



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:12 AM GMT

PDB ID : 2W8I
Title : CRYSTAL STRUCTURE OF WZA24-345.
Authors : Hagelueken, G.; Ingledew, W.J.; Huang, H.; Petrovic-Stojanovska, B.; Whitfield, C.; Elmkami, H.; Schiemann, O.; Naismith, J.H.
Deposited on : 2009-01-16
Resolution : 3.00 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

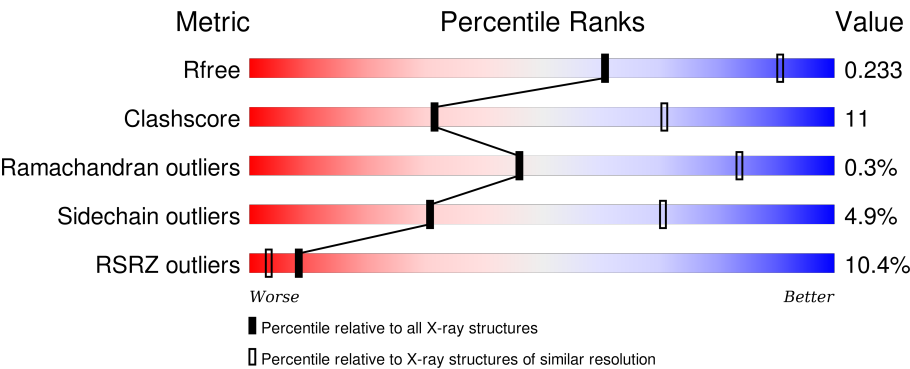
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 $\leq 5\%$. 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	329	<div><div>10%</div><div>74%</div><div>23%</div><div>..</div></div>
1	B	329	<div><div>11%</div><div>73%</div><div>23%</div><div>..</div></div>
1	C	329	<div><div>9%</div><div>71%</div><div>25%</div><div>..</div></div>
1	D	329	<div><div>10%</div><div>71%</div><div>24%</div><div>..</div></div>
1	E	329	<div><div>9%</div><div>72%</div><div>24%</div><div>..</div></div>

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Mol	Chain	Length	Quality of chain
1	F	329	<div><div></div><div>10%</div><div></div><div>71%</div><div></div><div>25%</div><div></div><div>• •</div></div>
1	G	329	<div><div></div><div>11%</div><div></div><div>73%</div><div></div><div>23%</div><div></div><div>• •</div></div>
1	H	329	<div><div></div><div>11%</div><div></div><div>71%</div><div></div><div>25%</div><div></div><div>• •</div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 19792 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 PUTATIVE OUTER MEMBRANE LIPOPROTEIN WZA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2474	1558	419	488	9			
1	B	322	Total	C	N	O	S	0	0	0
			2474	1558	419	488	9			
1	C	322	Total	C	N	O	S	0	0	0
			2474	1558	419	488	9			
1	D	322	Total	C	N	O	S	0	0	0
			2474	1558	419	488	9			
1	E	322	Total	C	N	O	S	0	0	0
			2474	1558	419	488	9			
1	F	322	Total	C	N	O	S	0	0	0
			2474	1558	419	488	9			
1	G	322	Total	C	N	O	S	0	0	0
			2474	1558	419	488	9			
1	H	322	Total	C	N	O	S	0	0	0
			2474	1558	419	488	9			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLY	-	EXPRESSION TAG	UNP Q9X4B7
A	18	ALA	-	EXPRESSION TAG	UNP Q9X4B7
A	19	MET	-	EXPRESSION TAG	UNP Q9X4B7
A	20	VAL	-	EXPRESSION TAG	UNP Q9X4B7
A	21	PRO	-	EXPRESSION TAG	UNP Q9X4B7
B	17	GLY	-	EXPRESSION TAG	UNP Q9X4B7
B	18	ALA	-	EXPRESSION TAG	UNP Q9X4B7
B	19	MET	-	EXPRESSION TAG	UNP Q9X4B7
B	20	VAL	-	EXPRESSION TAG	UNP Q9X4B7
B	21	PRO	-	EXPRESSION TAG	UNP Q9X4B7
C	17	GLY	-	EXPRESSION TAG	UNP Q9X4B7
C	18	ALA	-	EXPRESSION TAG	UNP Q9X4B7
C	19	MET	-	EXPRESSION TAG	UNP Q9X4B7

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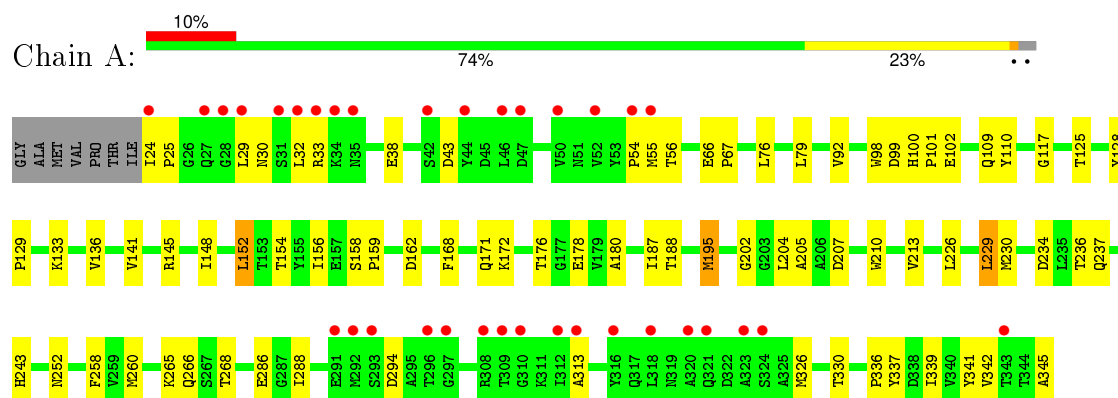
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Chain	Residue	Modelled	Actual	Comment	Reference
C	20	VAL	-	EXPRESSION TAG	UNP Q9X4B7
C	21	PRO	-	EXPRESSION TAG	UNP Q9X4B7
D	17	GLY	-	EXPRESSION TAG	UNP Q9X4B7
D	18	ALA	-	EXPRESSION TAG	UNP Q9X4B7
D	19	MET	-	EXPRESSION TAG	UNP Q9X4B7
D	20	VAL	-	EXPRESSION TAG	UNP Q9X4B7
D	21	PRO	-	EXPRESSION TAG	UNP Q9X4B7
E	17	GLY	-	EXPRESSION TAG	UNP Q9X4B7
E	18	ALA	-	EXPRESSION TAG	UNP Q9X4B7
E	19	MET	-	EXPRESSION TAG	UNP Q9X4B7
E	20	VAL	-	EXPRESSION TAG	UNP Q9X4B7
E	21	PRO	-	EXPRESSION TAG	UNP Q9X4B7
F	17	GLY	-	EXPRESSION TAG	UNP Q9X4B7
F	18	ALA	-	EXPRESSION TAG	UNP Q9X4B7
F	19	MET	-	EXPRESSION TAG	UNP Q9X4B7
F	20	VAL	-	EXPRESSION TAG	UNP Q9X4B7
F	21	PRO	-	EXPRESSION TAG	UNP Q9X4B7
G	17	GLY	-	EXPRESSION TAG	UNP Q9X4B7
G	18	ALA	-	EXPRESSION TAG	UNP Q9X4B7
G	19	MET	-	EXPRESSION TAG	UNP Q9X4B7
G	20	VAL	-	EXPRESSION TAG	UNP Q9X4B7
G	21	PRO	-	EXPRESSION TAG	UNP Q9X4B7
H	17	GLY	-	EXPRESSION TAG	UNP Q9X4B7
H	18	ALA	-	EXPRESSION TAG	UNP Q9X4B7
H	19	MET	-	EXPRESSION TAG	UNP Q9X4B7
H	20	VAL	-	EXPRESSION TAG	UNP Q9X4B7
H	21	PRO	-	EXPRESSION TAG	UNP Q9X4B7

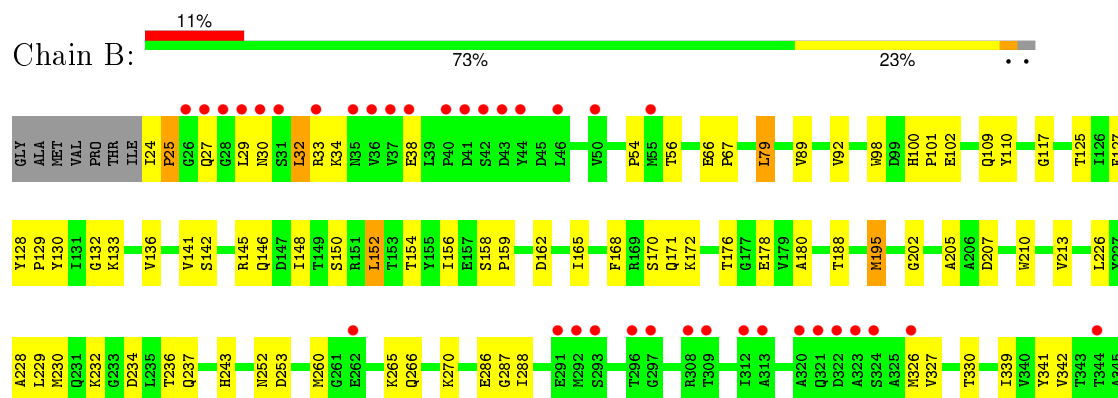
3 Residue-property plots [i](#)

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.

