



Full wwPDB X-ray Structure Validation Report ⓘ

May 31, 2022 – 06:14 pm BST

PDB ID : 7QFZ
Title : BrxR, a WYL-domain containing transcriptional regulator
Authors : Picton, D.M.; Blower, T.R.
Deposited on : 2021-12-07
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.28.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28.1

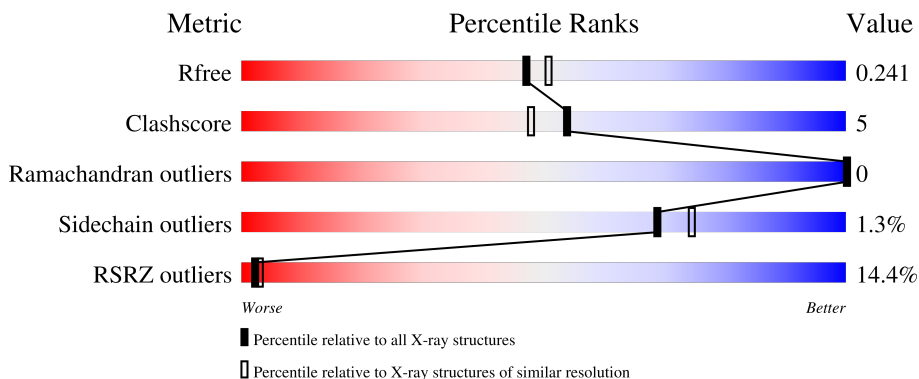
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



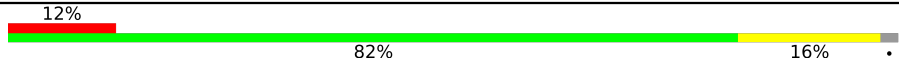

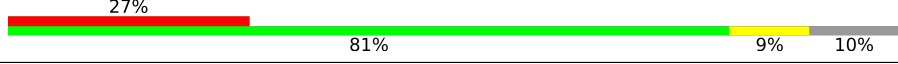
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	295	 4% 87% 10%
1	B	295	 14% 86% 10%
1	C	295	 6% 86% 12%
1	D	295	 6% 84% 15%
1	E	295	 17% 80% 16%

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Mol	Chain	Length	Quality of chain
1	F	295	 <p>12% 82% 16%</p>
1	G	295	 <p>25% 82% 13%</p>
1	H	295	 <p>27% 81% 9% 10%</p>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 19401 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 WYL domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	287	2323	1478	419	421	5	0	0	0
1	B	288	2330	1480	420	425	5	0	0	0
1	C	289	2338	1486	421	426	5	0	0	0
1	D	290	2342	1488	422	427	5	0	0	0
1	E	286	2312	1470	418	419	5	0	0	0
1	F	288	2330	1480	420	425	5	0	0	0
1	G	282	2291	1460	413	413	5	0	0	0
1	H	266	2171	1386	390	390	5	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP B7L3Y3
B	1	MET	-	initiating methionine	UNP B7L3Y3
C	1	MET	-	initiating methionine	UNP B7L3Y3
D	1	MET	-	initiating methionine	UNP B7L3Y3
E	1	MET	-	initiating methionine	UNP B7L3Y3
F	1	MET	-	initiating methionine	UNP B7L3Y3
G	1	MET	-	initiating methionine	UNP B7L3Y3
H	1	MET	-	initiating methionine	UNP B7L3Y3

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		

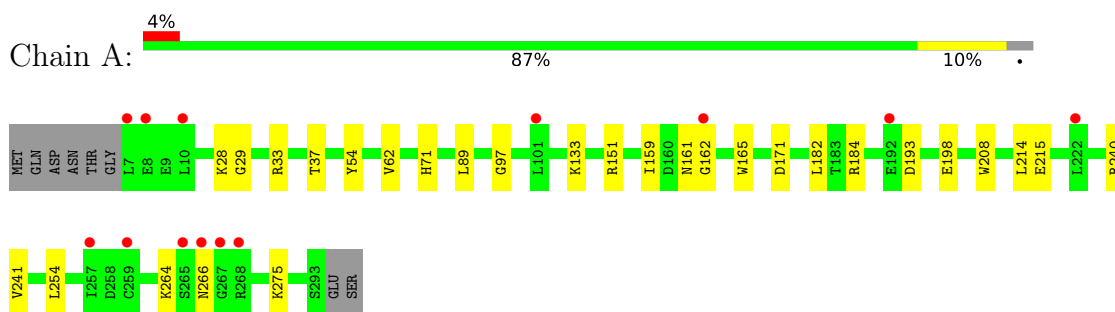
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	151	Total	O	0	0
			151	151		
3	B	155	Total	O	0	0
			155	155		
3	C	161	Total	O	0	0
			161	161		
3	D	157	Total	O	0	0
			157	157		
3	E	101	Total	O	0	0
			101	101		
3	F	79	Total	O	0	0
			79	79		
3	G	44	Total	O	0	0
			44	44		
3	H	36	Total	O	0	0
			36	36		

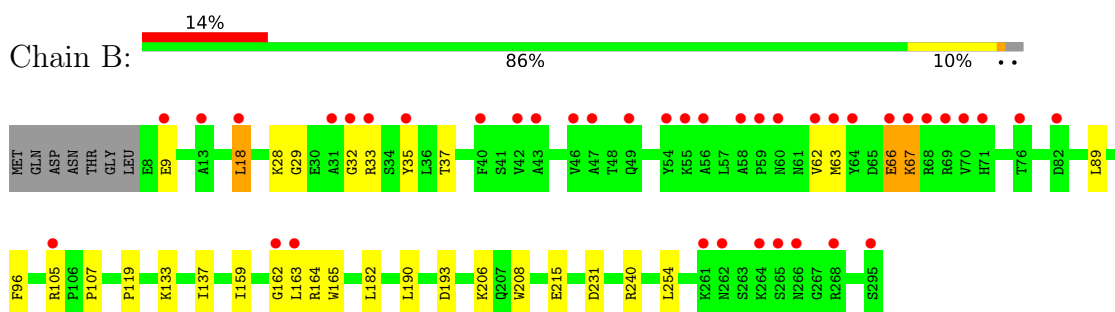
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

