



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:52 am BST

PDB ID : 4FIP
Title : Structure of the SAGA Ubp8(S144N)/Sgf11(1-72, Delta-ZnF)/Sus1/Sgf73 DUB module
Authors : Samara, N.L.; Ringel, A.E.; Wolberger, C.
Deposited on : 2012-06-10
Resolution : 2.69 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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

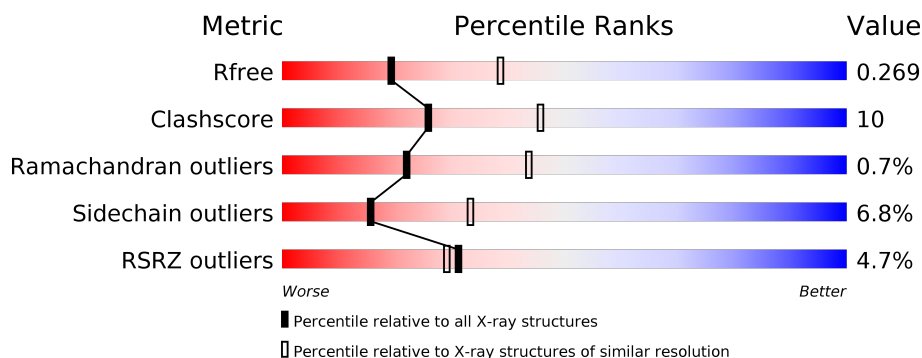
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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 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	476	
1	E	476	
2	B	96	
2	F	96	
3	C	72	
3	G	72	

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Mol	Chain	Length	Quality of chain
4	D	96	<div><div></div><div>7%</div><div>72%</div><div>18%</div><div>•</div><div>8%</div></div>
4	H	96	<div><div></div><div>11%</div><div>68%</div><div>19%</div><div>14%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10730 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 Ubiquitin carboxyl-terminal hydrolase 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3597	2276	618	667	36			
1	E	441	Total	C	N	O	S	0	0	0
			3534	2244	603	651	36			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	EXPRESSION TAG	UNP P50102
A	-3	ALA	-	EXPRESSION TAG	UNP P50102
A	-2	ALA	-	EXPRESSION TAG	UNP P50102
A	-1	ALA	-	EXPRESSION TAG	UNP P50102
A	0	ALA	-	EXPRESSION TAG	UNP P50102
A	144	ASN	SER	ENGINEERED MUTATION	UNP P50102
E	-4	GLY	-	EXPRESSION TAG	UNP P50102
E	-3	ALA	-	EXPRESSION TAG	UNP P50102
E	-2	ALA	-	EXPRESSION TAG	UNP P50102
E	-1	ALA	-	EXPRESSION TAG	UNP P50102
E	0	ALA	-	EXPRESSION TAG	UNP P50102
E	144	ASN	SER	ENGINEERED MUTATION	UNP P50102

- Molecule 2 is a protein called Protein SUS1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	90	Total	C	N	O	S	0	0	0
			727	455	119	151	2			
2	F	90	Total	C	N	O	S	0	1	0
			735	460	122	151	2			

- Molecule 3 is a protein called SAGA-associated factor 11.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	41	Total	C	N	O	0	0	0
			324	203	55	66			
3	G	43	Total	C	N	O	0	0	0
			342	213	57	72			

- Molecule 4 is a protein called SAGA-associated factor 73.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	88	Total	C	N	O	S	0	0	0
			695	439	115	137	4			
4	H	83	Total	C	N	O	S	1	0	0
			670	426	111	129	4			

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	Zn	0	0
			1	1		
5	A	6	Total	Zn	0	0
			6	6		
5	D	1	Total	Zn	0	0
			1	1		
5	E	6	Total	Zn	0	0
			6	6		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	34	Total	O	0	0
			34	34		
6	B	3	Total	O	0	0
			3	3		
6	C	1	Total	O	0	0
			1	1		
6	D	11	Total	O	0	0
			11	11		
6	E	34	Total	O	0	0
			34	34		
6	F	5	Total	O	0	0
			5	5		
6	G	1	Total	O	0	0
			1	1		