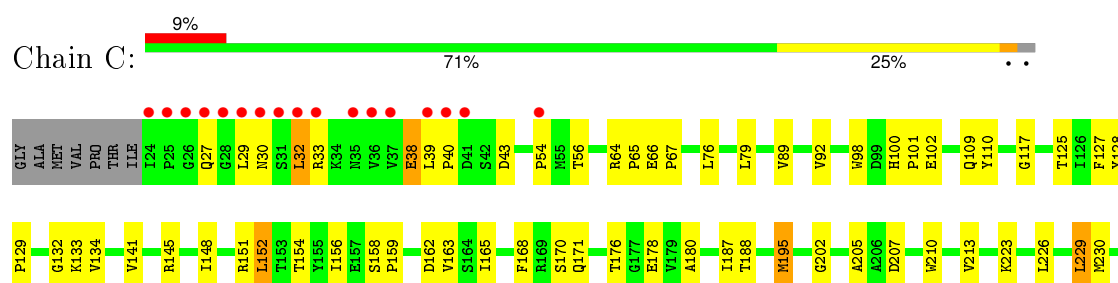
• Molecule 1: PUTATIVE OUTER MEMBRANE LIPOPROTEIN WZA

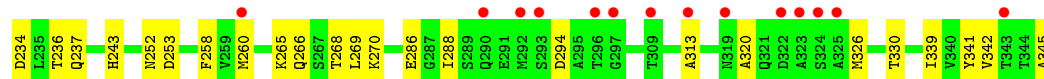


• Molecule 1: PUTATIVE OUTER MEMBRANE LIPOPROTEIN WZA

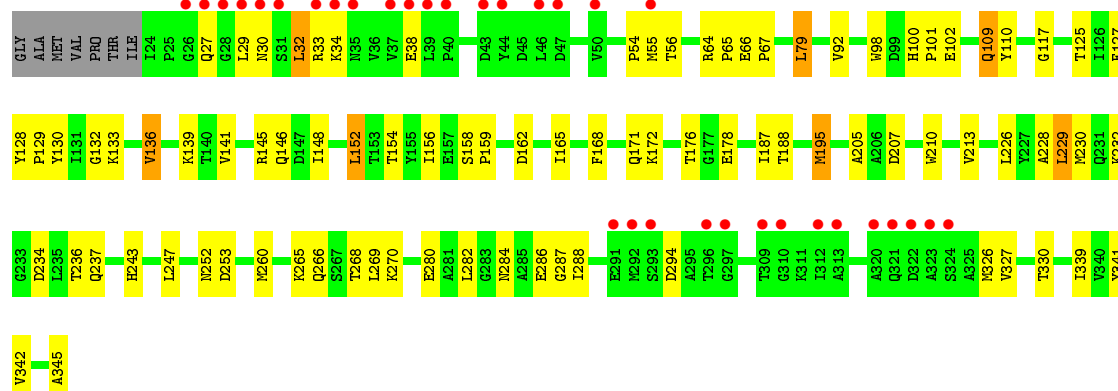


• Molecule 1: PUTATIVE OUTER MEMBRANE LIPOPROTEIN WZA

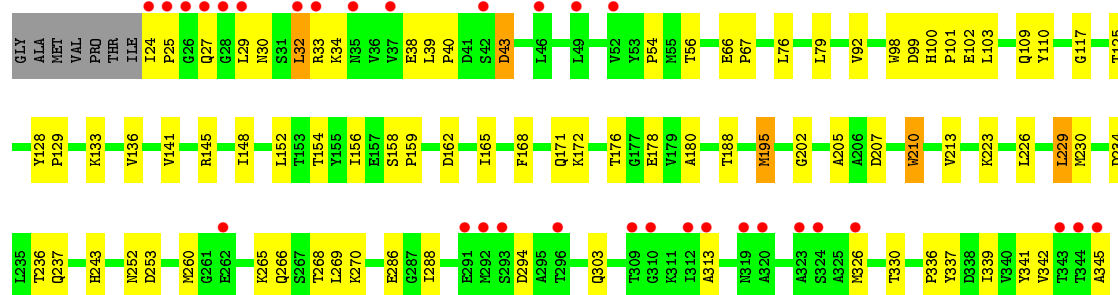




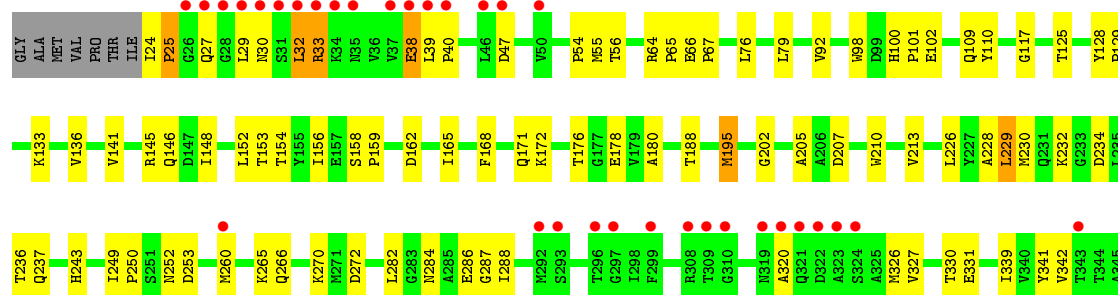
• Molecule 1: PUTATIVE OUTER MEMBRANE LIPOPROTEIN WZA



• Molecule 1: PUTATIVE OUTER MEMBRANE LIPOPROTEIN WZA

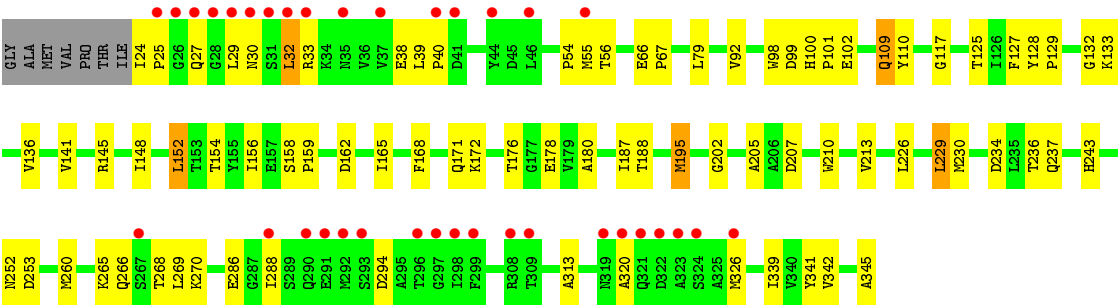


• Molecule 1: PUTATIVE OUTER MEMBRANE LIPOPROTEIN WZA

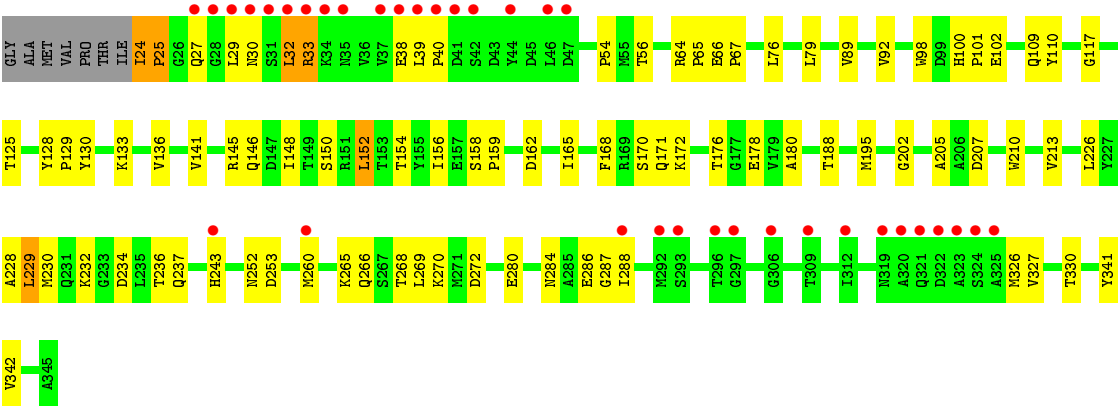


• Molecule 1: PUTATIVE OUTER MEMBRANE LIPOPROTEIN WZA





● Molecule 1: PUTATIVE OUTER MEMBRANE LIPOPROTEIN WZA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	140.08Å 140.20Å 165.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.38 – 3.00 41.38 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.2 (41.38-3.00) 98.2 (41.38-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.210 , 0.231 0.207 , 0.233	Depositor DCC
R_{free} test set	3284 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 22.9	EDS
Estimated twinning fraction	0.502 for K,H,-L 0.478 for k,h,-l	Xtriage
Reported twinning fraction	0.502 for K,H,-L	Depositor
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 64763 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19792	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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