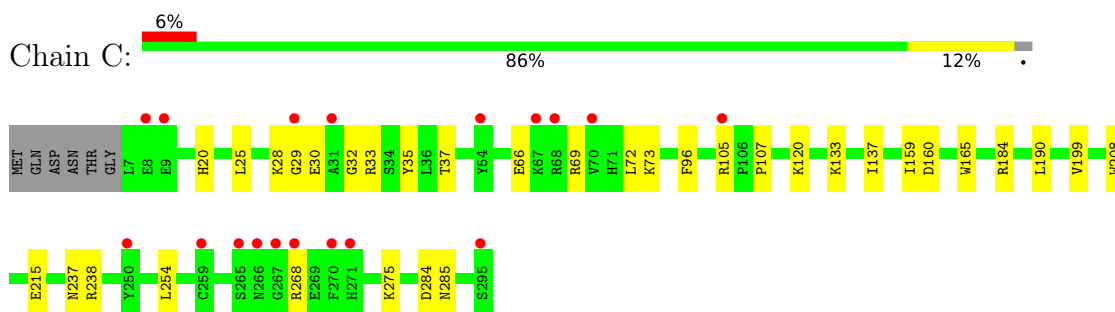
- Molecule 1: WYL domain-containing protein



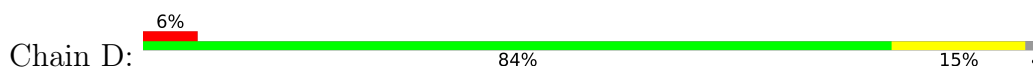
- Molecule 1: WYL domain-containing protein

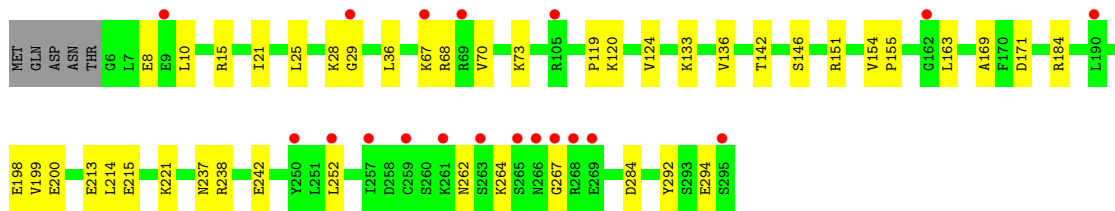


- Molecule 1: WYL domain-containing protein

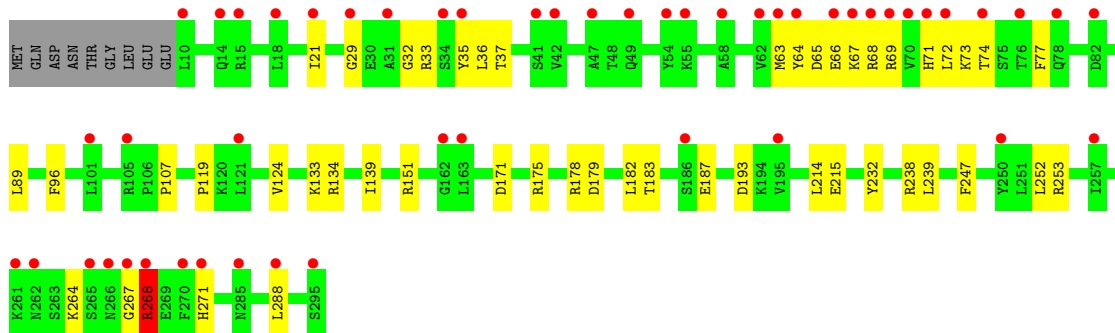
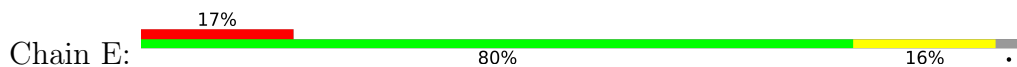


- Molecule 1: WYL domain-containing protein

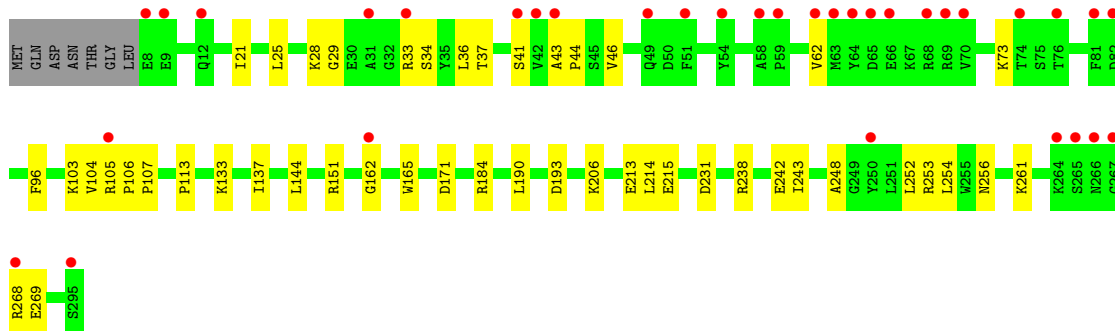
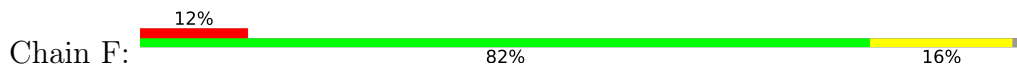




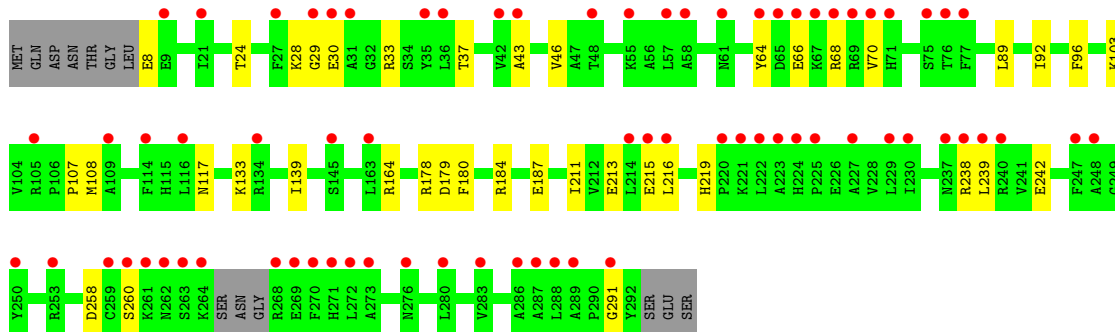
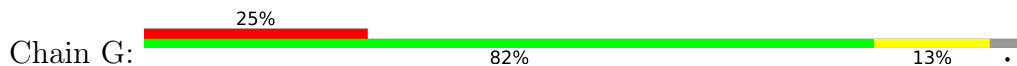
● Molecule 1: WYL domain-containing protein