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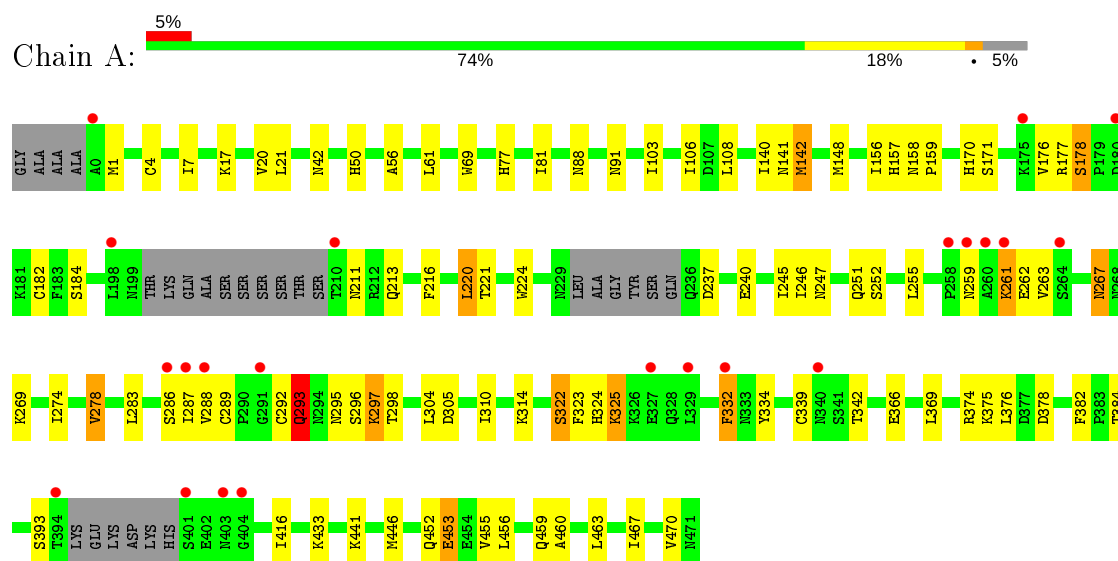
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	3	Total	O	0	0
			3	3		

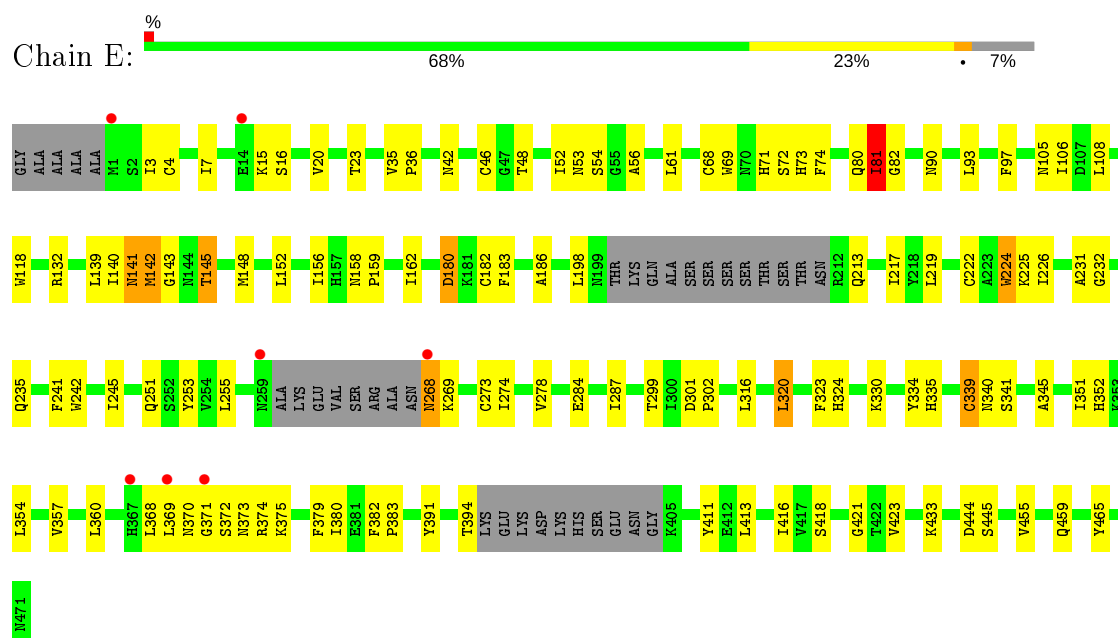
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Ubiquitin carboxyl-terminal hydrolase 8



- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 8




- Molecule 2: Protein SUS1

Chain B: 

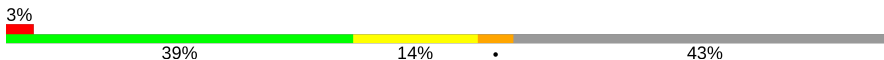


- Molecule 2: Protein SUS1

Chain F: 

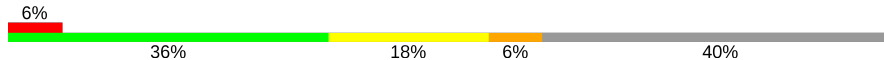


- Molecule 3: SAGA-associated factor 11

Chain C: 




- Molecule 3: SAGA-associated factor 11

Chain G: 



HIS

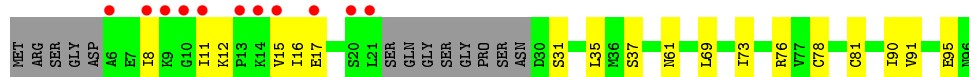
- Molecule 4: SAGA-associated factor 73

Chain D: 



- Molecule 4: SAGA-associated factor 73

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.97Å 79.97Å 274.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.18 – 2.69 47.18 – 2.69	Depositor EDS
% Data completeness (in resolution range)	91.0 (47.18-2.69) 91.0 (47.18-2.69)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.183 , 0.264 0.188 , 0.269	Depositor DCC
R_{free} test set	2199 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10730	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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: 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	0.71	1/3674 (0.0%)	0.78	1/4950 (0.0%)
1	E	0.68	2/3612 (0.1%)	0.77	2/4867 (0.0%)
2	B	0.62	0/733	0.75	0/988
2	F	0.62	0/744	0.75	0/1002
3	C	0.66	0/325	0.76	0/443
3	G	0.51	0/343	0.67	0/467
4	D	0.74	1/708 (0.1%)	0.83	0/954
4	H	0.67	0/683	0.76	0/919
All	All	0.68	4/10822 (0.0%)	0.77	3/14590 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	TRP	CD2-CE2	5.43	1.47	1.41
1	E	224	TRP	CD2-CE2	5.15	1.47	1.41
4	D	32	TRP	CD2-CE2	5.14	1.47	1.41
1	E	69	TRP	CD2-CE2	5.13	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	ASP	CB-CG-OD1	5.79	123.51	118.30
1	E	81	ILE	N-CA-C	5.55	125.98	111.00
1	E	132	ARG	NE-CZ-NH1	5.52	123.06	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3597	0	3504	66	0
1	E	3534	0	3445	92	0
2	B	727	0	734	16	0
2	F	735	0	747	19	0
3	C	324	0	341	15	0
3	G	342	0	353	27	0
4	D	695	0	685	11	0
4	H	670	0	672	13	0
5	A	6	0	0	0	0
5	D	1	0	0	0	0
5	E	6	0	0	0	0
5	H	1	0	0	0	0
6	A	34	0	0	0	0
6	B	3	0	0	0	0
6	C	1	0	0	0	0
6	D	11	0	0	0	0
6	E	34	0	0	0	0
6	F	5	0	0	0	0
6	G	1	0	0	0	0
6	H	3	0	0	0	0
All	All	10730	0	10481	221	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 10.

