	100
2	G	52/65 (80%)	46 (88%)	6 (12%)	0	100	100
2	H	52/65 (80%)	47 (90%)	5 (10%)	0	100	100
All	All	1286/1708 (75%)	1076 (84%)	185 (14%)	25 (2%)	10	50

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	343	ASP
1	B	136	ILE
1	B	325	ASN
1	B	343	ASP
1	E	184	SER
1	E	343	ASP

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Mol	Chain	Res	Type
1	F	136	ILE
1	F	343	ASP
1	A	277	ALA
1	B	182	THR
1	E	136	ILE
1	F	181	ASN
1	F	325	ASN
1	A	136	ILE
1	A	141	SER
1	A	183	LEU
1	A	263	ASP
1	B	181	ASN
1	E	181	ASN
1	E	325	ASN
1	A	325	ASN
1	B	15	SER
1	E	74	ALA
1	F	74	ALA
1	F	15	SER

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	247/317 (78%)	221 (90%)	26 (10%)	8 35
1	B	248/317 (78%)	230 (93%)	18 (7%)	17 57
1	E	249/317 (78%)	230 (92%)	19 (8%)	16 55
1	F	247/317 (78%)	228 (92%)	19 (8%)	16 54
2	C	51/62 (82%)	50 (98%)	1 (2%)	63 88
2	D	51/62 (82%)	50 (98%)	1 (2%)	63 88
2	G	51/62 (82%)	50 (98%)	1 (2%)	63 88
2	H	51/62 (82%)	50 (98%)	1 (2%)	63 88
All	All	1195/1516 (79%)	1109 (93%)	86 (7%)	18 57

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

Mol	Chain	Res	Type
1	A	16	THR
1	A	17	THR
1	A	41	GLN
1	A	50	GLN
1	A	54	ILE
1	A	78	THR
1	A	133	ILE
1	A	141	SER
1	A	158	GLU
1	A	163	VAL
1	A	174	LEU
1	A	227	ARG
1	A	236	THR
1	A	242	CYS
1	A	247	LEU
1	A	251	GLU
1	A	267	ASN
1	A	268	SER
1	A	275	LEU
1	A	278	GLU
1	A	287	ARG
1	A	308	ASP
1	A	310	HIS
1	A	312	VAL
1	A	325	ASN
1	A	330	PHE
1	B	5	VAL
1	B	76	LYS
1	B	158	GLU
1	B	163	VAL
1	B	177	LEU
1	B	216	LEU
1	B	236	THR
1	B	247	LEU
1	B	250	TYR
1	B	261	SER
1	B	264	MET
1	B	267	ASN
1	B	268	SER
1	B	278	GLU
1	B	308	ASP
1	B	311	VAL

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Mol	Chain	Res	Type
1	B	342	THR
1	B	346	VAL
2	C	62	GLN
2	D	62	GLN
1	E	5	VAL
1	E	76	LYS
1	E	158	GLU
1	E	163	VAL
1	E	177	LEU
1	E	216	LEU
1	E	236	THR
1	E	247	LEU
1	E	250	TYR
1	E	261	SER
1	E	264	MET
1	E	266	VAL
1	E	267	ASN
1	E	268	SER
1	E	278	GLU
1	E	308	ASP
1	E	311	VAL
1	E	342	THR
1	E	346	VAL
1	F	5	VAL
1	F	11	SER
1	F	76	LYS
1	F	158	GLU
1	F	163	VAL
1	F	177	LEU
1	F	216	LEU
1	F	236	THR
1	F	247	LEU
1	F	250	TYR
1	F	261	SER
1	F	266	VAL
1	F	267	ASN
1	F	268	SER
1	F	278	GLU
1	F	308	ASP
1	F	311	VAL
1	F	342	THR
1	F	346	VAL

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Mol	Chain	Res	Type
2	G	62	GLN
2	H	62	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	41	GLN
1	A	222	ASN
1	A	267	ASN
1	A	310	HIS
1	B	18	HIS
1	B	41	GLN
1	B	310	HIS
2	C	62	GLN
2	D	62	GLN
1	E	18	HIS
1	E	41	GLN
1	E	310	HIS
1	F	18	HIS
1	F	41	GLN
1	F	310	HIS
2	G	62	GLN
2	H	62	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 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	276/362 (76%)	-0.62	3 (1%) 82 72	19, 55, 153, 210	0
1	B	277/362 (76%)	-0.49	4 (1%) 78 65	18, 59, 203, 254	0
1	E	279/362 (77%)	-0.52	3 (1%) 82 72	41, 67, 206, 256	0
1	F	276/362 (76%)	-0.47	2 (0%) 89 83	39, 67, 214, 264	0
2	C	54/65 (83%)	-0.35	1 (1%) 70 55	21, 66, 172, 225	0
2	D	54/65 (83%)	-0.42	0 100 100	22, 67, 162, 214	0
2	G	54/65 (83%)	-0.22	2 (3%) 45 30	41, 74, 169, 221	0
2	H	54/65 (83%)	-0.40	0 100 100	42, 78, 171, 217	0
All	All	1324/1708 (77%)	-0.49	15 (1%) 82 72	18, 64, 196, 264	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	157	GLY	3.9
1	A	157	GLY	3.6
2	G	90	GLN	3.5
1	E	155	GLY	2.5
2	G	38	LEU	2.5
1	B	215	LYS	2.5
1	E	214	GLY	2.3
1	B	183	LEU	2.3
1	A	155	GLY	2.2
1	F	218	GLU	2.2
2	C	90	GLN	2.1
1	A	158	GLU	2.1
1	B	218	GLU	2.1
1	B	136	ILE	2.0
1	F	136	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	ZN	A	363	1/1	0.94	0.31	3.20	193,193,193,193	0
3	ZN	E	363	1/1	0.91	0.18	-	223,223,223,223	0

6.5 Other polymers (i)

There are no such residues in this entry.