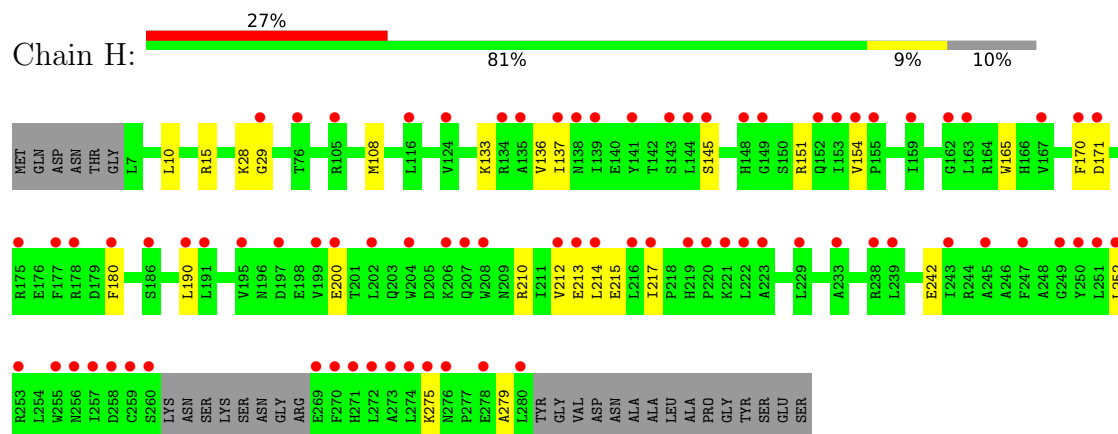
● Molecule 1: WYL domain-containing protein



● Molecule 1: WYL domain-containing protein



- Molecule 1: WYL domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	131.12Å 131.12Å 358.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.35 – 2.15 82.35 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (82.35-2.15) 99.9 (82.35-2.15)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.220 , 0.244 0.216 , 0.241	Depositor DCC
R_{free} test set	8437 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19401	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.46	0/2377	0.71	2/3219 (0.1%)
1	B	0.45	0/2384	0.71	1/3228 (0.0%)
1	C	0.49	0/2392	0.71	2/3239 (0.1%)
1	D	0.46	0/2396	0.72	2/3244 (0.1%)
1	E	0.44	0/2366	0.71	2/3204 (0.1%)
1	F	0.39	0/2384	0.67	1/3228 (0.0%)
1	G	0.36	0/2344	0.65	2/3173 (0.1%)
1	H	0.38	0/2221	0.66	1/3007 (0.0%)
All	All	0.43	0/18864	0.69	13/25542 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	LYS	C-N-CA	-9.15	103.08	122.30
1	D	28	LYS	C-N-CA	-7.88	105.75	122.30
1	H	28	LYS	C-N-CA	-7.68	106.17	122.30
1	C	28	LYS	C-N-CA	-7.65	106.23	122.30
1	G	117	ASN	N-CA-CB	6.95	123.11	110.60
1	C	199	VAL	CB-CA-C	6.70	124.13	111.40
1	F	28	LYS	C-N-CA	-6.54	108.57	122.30
1	B	28	LYS	C-N-CA	-6.23	109.22	122.30
1	G	28	LYS	C-N-CA	-6.22	109.24	122.30
1	D	146	SER	C-N-CA	-6.20	109.29	122.30
1	A	266	ASN	CB-CA-C	-6.15	98.11	110.40
1	E	268	ARG	N-CA-CB	6.03	121.46	110.60
1	E	74	THR	CB-CA-C	-5.04	98.00	111.60

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	2323	0	2310	24	0
1	B	2330	0	2310	22	0
1	C	2338	0	2321	23	0
1	D	2342	0	2324	27	0
1	E	2312	0	2298	37	0
1	F	2330	0	2310	49	0
1	G	2291	0	2279	27	0
1	H	2171	0	2164	20	0
2	A	10	0	0	1	0
2	B	10	0	0	0	0
2	C	10	0	0	1	0
2	D	10	0	0	1	0
2	E	10	0	0	0	0
2	F	10	0	0	2	0
2	G	10	0	0	1	0
2	H	10	0	0	1	0
3	A	151	0	0	1	0
3	B	155	0	0	1	0
3	C	161	0	0	2	0
3	D	157	0	0	3	0
3	E	101	0	0	3	0
3	F	79	0	0	2	0
3	G	44	0	0	5	0
3	H	36	0	0	0	0
All	All	19401	0	18316	194	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 5.