All (221) 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)
2:F:89:LEU:HD11	3:G:11:ILE:HD11	1.20	1.19
1:E:105:ASN:HD22	3:G:40:THR:HG21	1.03	1.09
3:G:36:GLN:O	3:G:40:THR:HG23	1.60	1.02
2:B:12:ILE:HG22	4:D:11:ILE:HD11	1.47	0.96
1:A:251:GLN:O	1:A:255:LEU:HD13	1.65	0.95
4:H:12:LYS:O	4:H:15:VAL:HG22	1.66	0.94
1:E:142:MET:CE	1:E:231:ALA:HB1	2.01	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:93:VAL:HG11	3:G:8:ILE:HD11	1.55	0.89
2:F:61:ILE:O	2:F:64:THR:HG22	1.73	0.89
2:F:93:VAL:HG11	3:G:8:ILE:CD1	2.04	0.87
1:E:105:ASN:ND2	3:G:40:THR:HG21	1.89	0.87
1:E:287:ILE:CG2	1:E:345:ALA:HB1	2.07	0.85
1:E:140:ILE:HD11	1:E:142:MET:HE1	1.58	0.82
2:B:12:ILE:HD13	2:B:89:LEU:HD21	1.62	0.81
2:F:89:LEU:CD1	3:G:11:ILE:HD11	2.08	0.81
1:A:213:GLN:HE22	1:E:139:LEU:HA	1.45	0.80
2:B:12:ILE:HD13	2:B:89:LEU:CD2	2.13	0.79
1:E:140:ILE:CD1	1:E:142:MET:HE1	2.15	0.76
1:E:142:MET:HE1	1:E:231:ALA:HB1	1.66	0.75
2:B:41:LYS:HB3	2:B:72:MET:HE1	1.67	0.75
2:B:41:LYS:HB3	2:B:72:MET:CE	2.18	0.73
3:C:7:THR:HG23	3:C:10:SER:HB3	1.71	0.72
3:G:11:ILE:HD12	3:G:12:SER:N	2.06	0.70
1:E:320:LEU:O	1:E:323:PHE:HB3	1.91	0.70
1:E:142:MET:HE2	1:E:231:ALA:HB1	1.74	0.69
1:A:142:MET:HE3	1:A:224:TRP:HB2	1.75	0.69
2:B:8:LEU:O	2:B:12:ILE:HG23	1.93	0.69
1:A:376:LEU:HD12	1:A:376:LEU:N	2.07	0.69
3:G:11:ILE:HD12	3:G:11:ILE:C	2.12	0.69
1:A:148:MET:HE3	1:A:220:LEU:HD21	1.77	0.67
1:E:235:GLN:OE1	1:E:423:VAL:HG12	1.93	0.67
2:F:89:LEU:HD11	3:G:11:ILE:CD1	2.13	0.67
2:B:32:ARG:NH1	2:B:80:THR:HG21	2.10	0.67
1:A:171:SER:O	1:A:177:ARG:NH1	2.28	0.66
1:E:287:ILE:HG22	1:E:345:ALA:HB1	1.77	0.66
1:E:140:ILE:CD1	1:E:142:MET:CE	2.74	0.65
1:E:71:HIS:HB2	1:E:73:HIS:CE1	2.31	0.65
1:E:224:TRP:CD1	1:E:231:ALA:HB2	2.32	0.64
1:E:416:ILE:HD12	1:E:455:VAL:HG13	1.79	0.64
1:A:322:SER:O	1:A:325:LYS:HD2	1.98	0.64
1:E:156:ILE:O	1:E:162:ILE:HD11	1.98	0.63
1:A:20:VAL:HG13	1:A:61:LEU:HD21	1.81	0.62
1:E:379:PHE:C	1:E:380:ILE:HD12	2.20	0.62
2:B:12:ILE:HD11	3:C:15:ILE:HD11	1.82	0.61
2:B:12:ILE:CD1	2:B:89:LEU:HD21	2.29	0.61
3:C:11:ILE:HD12	3:C:11:ILE:O	2.01	0.61
4:H:11:ILE:HG23	4:H:15:VAL:CG2	2.30	0.61