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	0.42	0/2517	0.59	0/3425
1	B	0.43	0/2517	0.59	0/3425
1	C	0.42	0/2517	0.60	0/3425
1	D	0.41	0/2517	0.59	0/3425
1	E	0.42	0/2517	0.59	0/3425
1	F	0.43	1/2517 (0.0%)	0.61	2/3425 (0.1%)
1	G	0.41	0/2517	0.59	0/3425
1	H	0.43	1/2517 (0.0%)	0.60	1/3425 (0.0%)
All	All	0.42	2/20136 (0.0%)	0.59	3/27400 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	33	ARG	CG-CD	5.63	1.66	1.51
1	H	33	ARG	CG-CD	5.51	1.65	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	33	ARG	CA-CB-CG	5.67	125.88	113.40
1	H	33	ARG	CG-CD-NE	5.23	122.79	111.80
1	F	33	ARG	CG-CD-NE	5.16	122.63	111.80

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	2474	0	2464	62	1
1	B	2474	0	2464	59	9
1	C	2474	0	2464	63	2
1	D	2474	0	2464	67	4
1	E	2474	0	2464	66	1
1	F	2474	0	2464	64	9
1	G	2474	0	2464	61	0
1	H	2474	0	2464	62	5
All	All	19792	0	19712	421	16