All (194) 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:E:253:ARG:HH11	1:F:268:ARG:HD2	1.28	0.98
1:A:97:GLY:HA3	3:A:471:HOH:O	1.66	0.95
1:E:271:HIS:CE1	1:F:144:LEU:CD1	2.52	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:271:HIS:CE1	1:F:144:LEU:HD13	2.05	0.90
1:E:29:GLY:HA3	1:F:133:LYS:HE3	1.55	0.88
1:F:261:LYS:HG3	3:F:403:HOH:O	1.75	0.87
1:G:30:GLU:OE1	1:G:70:VAL:HG11	1.82	0.80
1:B:159:ILE:HD11	1:B:208:TRP:HH2	1.53	0.73
1:E:288:LEU:HA	1:F:268:ARG:HH12	1.53	0.73
1:A:62:VAL:CG1	1:A:71:HIS:HB3	2.18	0.73
1:G:30:GLU:HB2	1:G:70:VAL:CG1	2.18	0.73
1:A:159:ILE:HD11	1:A:208:TRP:HH2	1.53	0.72
1:G:8:GLU:N	3:G:402:HOH:O	2.22	0.72
1:A:254:LEU:O	1:B:163:LEU:HD21	1.90	0.72
1:H:213:GLU:HG2	1:H:242:GLU:HG2	1.73	0.71
1:E:288:LEU:HA	1:F:268:ARG:NH1	2.06	0.71
1:B:215:GLU:OE2	1:B:240:ARG:NH1	2.26	0.68
1:F:105:ARG:HG3	1:F:106:PRO:HD2	1.76	0.68
1:C:29:GLY:HA3	1:D:133:LYS:HE3	1.74	0.68
1:A:62:VAL:HG11	1:A:71:HIS:HB3	1.76	0.67
1:G:216:LEU:HD12	1:G:239:LEU:HD23	1.78	0.65
1:C:159:ILE:HD11	1:C:208:TRP:HH2	1.61	0.65
1:E:133:LYS:HE3	1:F:29:GLY:HA3	1.77	0.65
1:F:105:ARG:CG	1:F:106:PRO:HD2	2.27	0.65
1:A:215:GLU:OE2	1:A:240:ARG:NH1	2.31	0.63
1:C:33:ARG:NH1	3:C:401:HOH:O	2.30	0.63
1:H:137:ILE:HG22	1:H:190:LEU:HA	1.82	0.62
1:E:134:ARG:NH1	3:E:402:HOH:O	2.32	0.62
1:F:268:ARG:HD3	1:F:269:GLU:H	1.63	0.62
1:F:151:ARG:HD3	1:F:171:ASP:OD1	1.99	0.62
1:A:29:GLY:HA3	1:B:133:LYS:HE3	1.80	0.62
1:C:184:ARG:NH1	2:C:302:SO4:O1	2.33	0.61
1:C:133:LYS:HE3	1:D:29:GLY:HA3	1.82	0.60
1:F:184:ARG:NH1	2:F:302:SO4:O2	2.35	0.60
1:G:29:GLY:HA3	1:H:133:LYS:HE3	1.82	0.60
1:G:215:GLU:OE2	1:G:238:ARG:NE	2.36	0.59
1:F:151:ARG:NH2	2:F:301:SO4:O2	2.36	0.58
1:E:183:THR:HG23	3:E:446:HOH:O	2.04	0.58
1:B:206:LYS:HE3	3:B:517:HOH:O	2.03	0.58
1:F:162:GLY:HA3	1:F:254:LEU:HD22	1.85	0.57
1:E:175:ARG:NH2	3:E:404:HOH:O	2.36	0.57
1:G:64:TYR:CE2	1:G:66:GLU:HG2	2.39	0.56
1:E:271:HIS:ND1	1:F:144:LEU:HD11	2.20	0.56
1:A:151:ARG:HD3	1:A:171:ASP:OD1	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:SER:HA	1:F:37:THR:HG22	1.88	0.56
1:A:133:LYS:HE3	1:B:29:GLY:HA3	1.88	0.55
1:H:217:ILE:HG21	1:H:275:LYS:HB2	1.88	0.55
1:F:25:LEU:HD11	1:F:62:VAL:CG2	2.37	0.55
1:B:159:ILE:HD11	1:B:208:TRP:CH2	2.39	0.55
1:H:217:ILE:CG2	1:H:275:LYS:HB2	2.36	0.55
1:B:105:ARG:NH1	1:D:198:GLU:OE2	2.40	0.55
1:A:151:ARG:NH2	2:A:301:SO4:O2	2.40	0.54
1:A:159:ILE:HD11	1:A:208:TRP:CH2	2.38	0.54
1:G:178:ARG:HG2	1:G:179:ASP:N	2.22	0.54
1:F:215:GLU:OE2	1:F:238:ARG:NH1	2.37	0.54
1:C:215:GLU:OE2	1:C:275:LYS:HD3	2.08	0.54
1:H:10:LEU:O	1:H:15:ARG:NH1	2.41	0.54
1:D:151:ARG:NH2	2:D:301:SO4:O3	2.39	0.53
1:E:268:ARG:HG2	1:F:253:ARG:HD3	1.89	0.53
1:H:212:VAL:HG13	1:H:279:ALA:HB1	1.90	0.53
1:H:151:ARG:HD3	1:H:171:ASP:OD1	2.08	0.53
1:C:159:ILE:HD11	1:C:208:TRP:CH2	2.43	0.53
1:D:136:VAL:HG22	1:D:154:VAL:HG22	1.91	0.52
1:D:68:ARG:HB2	1:D:70:VAL:HG22	1.90	0.52
1:D:199:VAL:HG22	1:D:200:GLU:HG3	1.90	0.52
1:H:212:VAL:CG1	1:H:279:ALA:HB1	2.40	0.52
1:B:163:LEU:O	1:B:164:ARG:HD2	2.09	0.52
1:F:256:ASN:OD1	1:F:268:ARG:HG2	2.10	0.51
1:E:21:ILE:HD11	1:E:36:LEU:HD11	1.92	0.51
1:G:213:GLU:HG2	1:G:242:GLU:HG2	1.91	0.51
1:G:258:ASP:CG	3:G:407:HOH:O	2.48	0.51
1:G:184:ARG:NH1	2:G:302:SO4:O3	2.44	0.51
1:A:214:LEU:HB2	1:A:241:VAL:HG22	1.92	0.51
1:C:120:LYS:HA	1:C:120:LYS:HE2	1.92	0.50
1:E:271:HIS:ND1	1:F:144:LEU:CD1	2.73	0.50
1:F:137:ILE:HG22	1:F:190:LEU:HA	1.93	0.50
1:B:162:GLY:HA3	1:B:254:LEU:HD22	1.94	0.50
1:E:214:LEU:HD13	1:E:252:LEU:HD21	1.94	0.50
1:G:216:LEU:HB2	1:G:239:LEU:HB3	1.93	0.50
1:C:96:PHE:CE2	1:C:107:PRO:HB3	2.47	0.50
1:G:219:HIS:NE2	1:G:258:ASP:OD2	2.36	0.49
1:A:184:ARG:NH1	1:B:231:ASP:OD2	2.44	0.49
1:G:33:ARG:O	1:G:37:THR:HG23	2.12	0.49
1:E:271:HIS:CE1	1:F:144:LEU:HD11	2.46	0.49
1:F:105:ARG:CG	1:F:106:PRO:CD	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:214:LEU:HD13	1:F:252:LEU:HD21	1.95	0.49
1:G:133:LYS:HE3	1:H:29:GLY:HA3	1.94	0.49
1:E:183:THR:OG1	1:F:231:ASP:OD1	2.23	0.48
1:C:215:GLU:OE2	1:C:238:ARG:NE	2.40	0.48
1:E:124:VAL:HG22	1:E:182:LEU:HD23	1.94	0.48
1:E:151:ARG:HD3	1:E:171:ASP:OD1	2.13	0.48
1:A:89:LEU:HB3	1:B:165:TRP:CZ2	2.48	0.48
1:H:136:VAL:HG22	1:H:154:VAL:HG22	1.94	0.48
1:E:288:LEU:O	1:F:268:ARG:NH2	2.46	0.48
1:C:254:LEU:O	1:D:163:LEU:HD21	2.15	0.47
1:F:105:ARG:HG3	1:F:106:PRO:CD	2.43	0.47
1:E:267:GLY:O	1:E:268:ARG:NH1	2.48	0.47
1:C:20:HIS:HD2	3:D:405:HOH:O	1.98	0.47
1:G:24:THR:HG22	1:G:30:GLU:O	2.15	0.47
1:A:198:GLU:OE2	1:C:105:ARG:NH1	2.48	0.47
1:F:37:THR:O	1:F:41:SER:HA	2.15	0.47
1:C:215:GLU:CD	1:C:275:LYS:HD3	2.35	0.46
1:H:170:PHE:CD2	1:H:200:GLU:HG2	2.50	0.46
1:A:33:ARG:O	1:A:37:THR:HG23	2.16	0.46
1:B:32:GLY:H	1:B:35:TYR:HD2	1.63	0.46
1:C:32:GLY:H	1:C:35:TYR:HD2	1.63	0.46