1:A:141:ASN:HD22	1:E:145:THR:HB	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:287:ILE:HG23	1:E:345:ALA:HB1	1.82	0.60
2:F:89:LEU:O	2:F:93:VAL:HG12	2.01	0.60
2:F:25:ILE:HD13	2:F:85:ILE:HG12	1.84	0.60
4:D:12:LYS:O	4:D:15:VAL:HG12	2.01	0.59
1:A:246:ILE:HD12	1:A:304:LEU:HD13	1.84	0.59
1:A:286:SER:HA	1:A:298:THR:HG22	1.84	0.59
1:E:148:MET:CE	1:E:241:PHE:CE1	2.86	0.58
1:E:52:ILE:N	1:E:52:ILE:HD13	2.17	0.58
1:E:268:ASN:N	1:E:269:LYS:HA	2.18	0.58
1:A:292:CYS:O	1:A:293:GLN:HB2	2.04	0.58
1:A:142:MET:CE	1:A:224:TRP:HB2	2.33	0.57
1:A:288:VAL:HG12	1:A:289:CYS:O	2.04	0.57
3:G:7:THR:HG22	3:G:10:SER:HB2	1.86	0.57
1:A:274:ILE:O	1:A:278:VAL:HG13	2.04	0.57
1:A:148:MET:CE	1:A:220:LEU:HD21	2.34	0.57
1:E:152:LEU:HD11	1:E:219:LEU:CD2	2.34	0.57
1:E:148:MET:HE2	1:E:241:PHE:CE1	2.40	0.56
4:D:48:HIS:NE2	4:D:67:ASP:OD1	2.37	0.56
1:A:156:ILE:C	1:A:156:ILE:HD12	2.26	0.56
2:F:75:ASP:OD1	2:F:75:ASP:N	2.39	0.56
3:C:6:ILE:HG22	3:C:6:ILE:O	2.05	0.56
2:B:57:ASN:HD22	2:B:60:GLN:H	1.55	0.55
2:F:93:VAL:CG1	3:G:8:ILE:HD11	2.33	0.55
1:A:156:ILE:HD12	1:A:157:HIS:ND1	2.21	0.55
1:E:335:HIS:HE1	1:E:340:ASN:HD22	1.53	0.55
3:G:7:THR:CG2	3:G:10:SER:HB2	2.37	0.55
1:E:46:CYS:HB2	1:E:68:CYS:HB3	1.89	0.54
1:A:56:ALA:H	3:C:25:GLN:NE2	2.05	0.54
1:E:284:GLU:HB2	1:E:352:HIS:HB2	1.90	0.54
2:F:7:GLN:O	2:F:7:GLN:CG	2.54	0.54
3:C:28:VAL:O	3:C:32:THR:HG23	2.06	0.54
1:A:376:LEU:N	1:A:376:LEU:CD1	2.71	0.54
2:F:78[A]:ARG:HG2	2:F:82:LEU:HD12	1.89	0.54
1:A:42:ASN:HB2	4:D:35:LEU:HD11	1.89	0.54
2:B:89:LEU:HD11	3:C:11:ILE:HD11	1.89	0.53
3:G:24:ILE:O	3:G:28:VAL:HG23	2.08	0.53
1:A:334:TYR:O	1:A:342:THR:HG22	2.09	0.53
1:E:287:ILE:CG2	1:E:345:ALA:CB	2.84	0.53
3:G:36:GLN:O	3:G:40:THR:CG2	2.46	0.53
3:C:9:ASP:OD2	4:D:5:ASP:N	2.42	0.53
1:A:324:HIS:O	1:A:324:HIS:CG	2.62	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:TRP:CE2	1:E:217:ILE:HG21	2.43	0.52
1:A:366:GLU:OE2	1:A:374:ARG:NH2	2.43	0.52
4:H:12:LYS:HB2	4:H:15:VAL:HG13	1.91	0.52
2:F:82:LEU:HG	3:G:16:LEU:HD22	1.92	0.52
3:C:7:THR:CG2	3:C:10:SER:HB3	2.37	0.51
1:E:42:ASN:HB3	4:H:35:LEU:HD11	1.92	0.51
1:E:48:THR:HG21	1:E:73:HIS:CD2	2.46	0.51