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (421) 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:F:168:PHE:CG	1:F:188:THR:HG22	2.21	0.76
1:H:128:TYR:CD2	1:H:129:PRO:HD2	2.22	0.74
1:B:168:PHE:CG	1:B:188:THR:HG22	2.23	0.73
1:A:148:ILE:O	1:A:152:LEU:HB2	1.89	0.73
1:H:171:GLN:HB3	1:H:243:HIS:HB3	1.71	0.73
1:A:168:PHE:CG	1:A:188:THR:HG22	2.24	0.72
1:E:148:ILE:O	1:E:152:LEU:HB2	1.89	0.72
1:G:148:ILE:O	1:G:152:LEU:HB2	1.90	0.72
1:A:171:GLN:HB3	1:A:243:HIS:HB3	1.72	0.71
1:B:148:ILE:O	1:B:152:LEU:HB2	1.90	0.71
1:G:171:GLN:HB3	1:G:243:HIS:HB3	1.73	0.71
1:C:171:GLN:HB3	1:C:243:HIS:HB3	1.73	0.71
1:E:168:PHE:CG	1:E:188:THR:HG22	2.25	0.71
1:H:128:TYR:CG	1:H:129:PRO:HD2	2.26	0.70
1:D:129:PRO:HG3	1:E:98:TRP:CD2	2.27	0.70
1:D:148:ILE:O	1:D:152:LEU:HB2	1.93	0.69
1:B:32:LEU:O	1:B:33:ARG:HG3	1.92	0.69
1:G:168:PHE:CG	1:G:188:THR:HG22	2.27	0.69
1:H:168:PHE:CG	1:H:188:THR:HG22	2.27	0.69
1:F:128:TYR:CD2	1:F:129:PRO:HD2	2.28	0.68
1:A:98:TRP:CD2	1:B:129:PRO:HG3	2.27	0.68
1:D:168:PHE:CG	1:D:188:THR:HG22	2.28	0.68
1:E:171:GLN:HB3	1:E:243:HIS:HB3	1.75	0.68
1:A:110:TYR:CE1	1:B:110:TYR:CE1	2.82	0.68
1:B:100:HIS:HD2	1:B:102:GLU:OE2	1.77	0.68
1:F:148:ILE:O	1:F:152:LEU:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:ILE:O	1:C:152:LEU:HB2	1.93	0.67
1:D:171:GLN:HB3	1:D:243:HIS:HB3	1.76	0.67
1:H:24:ILE:N	1:H:25:PRO:HD3	2.10	0.67
1:H:32:LEU:O	1:H:33:ARG:HG3	1.95	0.67
1:G:100:HIS:HD2	1:G:102:GLU:OE2	1.78	0.67
1:H:148:ILE:O	1:H:152:LEU:HB2	1.95	0.65
1:F:32:LEU:O	1:F:33:ARG:HG3	1.97	0.65
1:D:32:LEU:O	1:D:33:ARG:HG3	1.97	0.65
1:F:128:TYR:CG	1:F:129:PRO:HD2	2.33	0.64
1:A:32:LEU:O	1:A:33:ARG:HG3	1.98	0.64
1:H:100:HIS:HD2	1:H:102:GLU:OE2	1.82	0.63
1:C:100:HIS:HD2	1:C:102:GLU:OE2	1.81	0.63
1:B:171:GLN:HB3	1:B:243:HIS:HB3	1.80	0.63
1:D:178:GLU:HB3	1:D:205:ALA:HB3	1.80	0.63
1:G:98:TRP:CD2	1:H:129:PRO:HG3	2.34	0.63
1:H:178:GLU:HB3	1:H:205:ALA:HB3	1.80	0.63
1:E:32:LEU:O	1:E:33:ARG:HG3	1.98	0.63
1:F:24:ILE:N	1:F:24:ILE:HD12	2.14	0.63
1:E:129:PRO:HG3	1:F:98:TRP:CD2	2.34	0.63
1:G:32:LEU:O	1:G:33:ARG:HG3	1.98	0.62
1:F:100:HIS:HD2	1:F:102:GLU:OE2	1.82	0.62
1:A:100:HIS:HD2	1:A:102:GLU:OE2	1.82	0.62
1:B:178:GLU:HB3	1:B:205:ALA:HB3	1.82	0.62
1:B:128:TYR:CG	1:B:129:PRO:HD2	2.34	0.62
1:C:341:TYR:OH	1:F:27:GLN:HB2	1.99	0.62
1:G:110:TYR:CE1	1:H:110:TYR:CE1	2.87	0.62
1:B:98:TRP:CD2	1:G:129:PRO:HG3	2.34	0.62
1:A:178:GLU:HB3	1:A:205:ALA:HB3	1.82	0.62
1:E:265:LYS:HE2	1:F:286:GLU:HG2	1.82	0.61
1:C:265:LYS:HE2	1:H:286:GLU:HG2	1.82	0.61
1:C:32:LEU:O	1:C:33:ARG:HG3	2.01	0.61
1:F:171:GLN:HB3	1:F:243:HIS:HB3	1.83	0.61
1:C:98:TRP:CD2	1:F:129:PRO:HG3	2.35	0.61
1:G:234:ASP:OD1	1:G:236:THR:HB	2.01	0.60
1:A:128:TYR:CG	1:A:129:PRO:HD2	2.37	0.60
1:E:213:VAL:HG21	1:E:226:LEU:HG	1.84	0.60
1:A:234:ASP:OD1	1:A:236:THR:HB	2.00	0.60
1:G:341:TYR:OH	1:H:27:GLN:HB2	2.02	0.60
1:C:178:GLU:HB3	1:C:205:ALA:HB3	1.83	0.60
1:F:178:GLU:HB3	1:F:205:ALA:HB3	1.83	0.60
1:E:100:HIS:HD2	1:E:102:GLU:OE2	1.85	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:178:GLU:HB3	1:E:205:ALA:HB3	1.83	0.60
1:E:128:TYR:CG	1:E:129:PRO:HD2	2.37	0.59
1:A:313:ALA:HB2	1:D:327:VAL:HG21	1.83	0.59
1:G:178:GLU:HB3	1:G:205:ALA:HB3	1.84	0.59
1:A:101:PRO:HD2	1:A:102:GLU:OE1	2.01	0.59
1:D:213:VAL:HG21	1:D:226:LEU:HG	1.85	0.59
1:B:128:TYR:CD2	1:B:129:PRO:HD2	2.38	0.58
1:D:100:HIS:HD2	1:D:102:GLU:OE2	1.86	0.58
1:G:125:THR:OG1	1:G:133:LYS:HE2	2.03	0.58
1:H:24:ILE:N	1:H:25:PRO:CD	2.66	0.58
1:A:341:TYR:OH	1:B:27:GLN:HB2	2.03	0.58
1:B:213:VAL:HG21	1:B:226:LEU:HG	1.86	0.58
1:C:128:TYR:CG	1:C:129:PRO:HD2	2.38	0.58
1:C:286:GLU:HG2	1:F:265:LYS:HE2	1.86	0.58
1:A:125:THR:OG1	1:A:133:LYS:HE2	2.03	0.57
1:B:101:PRO:HD2	1:B:102:GLU:OE1	2.05	0.57
1:C:129:PRO:HG3	1:H:98:TRP:CD2	2.39	0.57
1:E:313:ALA:HB2	1:F:327:VAL:HG21	1.86	0.57
1:C:168:PHE:CG	1:C:188:THR:HG22	2.38	0.57
1:E:234:ASP:OD1	1:E:236:THR:HB	2.04	0.57
1:C:128:TYR:CD2	1:C:129:PRO:HD2	2.40	0.57
1:D:54:PRO:O	1:D:56:THR:HG23	2.04	0.57
1:G:101:PRO:HD2	1:G:102:GLU:OE1	2.04	0.57
1:D:101:PRO:HD2	1:D:102:GLU:OE1	2.04	0.57
1:D:128:TYR:CG	1:D:129:PRO:HD2	2.40	0.56
1:E:128:TYR:CD2	1:E:129:PRO:HD2	2.40	0.56
1:F:234:ASP:OD1	1:F:236:THR:HB	2.04	0.56
1:D:27:GLN:HB2	1:E:341:TYR:OH	2.05	0.56
1:F:54:PRO:O	1:F:56:THR:HG23	2.06	0.56
1:D:128:TYR:CD2	1:D:129:PRO:HD2	2.41	0.56
1:E:54:PRO:O	1:E:56:THR:HG23	2.06	0.56
1:C:234:ASP:OD1	1:C:236:THR:HB	2.06	0.56
1:H:234:ASP:OD1	1:H:236:THR:HB	2.06	0.56
1:D:110:TYR:CE1	1:E:110:TYR:CE1	2.93	0.56
1:C:213:VAL:HG21	1:C:226:LEU:HG	1.88	0.55
1:H:195:MET:HA	1:H:195:MET:CE	2.36	0.55
1:H:125:THR:OG1	1:H:133:LYS:HE2	2.06	0.55
1:A:265:LYS:HE2	1:D:286:GLU:HG2	1.88	0.55
1:E:125:THR:OG1	1:E:133:LYS:HE2	2.06	0.55
1:A:54:PRO:O	1:A:56:THR:HG23	2.06	0.55
1:D:234:ASP:OD1	1:D:236:THR:HB	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:101:PRO:HD2	1:E:102:GLU:OE1	2.05	0.55
1:G:128:TYR:CG	1:G:129:PRO:HD2	2.42	0.55
1:E:180:ALA:HB3	1:E:202:GLY:HA3	1.88	0.55
1:G:213:VAL:HG21	1:G:226:LEU:HG	1.89	0.55
1:B:234:ASP:OD1	1:B:236:THR:HB	2.06	0.55
1:A:213:VAL:HG21	1:A:226:LEU:HG	1.89	0.55
1:B:54:PRO:O	1:B:56:THR:HG23	2.07	0.55
1:B:286:GLU:HG2	1:G:265:LYS:HE2	1.88	0.54
1:A:92:VAL:CG1	1:A:117:GLY:HA3	2.37	0.54
1:A:195:MET:CE	1:A:195:MET:HA	2.37	0.54
1:A:260:MET:O	1:A:341:TYR:HA	2.06	0.54
1:F:195:MET:HA	1:F:195:MET:CE	2.38	0.54
1:F:213:VAL:HG21	1:F:226:LEU:HG	1.90	0.54
1:A:98:TRP:CG	1:B:129:PRO:HG3	2.43	0.54
1:A:110:TYR:CD1	1:B:110:TYR:CE1	2.95	0.54
1:B:110:TYR:CE1	1:G:110:TYR:CE1	2.95	0.54
1:H:101:PRO:HD2	1:H:102:GLU:OE1	2.08	0.54
1:C:110:TYR:CE1	1:F:110:TYR:CE1	2.96	0.54
1:C:260:MET:O	1:C:341:TYR:HA	2.09	0.54
1:A:99:ASP:OD2	1:B:130:TYR:OH	2.25	0.54
1:G:54:PRO:O	1:G:56:THR:HG23	2.08	0.53
1:G:260:MET:O	1:G:341:TYR:HA	2.08	0.53
1:D:195:MET:CE	1:D:195:MET:HA	2.38	0.53
1:C:101:PRO:HD2	1:C:102:GLU:OE1	2.08	0.53
1:G:226:LEU:HB3	1:G:230:MET:HE2	1.90	0.53
1:H:213:VAL:HG21	1:H:226:LEU:HG	1.90	0.53
1:G:92:VAL:CG1	1:G:117:GLY:HA3	2.38	0.53
1:F:260:MET:O	1:F:341:TYR:HA	2.09	0.53
1:B:260:MET:O	1:B:341:TYR:HA	2.08	0.53
1:C:29:LEU:HD23	1:C:30:ASN:N	2.24	0.53
1:H:54:PRO:O	1:H:56:THR:HG23	2.09	0.53
1:D:260:MET:O	1:D:341:TYR:HA	2.09	0.53
1:A:129:PRO:HG3	1:D:98:TRP:CD2	2.44	0.53
1:E:260:MET:O	1:E:341:TYR:HA	2.08	0.53
1:A:128:TYR:CD2	1:A:129:PRO:HD2	2.44	0.53
1:H:260:MET:O	1:H:341:TYR:HA	2.09	0.53
1:B:195:MET:CE	1:B:195:MET:HA	2.39	0.52
1:D:229:LEU:HG	1:D:237:GLN:HB2	1.92	0.52
1:C:54:PRO:O	1:C:56:THR:HG23	2.09	0.52
1:A:226:LEU:HB3	1:A:230:MET:HE2	1.91	0.52
1:D:125:THR:OG1	1:D:133:LYS:HE2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:29:LEU:HD23	1:G:30:ASN:N	2.24	0.52
1:C:195:MET:HA	1:C:195:MET:CE	2.39	0.52
1:G:99:ASP:OD2	1:H:130:TYR:OH	2.27	0.52
1:B:125:THR:OG1	1:B:133:LYS:HE2	2.10	0.52
1:E:266:GLN:CB	1:F:287:GLY:HA3	2.39	0.52
1:B:207:ASP:HB2	1:B:252:ASN:ND2	2.25	0.52
1:G:286:GLU:HG2	1:H:265:LYS:HE2	1.91	0.52
1:E:110:TYR:CD2	1:E:110:TYR:C	2.83	0.51
1:G:100:HIS:CD2	1:G:102:GLU:OE2	2.63	0.51
1:F:101:PRO:HD2	1:F:102:GLU:OE1	2.10	0.51
1:G:165:ILE:HG21	1:G:168:PHE:CD1	2.46	0.51
1:A:286:GLU:HG2	1:B:265:LYS:HE2	1.92	0.51
1:F:125:THR:OG1	1:F:133:LYS:HE2	2.10	0.51
1:E:339:ILE:HD11	1:F:330:THR:CG2	2.40	0.51
1:G:24:ILE:HG22	1:G:25:PRO:O	2.10	0.51
1:A:207:ASP:HB2	1:A:252:ASN:ND2	2.26	0.51
1:B:92:VAL:CG1	1:B:117:GLY:HA3	2.40	0.51
1:C:125:THR:OG1	1:C:133:LYS:HE2	2.10	0.51
1:D:265:LYS:HE2	1:E:286:GLU:HG2	1.93	0.51
1:G:195:MET:CE	1:G:195:MET:HA	2.41	0.51
1:F:165:ILE:HG21	1:F:168:PHE:CD1	2.46	0.51
1:F:229:LEU:HG	1:F:237:GLN:HB2	1.92	0.51
1:B:327:VAL:HG21	1:G:313:ALA:HB2	1.93	0.51
1:A:110:TYR:CE1	1:D:110:TYR:CE1	2.99	0.51
1:G:110:TYR:CD2	1:G:110:TYR:C	2.84	0.51
1:B:100:HIS:CD2	1:B:102:GLU:OE2	2.61	0.50
1:G:207:ASP:HB2	1:G:252:ASN:ND2	2.26	0.50
1:D:129:PRO:HG3	1:E:98:TRP:CG	2.46	0.50
1:G:128:TYR:CD2	1:G:129:PRO:HD2	2.46	0.50
1:F:226:LEU:HB3	1:F:230:MET:HE2	1.94	0.50
1:H:158:SER:N	1:H:159:PRO:HD3	2.27	0.50
1:E:195:MET:CE	1:E:195:MET:HA	2.41	0.50
1:C:265:LYS:HE2	1:H:286:GLU:OE2	2.12	0.50
1:C:313:ALA:HB2	1:H:327:VAL:HG21	1.92	0.50
1:E:145:ARG:HD3	1:E:162:ASP:HA	1.92	0.50
1:A:229:LEU:HG	1:A:237:GLN:HB2	1.93	0.50
1:G:110:TYR:CD1	1:H:110:TYR:CE1	3.00	0.50
1:C:110:TYR:CE1	1:H:110:TYR:CE1	3.00	0.50
1:H:110:TYR:CD2	1:H:110:TYR:C	2.85	0.49
1:C:92:VAL:CG1	1:C:117:GLY:HA3	2.42	0.49
1:C:229:LEU:HG	1:C:237:GLN:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:229:LEU:HG	1:E:237:GLN:HB2	1.94	0.49
1:C:110:TYR:CD2	1:C:110:TYR:C	2.86	0.49
1:C:320:ALA:O	1:E:27:GLN:HG2	2.13	0.49
1:E:226:LEU:HB3	1:E:230:MET:HE2	1.94	0.49
1:G:145:ARG:HD3	1:G:162:ASP:HA	1.95	0.49
1:C:145:ARG:HD3	1:C:162:ASP:HA	1.93	0.49
1:H:229:LEU:HG	1:H:237:GLN:HB2	1.94	0.49
1:C:165:ILE:HG21	1:C:168:PHE:CD1	2.48	0.48
1:C:266:GLN:CB	1:H:287:GLY:HA3	2.44	0.48
1:H:165:ILE:HG21	1:H:168:PHE:CD1	2.48	0.48
1:E:129:PRO:HG3	1:F:98:TRP:CG	2.48	0.48
1:D:158:SER:N	1:D:159:PRO:HD3	2.27	0.48
1:D:145:ARG:HD3	1:D:162:ASP:HA	1.96	0.48
1:C:207:ASP:HB2	1:C:252:ASN:ND2	2.29	0.48
1:H:145:ARG:HD3	1:H:162:ASP:HA	1.95	0.48
1:G:172:LYS:O	1:G:243:HIS:HA	2.13	0.48
1:F:100:HIS:CD2	1:F:102:GLU:OE2	2.67	0.48
1:E:92:VAL:CG1	1:E:117:GLY:HA3	2.44	0.48
1:A:339:ILE:HD11	1:D:330:THR:CG2	2.44	0.48