1:F:25:LEU:CD1	1:F:62:VAL:HG22	2.45	0.46
1:E:178:ARG:NH1	1:E:179:ASP:O	2.49	0.46
1:A:29:GLY:HA3	1:B:133:LYS:CE	2.46	0.46
1:A:215:GLU:OE1	1:A:275:LYS:HD3	2.15	0.46
1:F:206:LYS:HE3	3:F:472:HOH:O	2.15	0.46
1:F:21:ILE:HD11	1:F:36:LEU:HD11	1.97	0.46
1:F:213:GLU:HG2	1:F:242:GLU:HG2	1.97	0.46
1:F:33:ARG:HH21	1:F:44:PRO:C	2.19	0.45
1:H:214:LEU:HD13	1:H:252:LEU:HD21	1.98	0.45
1:F:105:ARG:HG2	1:F:106:PRO:HD2	1.98	0.45
1:A:161:ASN:O	1:A:162:GLY:C	2.54	0.45
1:F:25:LEU:CD1	1:F:62:VAL:CG2	2.94	0.45
1:G:68:ARG:O	1:G:70:VAL:HG23	2.16	0.45
1:G:178:ARG:HD3	1:G:180:PHE:CZ	2.51	0.45
1:D:10:LEU:O	1:D:15:ARG:NH1	2.48	0.45
1:E:133:LYS:CE	1:F:29:GLY:HA3	2.46	0.45
1:F:96:PHE:CE2	1:F:107:PRO:HB3	2.52	0.45
1:C:30:GLU:HB3	1:C:72:LEU:HD23	1.99	0.45
1:A:165:TRP:CZ2	1:B:89:LEU:HB3	2.51	0.45
1:D:237:ASN:ND2	3:D:409:HOH:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:253:ARG:HD3	1:F:268:ARG:NE	2.32	0.45
1:G:43:ALA:HB3	1:G:46:VAL:HG23	1.98	0.45
1:G:211:ILE:O	3:G:401:HOH:O	2.21	0.45
1:E:64:TYR:HE2	1:E:71:HIS:NE2	2.15	0.45
1:E:215:GLU:OE2	1:E:238:ARG:HD3	2.17	0.45
1:B:119:PRO:HB3	1:B:182:LEU:HB3	1.99	0.45
1:D:215:GLU:OE2	1:D:238:ARG:NH1	2.42	0.45
1:E:247:PHE:CE2	1:F:113:PRO:HG3	2.52	0.45
1:B:67:LYS:HA	1:B:67:LYS:HD2	1.72	0.44
1:G:103:LYS:NZ	3:G:413:HOH:O	2.49	0.44
1:G:260:SER:HA	1:G:291:GLY:O	2.18	0.44
1:H:210:ARG:NE	1:H:212:VAL:HG22	2.32	0.44
1:D:213:GLU:HG2	1:D:242:GLU:HG2	1.99	0.44
1:D:214:LEU:HD13	1:D:252:LEU:HD21	2.00	0.44
1:A:54:TYR:HE2	1:A:62:VAL:CG2	2.31	0.44
1:A:162:GLY:HA3	1:A:254:LEU:HD22	1.99	0.44
1:D:25:LEU:O	1:D:73:LYS:HD2	2.18	0.44
1:D:151:ARG:HD3	1:D:171:ASP:OD1	2.17	0.44
1:C:25:LEU:O	1:C:73:LYS:HD3	2.18	0.43
1:D:119:PRO:HB2	1:D:124:VAL:CG2	2.48	0.43
1:B:66:GLU:H	1:B:66:GLU:HG3	1.47	0.43
1:H:170:PHE:CE2	1:H:200:GLU:HG2	2.53	0.43
1:D:142:THR:O	1:D:184:ARG:HD2	2.18	0.43
1:A:165:TRP:HB3	1:A:182:LEU:HD22	2.00	0.43
1:C:160:ASP:HB2	1:C:165:TRP:CZ2	2.52	0.43
1:D:264:LYS:HD3	1:D:267:GLY:HA2	2.00	0.43
1:E:253:ARG:NH1	1:F:268:ARG:HD2	2.12	0.43
1:F:103:LYS:HE2	1:F:104:VAL:O	2.18	0.43
1:D:292:TYR:OH	1:D:294:GLU:HG3	2.19	0.43
1:F:25:LEU:O	1:F:73:LYS:HD2	2.19	0.43
3:G:421:HOH:O	1:H:108:MET:HE3	2.19	0.43
1:C:33:ARG:O	1:C:37:THR:HG23	2.19	0.43
1:G:96:PHE:CE2	1:G:107:PRO:HB3	2.54	0.43
1:G:30:GLU:HB2	1:G:70:VAL:HG12	2.00	0.42
1:D:8:GLU:H	1:D:8:GLU:CD	2.22	0.42
1:F:243:ILE:HD12	1:F:248:ALA:HA	2.02	0.42
1:C:137:ILE:HG22	1:C:190:LEU:HA	2.02	0.42
1:E:232:TYR:HB3	1:E:239:LEU:HD22	2.01	0.42
1:G:92:ILE:HB	1:G:108:MET:HE2	2.02	0.42
1:E:33:ARG:O	1:E:37:THR:HG23	2.20	0.42
1:E:288:LEU:CA	1:F:268:ARG:HH12	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:LEU:HD12	1:B:18:LEU:HA	1.77	0.42
1:H:210:ARG:HE	1:H:212:VAL:HG22	1.85	0.42
1:C:237:ASN:ND2	3:C:403:HOH:O	2.39	0.41
1:D:21:ILE:HD11	1:D:36:LEU:HD11	2.02	0.41
1:E:89:LEU:HB3	1:F:165:TRP:CZ2	2.55	0.41
1:D:120:LYS:O	1:D:124:VAL:HG23	2.20	0.41
1:F:162:GLY:HA3	1:F:254:LEU:CD2	2.50	0.41
1:D:262:ASN:OD1	1:D:262:ASN:O	2.38	0.41
1:D:155:PRO:HA	1:D:169:ALA:HB2	2.03	0.41
1:D:221:LYS:HD2	1:D:264:LYS:HE3	2.03	0.41
1:E:32:GLY:H	1:E:35:TYR:HD2	1.68	0.41
1:H:145:SER:OG	2:H:301:SO4:O1	2.35	0.41
1:B:96:PHE:CE2	1:B:107:PRO:HB3	2.56	0.41
1:G:89:LEU:HB3	1:H:165:TRP:CZ2	2.56	0.41
1:H:151:ARG:HD2	1:H:180:PHE:CE1	2.56	0.41
1:B:33:ARG:O	1:B:37:THR:HG23	2.21	0.41
1:B:137:ILE:HG22	1:B:190:LEU:HA	2.03	0.41
1:C:29:GLY:HA3	1:D:133:LYS:CE	2.48	0.41
1:G:139:ILE:HA	1:G:187:GLU:O	2.21	0.41
1:E:139:ILE:HA	1:E:187:GLU:O	2.22	0.40
1:C:284:ASP:O	1:C:285:ASN:HB2	2.21	0.40
1:E:73:LYS:HG3	1:E:77:PHE:CD2	2.56	0.40
1:F:43:ALA:HB3	1:F:46:VAL:HG23	2.03	0.40
1:A:264:LYS:HE2	1:A:264:LYS:HB2	1.77	0.40
1:E:96:PHE:CE2	1:E:107:PRO:HB3	2.56	0.40
1:E:119:PRO:HB3	1:E:182:LEU:HB3	2.03	0.40
1:D:284:ASP:OD1	3:D:401:HOH: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	285/295 (97%)	274 (96%)	11 (4%)	0	100	100
1	B	286/295 (97%)	274 (96%)	12 (4%)	0	100	100
1	C	287/295 (97%)	280 (98%)	7 (2%)	0	100	100
1	D	288/295 (98%)	280 (97%)	8 (3%)	0	100	100
1	E	284/295 (96%)	274 (96%)	10 (4%)	0	100	100
1	F	286/295 (97%)	278 (97%)	8 (3%)	0	100	100
1	G	278/295 (94%)	270 (97%)	8 (3%)	0	100	100
1	H	262/295 (89%)	255 (97%)	7 (3%)	0	100	100
All	All	2256/2360 (96%)	2185 (97%)	71 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	247/254 (97%)	246 (100%)	1 (0%)	91	93
1	B	248/254 (98%)	241 (97%)	7 (3%)	43	44
1	C	249/254 (98%)	246 (99%)	3 (1%)	71	76
1	D	249/254 (98%)	248 (100%)	1 (0%)	91	93
1	E	246/254 (97%)	236 (96%)	10 (4%)	30	29
1	F	248/254 (98%)	247 (100%)	1 (0%)	91	93
1	G	243/254 (96%)	242 (100%)	1 (0%)	91	93
1	H	232/254 (91%)	231 (100%)	1 (0%)	91	93
All	All	1962/2032 (97%)	1937 (99%)	25 (1%)	69	74