1:A:88:ASN:HB3	1:A:91:ASN:OD1	2.10	0.51
1:E:141:ASN:HD22	1:E:143:GLY:H	1.58	0.51
4:H:15:VAL:C	4:H:17:GLU:H	2.13	0.51
1:E:148:MET:HE3	1:E:241:PHE:CE1	2.47	0.50
2:F:7:GLN:CD	2:F:7:GLN:O	2.50	0.50
1:A:384:THR:CG2	1:A:456:LEU:HD11	2.41	0.50
3:G:6:ILE:O	3:G:6:ILE:HG13	2.12	0.50
1:E:42:ASN:CB	4:H:35:LEU:HD11	2.41	0.50
1:A:77:HIS:O	1:A:81:ILE:HG22	2.11	0.50
4:D:38:SER:O	4:D:42:THR:OG1	2.22	0.49
4:D:46:TYR:HB2	4:D:49:MET:HB2	1.93	0.49
1:E:4:CYS:HB3	1:E:7:ILE:HG22	1.94	0.49
1:A:366:GLU:HG3	1:A:376:LEU:HD11	1.93	0.49
1:A:246:ILE:CD1	1:A:304:LEU:HD13	2.43	0.49
1:E:351:ILE:HD12	1:E:391:TYR:O	2.12	0.49
1:E:380:ILE:N	1:E:380:ILE:HD12	2.28	0.49
1:E:71:HIS:CB	1:E:73:HIS:CE1	2.96	0.49
1:E:375:LYS:NZ	1:E:421:GLY:O	2.35	0.49
1:A:21:LEU:HD13	1:A:108:LEU:HD11	1.94	0.49
1:E:16:SER:O	1:E:20:VAL:HG13	2.13	0.49
1:A:247:ASN:O	1:A:251:GLN:HG2	2.13	0.48
1:E:140:ILE:HD12	1:E:142:MET:CE	2.43	0.48
1:E:416:ILE:HD12	1:E:455:VAL:CG1	2.43	0.48
3:G:7:THR:HG23	3:G:10:SER:N	2.28	0.48
1:E:334:TYR:CE1	1:E:345:ALA:HB2	2.49	0.48
3:C:45:LEU:N	3:C:45:LEU:HD12	2.28	0.48
3:C:6:ILE:HG23	3:C:11:ILE:CG2	2.43	0.48
1:E:141:ASN:O	1:E:232:GLY:HA2	2.14	0.48
1:A:287:ILE:N	1:A:287:ILE:HD12	2.28	0.48
2:B:41:LYS:HB3	2:B:72:MET:HE3	1.94	0.48
1:E:242:TRP:O	1:E:245:ILE:HG22	2.13	0.48
1:E:23:THR:CG2	1:E:61:LEU:HD12	2.44	0.48
1:A:141:ASN:HB3	1:E:145:THR:HG21	1.97	0.47
1:E:180:ASP:N	1:E:180:ASP:OD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:141:ASN:ND2	1:E:143:GLY:H	2.13	0.46
1:E:373:ASN:HB2	1:E:423:VAL:HG11	1.97	0.46
1:A:220:LEU:HD13	1:E:142:MET:HG3	1.97	0.46
1:A:263:VAL:O	1:A:267:ASN:HB2	2.15	0.46
1:A:261:LYS:HG3	1:A:262:GLU:N	2.31	0.46
3:C:6:ILE:O	4:D:8:ILE:HD13	2.16	0.46
1:A:170:HIS:CE1	1:A:184:SER:HB2	2.49	0.46
1:A:452:GLN:O	1:A:453:GLU:C	2.54	0.46
1:E:3:ILE:HG22	1:E:4:CYS:N	2.31	0.46
1:E:74:PHE:CD1	1:E:97:PHE:CE2	3.04	0.46
4:H:91:VAL:HG12	4:H:95:GLU:HG3	1.98	0.46
1:E:354:LEU:HB3	1:E:411:TYR:OH	2.16	0.46
1:E:152:LEU:HD11	1:E:219:LEU:HD22	1.97	0.45
1:E:158:ASN:HD21	1:E:357:VAL:HG21	1.80	0.45
4:D:21:LEU:C	4:D:21:LEU:CD2	2.85	0.45
1:E:251:GLN:O	1:E:255:LEU:HD13	2.16	0.45