1:C:226:LEU:HB3	1:C:230:MET:HE2	1.96	0.47
1:D:207:ASP:HB2	1:D:252:ASN:ND2	2.29	0.47
1:A:145:ARG:HD3	1:A:162:ASP:HA	1.95	0.47
1:A:266:GLN:CB	1:D:287:GLY:HA3	2.44	0.47
1:H:207:ASP:HB2	1:H:252:ASN:ND2	2.28	0.47
1:E:29:LEU:HD23	1:E:30:ASN:N	2.29	0.47
1:A:110:TYR:C	1:A:110:TYR:CD2	2.88	0.47
1:E:266:GLN:HB2	1:F:287:GLY:HA3	1.97	0.47
1:A:172:LYS:O	1:A:243:HIS:HA	2.14	0.47
1:F:110:TYR:C	1:F:110:TYR:CD2	2.87	0.47
1:F:158:SER:N	1:F:159:PRO:HD3	2.29	0.47
1:B:29:LEU:HD23	1:B:30:ASN:N	2.30	0.47
1:E:207:ASP:HB2	1:E:252:ASN:ND2	2.29	0.47
1:D:226:LEU:HB3	1:D:230:MET:HE2	1.96	0.47
1:E:158:SER:N	1:E:159:PRO:HD3	2.28	0.47
1:B:226:LEU:HB3	1:B:230:MET:HE2	1.97	0.47
1:A:29:LEU:HD23	1:A:30:ASN:N	2.30	0.47
1:C:158:SER:N	1:C:159:PRO:HD3	2.30	0.47
1:D:172:LYS:O	1:D:243:HIS:HA	2.15	0.47
1:A:180:ALA:HB3	1:A:202:GLY:HA3	1.97	0.47
1:F:29:LEU:HD23	1:F:30:ASN:N	2.30	0.46
1:D:130:TYR:OH	1:E:99:ASP:OD2	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:207:ASP:HB2	1:F:252:ASN:ND2	2.31	0.46
1:C:253:ASP:OD2	1:H:272:ASP:HB2	2.15	0.46
1:B:165:ILE:HG21	1:B:168:PHE:CD1	2.49	0.46
1:G:229:LEU:HG	1:G:237:GLN:HB2	1.97	0.46
1:E:172:LYS:O	1:E:243:HIS:HA	2.16	0.46
1:D:110:TYR:CE1	1:E:110:TYR:CD1	3.03	0.46
1:H:226:LEU:HB3	1:H:230:MET:HE2	1.97	0.46
1:G:32:LEU:HD12	1:G:32:LEU:HA	1.75	0.46
1:D:92:VAL:CG1	1:D:117:GLY:HA3	2.45	0.46
1:F:66:GLU:HG3	1:F:67:PRO:HD2	1.98	0.46
1:E:268:THR:HB	1:F:284:ASN:OD1	2.15	0.46
1:F:92:VAL:CG1	1:F:117:GLY:HA3	2.46	0.46
1:G:158:SER:N	1:G:159:PRO:HD3	2.31	0.46
1:C:110:TYR:CD1	1:F:110:TYR:CE1	3.04	0.46
1:H:29:LEU:HD23	1:H:30:ASN:N	2.30	0.46
1:D:110:TYR:CD2	1:D:110:TYR:C	2.89	0.45
1:H:100:HIS:CD2	1:H:102:GLU:OE2	2.66	0.45
1:C:260:MET:HA	1:C:266:GLN:HG2	1.97	0.45
1:A:260:MET:HA	1:A:266:GLN:HG2	1.98	0.45
1:B:158:SER:N	1:B:159:PRO:HD3	2.31	0.45
1:F:260:MET:HA	1:F:266:GLN:HG2	1.98	0.45
1:F:180:ALA:HB3	1:F:202:GLY:HA3	1.99	0.45
1:H:288:ILE:HG23	1:H:342:VAL:HG11	1.98	0.45
1:B:288:ILE:HG23	1:B:342:VAL:HG11	1.99	0.45
1:B:110:TYR:C	1:B:110:TYR:CD2	2.89	0.45
1:E:100:HIS:CD2	1:E:102:GLU:OE2	2.69	0.45
1:B:260:MET:HA	1:B:266:GLN:HG2	1.99	0.45
1:B:92:VAL:HG12	1:B:117:GLY:HA3	1.98	0.45
1:B:24:ILE:HD12	1:B:24:ILE:O	2.16	0.45
1:A:158:SER:N	1:A:159:PRO:HD3	2.31	0.45
1:A:195:MET:HE2	1:A:195:MET:HA	1.98	0.45
1:H:268:THR:O	1:H:269:LEU:HD23	2.17	0.45
1:A:66:GLU:HG3	1:A:67:PRO:HD2	1.99	0.45
1:B:145:ARG:HD3	1:B:162:ASP:HA	1.99	0.45
1:B:98:TRP:CG	1:G:129:PRO:HG3	2.52	0.45
1:H:260:MET:HA	1:H:266:GLN:HG2	1.98	0.45
1:B:127:PHE:CE1	1:B:132:GLY:HA2	2.52	0.45
1:F:288:ILE:HG23	1:F:342:VAL:HG11	1.98	0.45
1:H:24:ILE:C	1:H:25:PRO:O	2.55	0.45
1:A:100:HIS:CD2	1:A:102:GLU:OE2	2.67	0.45
1:B:341:TYR:OH	1:G:27:GLN:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:172:LYS:O	1:F:243:HIS:HA	2.17	0.45
1:D:29:LEU:HD23	1:D:30:ASN:N	2.31	0.45
1:D:66:GLU:HG3	1:D:67:PRO:HD2	1.99	0.45
1:A:265:LYS:HE2	1:D:286:GLU:OE2	2.17	0.45
1:B:66:GLU:HG3	1:B:67:PRO:HD2	1.99	0.45
1:H:172:LYS:O	1:H:243:HIS:HA	2.17	0.44
1:F:24:ILE:N	1:F:24:ILE:CD1	2.80	0.44
1:F:24:ILE:HG22	1:F:25:PRO:O	2.17	0.44
1:E:260:MET:HA	1:E:266:GLN:HG2	1.98	0.44
1:A:92:VAL:HG12	1:A:117:GLY:HA3	1.99	0.44
1:H:92:VAL:CG1	1:H:117:GLY:HA3	2.47	0.44
1:A:129:PRO:HG3	1:D:98:TRP:CG	2.53	0.44
1:G:260:MET:HA	1:G:266:GLN:HG2	1.99	0.44
1:H:228:ALA:O	1:H:232:LYS:HB2	2.18	0.44
1:F:253:ASP:HA	1:F:270:LYS:HD3	1.99	0.44
1:H:64:ARG:HA	1:H:65:PRO:HD3	1.81	0.44
1:G:288:ILE:HG23	1:G:342:VAL:HG11	1.99	0.44
1:H:89:VAL:O	1:H:170:SER:HB3	2.17	0.44
1:C:268:THR:HB	1:H:284:ASN:OD1	2.17	0.44
1:F:32:LEU:HA	1:F:32:LEU:HD12	1.59	0.44
1:H:180:ALA:HB3	1:H:202:GLY:HA3	1.99	0.44
1:C:326:MET:HA	1:C:326:MET:CE	2.48	0.44
1:D:288:ILE:HG23	1:D:342:VAL:HG11	1.99	0.44
1:B:286:GLU:OE2	1:G:265:LYS:HE2	2.18	0.44
1:C:27:GLN:HG2	1:G:320:ALA:O	2.17	0.44
1:D:136:VAL:O	1:D:139:LYS:HB2	2.18	0.44
1:D:326:MET:HA	1:D:326:MET:CE	2.48	0.44
1:D:260:MET:HA	1:D:266:GLN:HG2	1.99	0.44
1:G:180:ALA:HB3	1:G:202:GLY:HA3	2.00	0.44
1:E:303:GLN:HG3	1:F:331:GLU:OE2	2.18	0.44
1:E:268:THR:O	1:E:269:LEU:HD23	2.17	0.43
1:A:268:THR:HB	1:D:284:ASN:OD1	2.18	0.43
1:B:228:ALA:O	1:B:232:LYS:HB2	2.17	0.43
1:H:66:GLU:HG3	1:H:67:PRO:HD2	1.99	0.43
1:C:162:ASP:O	1:C:163:VAL:HG23	2.19	0.43
1:C:89:VAL:O	1:C:170:SER:HB3	2.18	0.43
1:D:268:THR:O	1:D:269:LEU:HD23	2.18	0.43
1:A:294:ASP:HB2	1:A:345:ALA:HA	2.00	0.43
1:A:98:TRP:CE2	1:B:129:PRO:HG3	2.53	0.43
1:D:339:ILE:HD11	1:E:330:THR:CG2	2.49	0.43
1:A:326:MET:HA	1:A:326:MET:CE	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:228:ALA:O	1:F:232:LYS:HB2	2.18	0.43
1:E:24:ILE:HA	1:E:25:PRO:HD3	1.83	0.43
1:E:32:LEU:HD12	1:E:32:LEU:HA	1.32	0.43
1:F:24:ILE:C	1:F:25:PRO:O	2.53	0.43
1:A:234:ASP:OD1	1:A:236:THR:CB	2.67	0.43
1:A:288:ILE:HG23	1:A:342:VAL:HG11	2.00	0.43
1:F:326:MET:HA	1:F:326:MET:CE	2.48	0.43
1:G:326:MET:HA	1:G:326:MET:CE	2.48	0.43
1:C:66:GLU:HG3	1:C:67:PRO:HD2	2.00	0.43
1:D:195:MET:HE2	1:D:195:MET:HA	1.98	0.43
1:A:313:ALA:CB	1:D:327:VAL:HG21	2.49	0.43
1:G:98:TRP:CG	1:H:129:PRO:HG3	2.54	0.42
1:C:288:ILE:HG23	1:C:342:VAL:HG11	2.00	0.42
1:D:127:PHE:CE1	1:D:132:GLY:HA2	2.54	0.42
1:C:39:LEU:HB3	1:C:40:PRO:HD2	2.01	0.42
1:H:326:MET:CE	1:H:326:MET:HA	2.48	0.42
1:B:326:MET:HA	1:B:326:MET:CE	2.49	0.42
1:C:180:ALA:HB3	1:C:202:GLY:HA3	2.01	0.42
1:B:172:LYS:O	1:B:243:HIS:HA	2.18	0.42
1:E:102:GLU:HG2	1:E:103:LEU:N	2.34	0.42
1:B:229:LEU:HG	1:B:237:GLN:HB2	2.00	0.42
1:D:165:ILE:HG21	1:D:168:PHE:CD1	2.53	0.42
1:B:287:GLY:HA3	1:G:266:GLN:CB	2.50	0.42
1:H:195:MET:HA	1:H:195:MET:HE2	2.01	0.42
1:F:195:MET:HA	1:F:195:MET:HE2	2.00	0.42
1:E:165:ILE:HG21	1:E:168:PHE:CD1	2.54	0.42
1:D:32:LEU:HA	1:D:32:LEU:HD12	1.61	0.42
1:E:260:MET:CE	1:F:282:LEU:HB2	2.49	0.42
1:H:253:ASP:HA	1:H:270:LYS:HD3	2.02	0.42
1:A:258:PHE:CE1	1:D:280:GLU:HA	2.55	0.42
1:F:153:THR:HG22	1:F:153:THR:O	2.18	0.42
1:E:326:MET:HA	1:E:326:MET:CE	2.48	0.42
1:E:253:ASP:HA	1:E:270:LYS:HD3	2.01	0.42
1:C:171:GLN:HB2	1:C:187:ILE:HB	2.02	0.42
1:G:127:PHE:CE1	1:G:132:GLY:HA2	2.55	0.42
1:C:339:ILE:HD11	1:H:330:THR:CG2	2.48	0.42
1:D:92:VAL:HG12	1:D:117:GLY:HA3	2.01	0.42
1:B:330:THR:CG2	1:G:339:ILE:HD11	2.49	0.42
1:E:66:GLU:HG3	1:E:67:PRO:HD2	2.02	0.42
1:B:89:VAL:O	1:B:170:SER:HB3	2.19	0.42
1:G:294:ASP:HB2	1:G:345:ALA:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:288:ILE:HG23	1:E:342:VAL:HG11	2.01	0.42
1:D:79:LEU:HA	1:D:79:LEU:HD12	1.80	0.42
1:D:226:LEU:O	1:D:230:MET:HE2	2.19	0.42
1:B:79:LEU:HD12	1:B:79:LEU:HA	1.71	0.42
1:C:127:PHE:CE1	1:C:132:GLY:HA2	2.55	0.42
1:G:171:GLN:HB2	1:G:187:ILE:HB	2.02	0.42
1:B:32:LEU:HA	1:B:32:LEU:HD12	1.65	0.42
1:E:313:ALA:CB	1:F:327:VAL:HG21	2.47	0.42
1:E:39:LEU:HB3	1:E:40:PRO:HD2	2.02	0.42
1:C:253:ASP:HA	1:C:270:LYS:HD3	2.01	0.41
1:D:253:ASP:HA	1:D:270:LYS:HD3	2.01	0.41
1:D:171:GLN:HB2	1:D:187:ILE:HB	2.02	0.41
1:E:34:LYS:HG2	1:F:47:ASP:HB3	2.02	0.41
1:H:39:LEU:HB3	1:H:40:PRO:HD2	2.03	0.41
1:G:66:GLU:HG3	1:G:67:PRO:HD2	2.01	0.41
1:B:110:TYR:CD1	1:G:110:TYR:CE1	3.07	0.41
1:H:32:LEU:HD12	1:H:32:LEU:HA	1.59	0.41
1:D:27:GLN:HG2	1:F:320:ALA:O	2.21	0.41
1:G:92:VAL:HG12	1:G:117:GLY:HA3	2.02	0.41
1:A:330:THR:CG2	1:B:339:ILE:HD11	2.49	0.41
1:A:32:LEU:HA	1:A:32:LEU:HD12	1.36	0.41
1:C:326:MET:HA	1:C:326:MET:HE3	2.03	0.41
1:F:39:LEU:HB3	1:F:40:PRO:HD2	2.02	0.41
1:C:100:HIS:CD2	1:C:102:GLU:OE2	2.66	0.41
1:A:24:ILE:HA	1:A:25:PRO:HD3	1.82	0.41
1:F:145:ARG:HD3	1:F:162:ASP:HA	2.01	0.41
1:B:142:SER:O	1:B:146:GLN:HG3	2.20	0.41
1:D:109:GLN:N	1:D:109:GLN:NE2	2.69	0.41
1:C:223:LYS:HB2	1:C:223:LYS:HE2	1.91	0.41
1:A:171:GLN:HB2	1:A:187:ILE:HB	2.02	0.41
1:E:253:ASP:OD2	1:F:272:ASP:HB2	2.21	0.41
1:B:180:ALA:HB3	1:B:202:GLY:HA3	2.03	0.41
1:D:64:ARG:HA	1:D:65:PRO:HD3	1.80	0.41
1:C:27:GLN:HB2	1:H:341:TYR:OH	2.21	0.41
1:F:64:ARG:HA	1:F:65:PRO:HD3	1.82	0.41
1:F:249:ILE:HA	1:F:250:PRO:HD3	1.84	0.41
1:E:210:TRP:CD1	1:E:210:TRP:N	2.89	0.41
1:D:294:ASP:HB2	1:D:345:ALA:HA	2.03	0.41
1:E:102:GLU:HG2	1:E:103:LEU:HG	2.03	0.41
1:A:110:TYR:CE1	1:D:110:TYR:CD1	3.09	0.40
1:G:234:ASP:OD1	1:G:236:THR:CB	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:253:ASP:HA	1:G:270:LYS:HD3	2.04	0.40
1:G:39:LEU:HB3	1:G:40:PRO:HD2	2.02	0.40
1:E:336:PRO:O	1:E:337:TYR:HB2	2.22	0.40
1:A:336:PRO:O	1:A:337:TYR:HB2	2.21	0.40
1:A:260:MET:CE	1:D:282:LEU:HB2	2.52	0.40
1:A:204:LEU:HD11	1:A:230:MET:HE1	2.04	0.40
1:G:268:THR:O	1:G:269:LEU:HD23	2.21	0.40
1:D:228:ALA:O	1:D:232:LYS:HB2	2.22	0.40
1:C:294:ASP:HB2	1:C:345:ALA:HA	2.02	0.40
1:B:253:ASP:HA	1:B:270:LYS:HD3	2.04	0.40
1:C:330:THR:CG2	1:F:339:ILE:HD11	2.51	0.40
1:C:64:ARG:HA	1:C:65:PRO:HD3	1.82	0.40
1:E:195:MET:HA	1:E:195:MET:HE2	2.02	0.40
1:C:66:GLU:HA	1:C:67:PRO:HD3	1.96	0.40
1:E:294:ASP:HB2	1:E:345:ALA:HA	2.02	0.40
1:C:258:PHE:HE1	1:H:280:GLU:HA	1.87	0.40
1:E:223:LYS:HB2	1:E:223:LYS:HE2	1.93	0.40
1:D:247:LEU:HA	1:D:247:LEU:HD12	1.89	0.40
1:G:109:GLN:N	1:G:109:GLN:NE2	2.69	0.40
1:E:265:LYS:HE2	1:F:286:GLU:OE2	2.21	0.40
1:G:226:LEU:O	1:G:230:MET:HE2	2.21	0.40
1:H:228:ALA:HB3	1:H:237:GLN:HG3	2.03	0.40
1:C:268:THR:O	1:C:269:LEU:HD23	2.21	0.40
1:A:258:PHE:HE1	1:D:280:GLU:HA	1.87	0.40
1:C:134:VAL:HA	1:C:151:ARG:HH12	1.86	0.40
1:C:110:TYR:CE1	1:H:110:TYR:CD1	3.10	0.40