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	ASP
1	B	9	GLU

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Mol	Chain	Res	Type
1	B	18	LEU
1	B	62	VAL
1	B	63	MET
1	B	66	GLU
1	B	67	LYS
1	B	193	ASP
1	C	66	GLU
1	C	69	ARG
1	C	268	ARG
1	D	67	LYS
1	E	63	MET
1	E	65	ASP
1	E	66	GLU
1	E	67	LYS
1	E	68	ARG
1	E	69	ARG
1	E	72	LEU
1	E	193	ASP
1	E	264	LYS
1	E	268	ARG
1	F	193	ASP
1	G	164	ARG
1	H	215	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	ASN
1	C	266	ASN
1	E	256	ASN
1	E	271	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	B	301	-	4,4,4	0.18	0	6,6,6	0.39	0
2	SO4	H	302	-	4,4,4	0.14	0	6,6,6	0.18	0
2	SO4	D	301	-	4,4,4	0.23	0	6,6,6	0.55	0
2	SO4	D	302	-	4,4,4	0.25	0	6,6,6	0.64	0
2	SO4	E	302	-	4,4,4	0.20	0	6,6,6	0.34	0
2	SO4	F	302	-	4,4,4	0.12	0	6,6,6	0.23	0
2	SO4	H	301	-	4,4,4	0.16	0	6,6,6	0.11	0
2	SO4	A	302	-	4,4,4	0.17	0	6,6,6	0.73	0
2	SO4	A	301	-	4,4,4	0.16	0	6,6,6	0.22	0
2	SO4	G	301	-	4,4,4	0.19	0	6,6,6	0.28	0
2	SO4	C	301	-	4,4,4	0.15	0	6,6,6	0.37	0
2	SO4	G	302	-	4,4,4	0.16	0	6,6,6	0.21	0
2	SO4	B	302	-	4,4,4	0.21	0	6,6,6	0.64	0
2	SO4	F	301	-	4,4,4	0.23	0	6,6,6	0.21	0
2	SO4	C	302	-	4,4,4	0.13	0	6,6,6	0.67	0
2	SO4	E	301	-	4,4,4	0.13	0	6,6,6	0.25	0

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.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	SO4	1	0
2	F	302	SO4	1	0
2	H	301	SO4	1	0
2	A	301	SO4	1	0
2	G	302	SO4	1	0
2	F	301	SO4	1	0
2	C	302	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	287/295 (97%)	0.66	13 (4%) 33 42	33, 46, 68, 96	0
1	B	288/295 (97%)	1.05	40 (13%) 2 3	33, 45, 89, 118	0
1	C	289/295 (97%)	0.75	18 (6%) 20 27	32, 43, 73, 106	0
1	D	290/295 (98%)	0.79	19 (6%) 18 24	33, 45, 80, 100	0
1	E	286/295 (96%)	1.11	50 (17%) 1 1	39, 55, 101, 126	0
1	F	288/295 (97%)	0.98	34 (11%) 4 6	39, 56, 91, 118	0
1	G	282/295 (95%)	1.45	73 (25%) 0 0	48, 76, 105, 128	0
1	H	266/295 (90%)	1.66	80 (30%) 0 0	43, 83, 111, 133	0
All	All	2276/2360 (96%)	1.05	327 (14%) 2 3	32, 53, 102, 133	0

All (327) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	265	SER	15.1
1	H	199	VAL	9.8
1	G	69	ARG	9.7
1	G	70	VAL	9.6
1	F	267	GLY	9.2
1	C	267	GLY	9.1
1	H	170	PHE	9.0
1	H	154	VAL	8.6
1	G	66	GLU	8.4
1	H	214	LEU	8.4
1	F	70	VAL	8.3
1	H	250	TYR	8.2
1	H	190	LEU	8.1
1	B	67	LYS	7.7
1	G	268	ARG	7.5
1	E	68	ARG	7.4

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Mol	Chain	Res	Type	RSRZ
1	B	268	ARG	6.8
1	H	223	ALA	6.7
1	H	163	LEU	6.7
1	E	267	GLY	6.7
1	H	249	GLY	6.6
1	H	238	ARG	6.6
1	F	9	GLU	6.5
1	H	177	PHE	6.4
1	F	64	TYR	6.3
1	E	271	HIS	6.2
1	F	265	SER	6.2
1	G	263	SER	6.2
1	H	217	ILE	6.1
1	H	208	TRP	6.1
1	B	295	SER	6.0
1	G	64	TYR	5.9
1	D	267	GLY	5.9
1	G	68	ARG	5.8
1	C	266	ASN	5.7
1	D	295	SER	5.6
1	E	66	GLU	5.6
1	H	275	LYS	5.6
1	E	72	LEU	5.6
1	H	155	PRO	5.5
1	B	264	LYS	5.5
1	G	58	ALA	5.5
1	F	268	ARG	5.4
1	G	65	ASP	5.4
1	H	149	GLY	5.4
1	G	269	GLU	5.4
1	D	268	ARG	5.4
1	H	180	PHE	5.3
1	E	261	LYS	5.3
1	G	109	ALA	5.3
1	E	63	MET	5.3
1	G	222	LEU	5.3
1	H	219	HIS	5.2
1	H	269	GLU	5.2
1	E	42	VAL	5.2
1	A	267	GLY	5.1
1	F	266	ASN	5.0
1	H	259	CYS	5.0