All (16) 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:D:32:LEU:N	1:H:33:ARG:NE[3_455]	1.77	0.43
1:D:146:GLN:OE1	1:H:146:GLN:O[4_546]	1.92	0.28
1:B:32:LEU:N	1:F:33:ARG:NE[4_545]	1.96	0.24
1:B:150:SER:OG	1:F:146:GLN:NE2[3_446]	2.02	0.18
1:D:34:LYS:N	1:H:33:ARG:CD[3_455]	2.03	0.17
1:F:38:GLU:N	1:F:38:GLU:CB[2_455]	2.03	0.17
1:B:25:PRO:CD	1:C:38:GLU:OE2[4_545]	2.05	0.15
1:B:146:GLN:O	1:F:146:GLN:OE1[3_446]	2.05	0.15
1:B:34:LYS:N	1:F:33:ARG:CD[4_545]	2.07	0.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LEU:O	1:C:32:LEU:CG[4_545]	2.08	0.12
1:B:30:ASN:OD1	1:F:33:ARG:NH2[4_545]	2.10	0.10
1:D:146:GLN:NE2	1:H:150:SER:OG[4_546]	2.14	0.06
1:B:34:LYS:O	1:F:32:LEU:O[4_545]	2.16	0.04
1:B:32:LEU:C	1:F:33:ARG:CB[4_545]	2.16	0.04
1:B:32:LEU:CA	1:F:33:ARG:CB[4_545]	2.17	0.03
1:E:43:ASP:OD1	1:H:25:PRO:N[3_455]	2.18	0.02

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	320/329 (97%)	289 (90%)	30 (9%)	1 (0%)	46	84
1	B	320/329 (97%)	289 (90%)	30 (9%)	1 (0%)	46	84
1	C	320/329 (97%)	292 (91%)	28 (9%)	0	100	100
1	D	320/329 (97%)	291 (91%)	28 (9%)	1 (0%)	46	84
1	E	320/329 (97%)	292 (91%)	28 (9%)	0	100	100
1	F	320/329 (97%)	289 (90%)	29 (9%)	2 (1%)	30	72
1	G	320/329 (97%)	291 (91%)	28 (9%)	1 (0%)	46	84
1	H	320/329 (97%)	289 (90%)	30 (9%)	1 (0%)	46	84
All	All	2560/2632 (97%)	2322 (91%)	231 (9%)	7 (0%)	46	84

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	25	PRO
1	A	55	MET
1	B	25	PRO
1	F	55	MET
1	G	55	MET

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Mol	Chain	Res	Type
1	D	55	MET
1	F	25	PRO

5.3.2 Protein sidechains ⓘ

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	272/277 (98%)	258 (95%)	14 (5%)	29	69
1	B	272/277 (98%)	260 (96%)	12 (4%)	35	74
1	C	272/277 (98%)	258 (95%)	14 (5%)	29	69
1	D	272/277 (98%)	259 (95%)	13 (5%)	31	71
1	E	272/277 (98%)	258 (95%)	14 (5%)	29	69
1	F	272/277 (98%)	259 (95%)	13 (5%)	31	71
1	G	272/277 (98%)	259 (95%)	13 (5%)	31	71
1	H	272/277 (98%)	258 (95%)	14 (5%)	29	69
All	All	2176/2216 (98%)	2069 (95%)	107 (5%)	31	71

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLU
1	A	43	ASP
1	A	76	LEU
1	A	79	LEU
1	A	109	GLN
1	A	136	VAL
1	A	141	VAL
1	A	152	LEU
1	A	154	THR
1	A	156	ILE
1	A	176	THR
1	A	195	MET
1	A	210	TRP

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Mol	Chain	Res	Type
1	A	229	LEU
1	B	32	LEU
1	B	38	GLU
1	B	79	LEU
1	B	109	GLN
1	B	136	VAL
1	B	141	VAL
1	B	152	LEU
1	B	154	THR
1	B	156	ILE
1	B	176	THR
1	B	195	MET
1	B	210	TRP
1	C	32	LEU
1	C	38	GLU
1	C	43	ASP
1	C	76	LEU
1	C	79	LEU
1	C	109	GLN
1	C	141	VAL
1	C	152	LEU
1	C	154	THR
1	C	156	ILE
1	C	176	THR
1	C	195	MET
1	C	210	TRP
1	C	229	LEU
1	D	32	LEU
1	D	38	GLU
1	D	79	LEU
1	D	109	GLN
1	D	136	VAL
1	D	141	VAL
1	D	152	LEU
1	D	154	THR
1	D	156	ILE
1	D	176	THR
1	D	195	MET
1	D	210	TRP
1	D	229	LEU
1	E	32	LEU
1	E	38	GLU

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Mol	Chain	Res	Type
1	E	43	ASP
1	E	76	LEU
1	E	79	LEU
1	E	109	GLN
1	E	136	VAL
1	E	141	VAL
1	E	154	THR
1	E	156	ILE
1	E	176	THR
1	E	195	MET
1	E	210	TRP
1	E	229	LEU
1	F	32	LEU
1	F	38	GLU
1	F	76	LEU
1	F	79	LEU
1	F	109	GLN
1	F	136	VAL
1	F	141	VAL
1	F	154	THR
1	F	156	ILE
1	F	176	THR
1	F	195	MET
1	F	210	TRP
1	F	229	LEU
1	G	32	LEU
1	G	38	GLU
1	G	79	LEU
1	G	109	GLN
1	G	136	VAL
1	G	141	VAL
1	G	152	LEU
1	G	154	THR
1	G	156	ILE
1	G	176	THR
1	G	195	MET
1	G	210	TRP
1	G	229	LEU
1	H	24	ILE
1	H	32	LEU
1	H	38	GLU
1	H	76	LEU

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Mol	Chain	Res	Type
1	H	79	LEU
1	H	109	GLN
1	H	136	VAL
1	H	141	VAL
1	H	152	LEU
1	H	154	THR
1	H	156	ILE
1	H	176	THR
1	H	210	TRP
1	H	229	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	100	HIS
1	A	109	GLN
1	A	146	GLN
1	A	218	ASN
1	A	231	GLN
1	B	62	GLN
1	B	100	HIS
1	B	109	GLN
1	B	146	GLN
1	B	218	ASN
1	B	231	GLN
1	C	62	GLN
1	C	100	HIS
1	C	109	GLN
1	C	146	GLN
1	C	181	ASN
1	C	218	ASN
1	C	231	GLN
1	D	62	GLN
1	D	100	HIS
1	D	109	GLN
1	D	146	GLN
1	D	218	ASN
1	D	231	GLN
1	D	321	GLN
1	E	62	GLN
1	E	100	HIS

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Mol	Chain	Res	Type
1	E	109	GLN
1	E	146	GLN
1	E	181	ASN
1	E	218	ASN
1	E	231	GLN
1	F	62	GLN
1	F	100	HIS
1	F	109	GLN
1	F	146	GLN
1	F	218	ASN
1	F	231	GLN
1	G	62	GLN
1	G	100	HIS
1	G	109	GLN
1	G	146	GLN
1	G	218	ASN
1	G	231	GLN
1	H	62	GLN
1	H	100	HIS
1	H	109	GLN
1	H	146	GLN
1	H	181	ASN
1	H	218	ASN
1	H	231	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 ⓘ

There are no ligands in this entry.