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Mol	Chain	Res	Type	RSRZ
1	G	264	LYS	5.0
1	H	162	GLY	5.0
1	E	295	SER	4.9
1	H	255	TRP	4.9
1	H	195	VAL	4.8
1	H	206	LYS	4.8
1	E	14	GLN	4.8
1	H	145	SER	4.7
1	H	202	LEU	4.6
1	F	69	ARG	4.5
1	B	163	LEU	4.5
1	G	43	ALA	4.5
1	H	253	ARG	4.5
1	G	247	PHE	4.5
1	H	152	GLN	4.5
1	H	216	LEU	4.4
1	A	265	SER	4.4
1	E	54	TYR	4.4
1	G	289	ALA	4.4
1	B	66	GLU	4.4
1	H	141	TYR	4.4
1	F	68	ARG	4.4
1	G	105	ARG	4.4
1	G	31	ALA	4.4
1	G	223	ALA	4.3
1	H	252	LEU	4.3
1	E	31	ALA	4.2
1	E	266	ASN	4.2
1	G	61	ASN	4.2
1	B	35	TYR	4.2
1	B	68	ARG	4.2
1	H	212	VAL	4.1
1	G	220	PRO	4.1
1	G	163	LEU	4.1
1	G	21	ILE	4.1
1	G	75	SER	4.1
1	H	257	ILE	4.1
1	A	162	GLY	4.0
1	B	13	ALA	4.0
1	E	70	VAL	4.0
1	G	76	THR	4.0
1	D	263	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	77	PHE	4.0
1	G	238	ARG	4.0
1	G	248	ALA	4.0
1	D	162	GLY	3.9
1	H	135	ALA	3.9
1	H	271	HIS	3.9
1	H	134	ARG	3.9
1	B	46	VAL	3.9
1	B	49	GLN	3.9
1	G	237	ASN	3.9
1	G	9	GLU	3.8
1	H	280	LEU	3.8
1	B	62	VAL	3.8
1	G	30	GLU	3.7
1	G	230	ILE	3.7
1	A	8	GLU	3.7
1	B	58	ALA	3.7
1	B	162	GLY	3.7
1	F	12	GLN	3.6
1	F	63	MET	3.6
1	H	204	TRP	3.6
1	B	266	ASN	3.6
1	F	8	GLU	3.6
1	C	271	HIS	3.5
1	H	274	LEU	3.5
1	G	215	GLU	3.5
1	D	266	ASN	3.5
1	E	82	ASP	3.5
1	B	31	ALA	3.5
1	H	243	ILE	3.4
1	G	224	HIS	3.4
1	E	101	LEU	3.3
1	B	54	TYR	3.3
1	D	269	GLU	3.3
1	H	245	ALA	3.3
1	G	229	LEU	3.3
1	B	56	ALA	3.3
1	E	163	LEU	3.3
1	H	239	LEU	3.2
1	H	272	LEU	3.2
1	C	295	SER	3.2
1	G	214	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	63	MET	3.2
1	H	138	ASN	3.2
1	H	144	LEU	3.2
1	G	55	LYS	3.2
1	B	265	SER	3.2
1	H	276	ASN	3.2
1	A	268	ARG	3.2
1	H	137	ILE	3.2
1	E	76	THR	3.2
1	H	167	VAL	3.2
1	B	71	HIS	3.1
1	F	43	ALA	3.1
1	F	66	GLU	3.1
1	F	59	PRO	3.1
1	A	266	ASN	3.1
1	E	62	VAL	3.1
1	B	43	ALA	3.1
1	B	18	LEU	3.1
1	C	70	VAL	3.0
1	E	67	LYS	3.0
1	F	250	TYR	3.0
1	G	71	HIS	3.0
1	F	81	PHE	3.0
1	E	15	ARG	3.0
1	B	59	PRO	3.0
1	F	62	VAL	2.9
1	C	68	ARG	2.9
1	E	35	TYR	2.9
1	G	57	LEU	2.9
1	H	256	ASN	2.9
1	H	221	LYS	2.9
1	H	222	LEU	2.9
1	F	33	ARG	2.9
1	F	41	SER	2.9
1	H	233	ALA	2.9
1	G	288	LEU	2.9
1	B	82	ASP	2.9
1	E	74	THR	2.9
1	F	105	ARG	2.9
1	G	145	SER	2.8
1	F	76	THR	2.8
1	H	105	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	278	GLU	2.8
1	B	32	GLY	2.8
1	H	116	LEU	2.8
1	G	48	THR	2.8
1	G	259	CYS	2.8
1	G	225	PRO	2.8
1	H	220	PRO	2.8
1	E	71	HIS	2.8
1	G	271	HIS	2.8
1	B	261	LYS	2.8
1	H	143	SER	2.7
1	E	18	LEU	2.7
1	G	36	LEU	2.7
1	H	273	ALA	2.7
1	G	42	VAL	2.7
1	H	207	GLN	2.7
1	F	264	LYS	2.7
1	B	42	VAL	2.7
1	B	33	ARG	2.7
1	F	54	TYR	2.7
1	G	35	TYR	2.7
1	G	250	TYR	2.7
1	H	197	ASP	2.7
1	G	221	LYS	2.7
1	G	276	ASN	2.7
1	C	265	SER	2.6
1	C	29	GLY	2.6
1	E	162	GLY	2.6
1	B	76	THR	2.6
1	F	51	PHE	2.6
1	A	192	GLU	2.6
1	E	64	TYR	2.6
1	H	148	HIS	2.6
1	F	162	GLY	2.6
1	G	239	LEU	2.6
1	F	42	VAL	2.6
1	H	258	ASP	2.6
1	C	268	ARG	2.6
1	H	178	ARG	2.6
1	E	41	SER	2.6
1	B	262	ASN	2.6
1	G	272	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	286	ALA	2.5
1	H	29	GLY	2.5
1	H	175	ARG	2.5
1	H	260	SER	2.5
1	E	10	LEU	2.5
1	E	29	GLY	2.5
1	G	29	GLY	2.5
1	G	67	LYS	2.5
1	H	159	ILE	2.5
1	E	121	LEU	2.5
1	H	229	LEU	2.5
1	D	250	TYR	2.5
1	B	9	GLU	2.5
1	C	31	ALA	2.5
1	H	247	PHE	2.5
1	B	69	ARG	2.4
1	G	253	ARG	2.4
1	C	54	TYR	2.4
1	E	47	ALA	2.4
1	G	216	LEU	2.4
1	C	8	GLU	2.4
1	B	47	ALA	2.4
1	F	65	ASP	2.4
1	F	295	SER	2.4
1	B	60	ASN	2.4
1	D	257	ILE	2.4
1	E	58	ALA	2.4
1	H	153	ILE	2.4
1	G	262	ASN	2.4
1	G	260	SER	2.4
1	H	200	GLU	2.4
1	A	259	CYS	2.4
1	C	67	LYS	2.4
1	C	105	ARG	2.4
1	E	78	GLN	2.4
1	F	49	GLN	2.4
1	H	139	ILE	2.4
1	C	270	PHE	2.3
1	B	55	LYS	2.3
1	H	124	VAL	2.3
1	D	105	ARG	2.3
1	G	273	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	283	VAL	2.3
1	F	58	ALA	2.3
1	F	74	THR	2.3
1	A	10	LEU	2.3
1	A	101	LEU	2.3
1	E	270	PHE	2.3
1	G	261	LYS	2.3
1	D	69	ARG	2.3
1	E	186	SER	2.3
1	E	285	ASN	2.3
1	A	257	ILE	2.3
1	C	250	TYR	2.2
1	H	191	LEU	2.2
1	E	49	GLN	2.2
1	E	288	LEU	2.2
1	G	240	ARG	2.2
1	G	270	PHE	2.2
1	D	261	LYS	2.2
1	F	82	ASP	2.2
1	H	76	THR	2.2
1	E	69	ARG	2.2
1	F	31	ALA	2.2
1	D	190	LEU	2.2
1	G	280	LEU	2.2
1	B	64	TYR	2.2
1	E	250	TYR	2.2
1	G	114	PHE	2.2
1	H	213	GLU	2.2
1	C	9	GLU	2.2
1	D	9	GLU	2.2
1	E	265	SER	2.2
1	G	291	GLY	2.2
1	E	105	ARG	2.2
1	E	21	ILE	2.1
1	G	116	LEU	2.1
1	B	40	PHE	2.1
1	E	257	ILE	2.1
1	E	268	ARG	2.1
1	G	287	ALA	2.1
1	G	134	ARG	2.1
1	H	251	LEU	2.1
1	B	70	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	186	SER	2.1
1	E	262	ASN	2.1
1	E	55	LYS	2.1
1	G	227	ALA	2.1
1	D	29	GLY	2.1
1	A	7	LEU	2.1
1	A	222	LEU	2.1
1	B	105	ARG	2.1
1	H	171	ASP	2.1
1	D	67	LYS	2.1
1	D	259	CYS	2.1
1	E	195	VAL	2.0
1	G	27	PHE	2.0
1	H	270	PHE	2.0
1	E	34	SER	2.0
1	C	259	CYS	2.0
1	D	252	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	H	301	5/5	0.74	0.31	104,107,118,120	0
2	SO4	G	301	5/5	0.91	0.26	75,77,83,88	0
2	SO4	H	302	5/5	0.92	0.47	105,105,110,112	0
2	SO4	A	302	5/5	0.93	0.21	53,53,58,62	0
2	SO4	D	302	5/5	0.94	0.15	53,53,60,63	0
2	SO4	B	302	5/5	0.94	0.16	45,48,50,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	G	302	5/5	0.95	0.09	81,84,86,90	0
2	SO4	F	302	5/5	0.96	0.15	55,58,61,61	0
2	SO4	C	302	5/5	0.97	0.13	49,50,56,63	0
2	SO4	E	302	5/5	0.98	0.17	51,52,59,61	0
2	SO4	D	301	5/5	0.98	0.15	43,47,53,54	0
2	SO4	A	301	5/5	0.99	0.15	47,49,54,54	0
2	SO4	C	301	5/5	0.99	0.15	43,43,45,46	0
2	SO4	E	301	5/5	0.99	0.16	42,44,46,50	0
2	SO4	B	301	5/5	0.99	0.13	38,40,48,49	0
2	SO4	F	301	5/5	0.99	0.18	47,48,54,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.