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, 95th 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	322/329 (97%)	0.20	34 (10%) 8 3	11, 56, 193, 221	0
1	B	322/329 (97%)	0.31	36 (11%) 7 3	9, 56, 194, 221	0
1	C	322/329 (97%)	0.22	31 (9%) 10 4	13, 55, 194, 221	0
1	D	322/329 (97%)	0.23	33 (10%) 9 3	10, 56, 194, 221	0
1	E	322/329 (97%)	0.19	31 (9%) 10 4	11, 55, 195, 221	0
1	F	322/329 (97%)	0.25	33 (10%) 9 3	11, 56, 195, 222	0
1	G	322/329 (97%)	0.23	35 (10%) 7 3	11, 55, 193, 221	0
1	H	322/329 (97%)	0.34	35 (10%) 7 3	10, 55, 194, 222	0
All	All	2576/2632 (97%)	0.25	268 (10%) 8 3	9, 56, 195, 222	0

All (268) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	31	SER	16.2
1	F	31	SER	14.7
1	B	27	GLN	13.6
1	H	324	SER	11.2
1	D	29	LEU	11.1
1	C	27	GLN	10.9
1	B	29	LEU	10.9
1	C	28	GLY	10.9
1	B	323	ALA	8.7
1	B	31	SER	8.5
1	A	27	GLN	8.3
1	H	35	ASN	8.3
1	G	31	SER	7.8
1	F	29	LEU	7.6
1	F	27	GLN	7.4
1	G	27	GLN	7.1

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Mol	Chain	Res	Type	RSRZ
1	H	29	LEU	6.9
1	D	38	GLU	6.7
1	F	30	ASN	6.7
1	C	31	SER	6.6
1	H	293	SER	6.5
1	C	32	LEU	6.5
1	D	31	SER	6.4
1	E	324	SER	6.4
1	H	28	GLY	6.3
1	H	27	GLN	6.3
1	D	296	THR	6.3
1	B	42	SER	6.2
1	H	30	ASN	6.2
1	B	293	SER	6.1
1	G	324	SER	6.1
1	H	323	ALA	6.1
1	D	27	GLN	6.1
1	B	46	LEU	6.0
1	C	324	SER	6.0
1	G	33	ARG	6.0
1	F	293	SER	5.8
1	G	309	THR	5.8
1	A	291	GLU	5.7
1	D	33	ARG	5.7
1	A	33	ARG	5.6
1	F	324	SER	5.6
1	B	28	GLY	5.6
1	H	38	GLU	5.5
1	H	32	LEU	5.5
1	H	34	LYS	5.5
1	E	292	MET	5.5
1	E	296	THR	5.5
1	G	28	GLY	5.4
1	D	324	SER	5.4
1	D	39	LEU	5.3
1	D	50	VAL	5.2
1	G	29	LEU	5.2
1	D	292	MET	5.1
1	A	324	SER	5.1
1	E	27	GLN	4.9
1	D	323	ALA	4.9
1	E	28	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	28	GLY	4.8
1	E	323	ALA	4.8
1	G	326	MET	4.7
1	B	33	ARG	4.7
1	D	46	LEU	4.7
1	C	29	LEU	4.7
1	H	296	THR	4.7
1	D	37	VAL	4.6
1	G	32	LEU	4.6
1	E	309	THR	4.6
1	A	296	THR	4.6
1	B	43	ASP	4.5
1	E	33	ARG	4.5
1	A	35	ASN	4.5
1	B	26	GLY	4.5
1	E	29	LEU	4.5
1	E	320	ALA	4.4
1	F	296	THR	4.4
1	H	37	VAL	4.3
1	C	26	GLY	4.3
1	D	28	GLY	4.3
1	B	44	TYR	4.3
1	G	44	TYR	4.3
1	F	323	ALA	4.3
1	C	292	MET	4.2
1	A	29	LEU	4.2
1	D	297	GLY	4.2
1	B	320	ALA	4.2
1	G	323	ALA	4.2
1	D	320	ALA	4.2
1	C	319	ASN	4.2
1	D	293	SER	4.2
1	C	33	ARG	4.1
1	H	320	ALA	4.1
1	F	28	GLY	4.1
1	E	26	GLY	4.1
1	E	310	GLY	4.1
1	H	292	MET	4.1
1	G	291	GLU	4.0
1	F	297	GLY	4.0
1	B	296	THR	4.0
1	D	321	GLN	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	323	ALA	4.0
1	A	31	SER	4.0
1	C	309	THR	3.9
1	C	322	ASP	3.9
1	F	321	GLN	3.9
1	G	46	LEU	3.9
1	H	322	ASP	3.9
1	C	323	ALA	3.9
1	G	293	SER	3.9
1	A	292	MET	3.8
1	G	319	ASN	3.8
1	B	292	MET	3.8
1	D	35	ASN	3.7
1	E	313	ALA	3.7
1	D	44	TYR	3.7
1	E	24	ILE	3.7
1	C	296	THR	3.7
1	A	24	ILE	3.7
1	D	47	ASP	3.7
1	H	309	THR	3.7
1	H	42	SER	3.7
1	A	320	ALA	3.7
1	H	39	LEU	3.6
1	D	309	THR	3.6
1	D	30	ASN	3.6
1	C	25	PRO	3.6
1	F	320	ALA	3.6
1	H	44	TYR	3.5
1	F	35	ASN	3.5
1	F	39	LEU	3.5
1	F	322	ASP	3.5
1	A	44	TYR	3.5
1	E	37	VAL	3.5
1	F	34	LYS	3.5
1	D	40	PRO	3.4
1	C	293	SER	3.4
1	B	50	VAL	3.4
1	E	42	SER	3.3
1	G	37	VAL	3.3
1	B	38	GLU	3.3
1	A	55	MET	3.3
1	H	325	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	291	GLU	3.3
1	D	43	ASP	3.3
1	G	308	ARG	3.2
1	H	288	ILE	3.2
1	F	299	PHE	3.2
1	E	35	ASN	3.2
1	H	33	ARG	3.2
1	A	46	LEU	3.2
1	B	309	THR	3.2
1	C	54	PRO	3.2
1	F	40	PRO	3.1
1	C	36	VAL	3.1
1	G	296	THR	3.1
1	A	310	GLY	3.1
1	F	50	VAL	3.1
1	A	309	THR	3.0
1	B	313	ALA	3.0
1	A	308	ARG	3.0
1	E	293	SER	3.0
1	D	26	GLY	3.0
1	G	288	ILE	3.0
1	B	291	GLU	3.0
1	E	345	ALA	3.0
1	C	325	ALA	3.0
1	E	326	MET	3.0
1	G	41	ASP	2.9
1	H	41	ASP	2.9
1	C	30	ASN	2.9
1	A	50	VAL	2.9
1	F	47	ASP	2.9
1	D	310	GLY	2.8
1	G	30	ASN	2.8
1	B	55	MET	2.8
1	E	343	THR	2.8
1	E	32	LEU	2.8
1	E	291	GLU	2.8
1	F	292	MET	2.8
1	E	319	ASN	2.8
1	C	39	LEU	2.8
1	G	322	ASP	2.8
1	C	37	VAL	2.8
1	H	40	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	35	ASN	2.7
1	C	41	ASP	2.7
1	F	343	THR	2.7
1	A	34	LYS	2.7
1	B	36	VAL	2.7
1	B	35	ASN	2.7
1	G	321	GLN	2.7
1	D	313	ALA	2.6
1	C	24	ILE	2.6
1	A	343	THR	2.6
1	C	35	ASN	2.6
1	B	322	ASP	2.6
1	E	46	LEU	2.6
1	F	37	VAL	2.6
1	E	344	THR	2.5
1	F	38	GLU	2.5
1	D	34	LYS	2.5
1	A	313	ALA	2.5
1	D	55	MET	2.5
1	F	308	ARG	2.5
1	F	32	LEU	2.5
1	A	312	ILE	2.5
1	C	290	GLN	2.5
1	F	46	LEU	2.4
1	C	40	PRO	2.4
1	B	37	VAL	2.4
1	F	309	THR	2.4
1	A	54	PRO	2.4
1	B	312	ILE	2.4
1	E	312	ILE	2.4
1	G	55	MET	2.4
1	H	47	ASP	2.4
1	D	312	ILE	2.4
1	A	293	SER	2.4
1	B	324	SER	2.3
1	E	49	LEU	2.3
1	B	30	ASN	2.3
1	F	319	ASN	2.3
1	H	46	LEU	2.3
1	E	52	VAL	2.3
1	B	262	GLU	2.3
1	G	26	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	32	LEU	2.3
1	C	297	GLY	2.3
1	G	290	GLN	2.3
1	B	41	ASP	2.3
1	B	344	THR	2.3
1	C	343	THR	2.3
1	A	42	SER	2.3
1	B	308	ARG	2.2
1	E	262	GLU	2.2
1	G	292	MET	2.2
1	G	297	GLY	2.2
1	G	267	SER	2.2
1	A	316	TYR	2.2
1	H	321	GLN	2.2
1	H	297	GLY	2.2
1	A	321	GLN	2.1
1	A	297	GLY	2.1
1	B	40	PRO	2.1
1	H	319	ASN	2.1
1	H	312	ILE	2.1
1	E	25	PRO	2.1
1	A	318	LEU	2.1
1	A	52	VAL	2.1
1	B	326	MET	2.1
1	G	320	ALA	2.1
1	H	306	GLY	2.1
1	D	322	ASP	2.1
1	C	313	ALA	2.1
1	F	260	MET	2.1
1	H	243	HIS	2.1
1	H	260	MET	2.1
1	G	25	PRO	2.1
1	G	40	PRO	2.0
1	F	33	ARG	2.0
1	A	47	ASP	2.0
1	F	310	GLY	2.0
1	G	299	PHE	2.0
1	G	298	ILE	2.0
1	F	26	GLY	2.0
1	C	260	MET	2.0
1	B	321	GLN	2.0
1	B	297	GLY	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.