1:A:416:ILE:HD12	1:A:455:VAL:HG13	1.99	0.45
1:A:50:HIS:O	2:B:10:SER:HB2	2.17	0.45
1:E:80:GLN:HA	1:E:82:GLY:N	2.31	0.45
2:F:25:ILE:CD1	2:F:85:ILE:HG12	2.47	0.45
2:F:8:LEU:O	2:F:11:GLN:N	2.42	0.45
1:A:221:THR:HG21	1:E:225:LYS:HE3	1.98	0.44
2:B:66:GLU:N	2:B:67:PRO:CD	2.81	0.44
1:A:4:CYS:HB3	1:A:7:ILE:HG22	1.99	0.44
1:E:35:VAL:HG13	1:E:36:PRO:HD2	1.99	0.44
1:A:216:PHE:HE2	1:E:140:ILE:O	2.00	0.44
1:E:93:LEU:HD13	3:G:33:THR:HG21	2.00	0.44
1:A:286:SER:HA	1:A:298:THR:CG2	2.48	0.44
1:E:253:TYR:CG	1:E:273:CYS:HB3	2.53	0.44
3:G:29:ALA:O	3:G:33:THR:HG23	2.18	0.44
1:E:274:ILE:CD1	1:E:278:VAL:HG21	2.48	0.43
4:D:73:ILE:HD12	4:D:73:ILE:H	1.82	0.43
1:E:368:LEU:HD12	1:E:372:SER:O	2.18	0.43
1:E:56:ALA:H	3:G:25:GLN:NE2	2.16	0.43
1:E:213:GLN:N	1:E:213:GLN:OE1	2.52	0.43
1:E:23:THR:HG22	1:E:61:LEU:HD12	1.98	0.43
3:C:7:THR:HG23	3:C:10:SER:H	1.84	0.43
1:A:287:ILE:HD13	1:A:297:LYS:O	2.19	0.43
1:A:375:LYS:NZ	1:A:459:GLN:HE22	2.16	0.43
3:G:6:ILE:O	4:H:8:ILE:HB	2.18	0.43
1:A:296:SER:HA	1:A:297:LYS:HA	1.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:444:ASP:HA	1:E:445:SER:HA	1.81	0.43
3:G:8:ILE:HA	4:H:8:ILE:HD11	2.01	0.43
1:A:142:MET:CE	1:A:224:TRP:CB	2.97	0.43
1:A:140:ILE:HD12	1:E:213:GLN:H	1.83	0.43
1:A:295:ASN:O	1:A:298:THR:HG23	2.19	0.42
3:C:8:ILE:N	4:D:8:ILE:HD11	2.34	0.42
1:E:148:MET:HE2	1:E:241:PHE:CZ	2.54	0.42
1:E:71:HIS:HB2	1:E:73:HIS:ND1	2.34	0.42
1:A:156:ILE:CD1	1:A:157:HIS:CE1	3.02	0.42
1:A:245:ILE:HD13	1:A:245:ILE:HG21	1.70	0.42
2:B:75:ASP:O	2:B:79:GLU:HG2	2.19	0.42
1:E:90:ASN:HD21	3:G:22:THR:HG23	1.84	0.42
1:A:158:ASN:HA	1:A:159:PRO:HD3	1.82	0.42
1:E:413:LEU:HB2	1:E:465:TYR:CE1	2.55	0.42
2:F:7:GLN:O	2:F:7:GLN:HG3	2.18	0.42
2:F:78[B]:ARG:HG2	3:G:16:LEU:HD21	2.01	0.42
1:E:142:MET:HE1	1:E:231:ALA:CB	2.45	0.42
1:E:339:CYS:HB3	1:E:341:SER:OG	2.19	0.42
1:A:433:LYS:HD2	4:H:69:LEU:HD12	2.02	0.42
1:A:176:VAL:HG12	1:A:178:SER:H	1.85	0.41
1:E:316:LEU:HD21	1:E:360:LEU:CD1	2.50	0.41
4:H:78:CYS:HB3	4:H:81:CYS:HB2	2.01	0.41
1:E:222:CYS:O	1:E:226:ILE:HG13	2.20	0.41
1:A:382:PHE:CE2	1:A:456:LEU:HD23	2.55	0.41
1:A:221:THR:HG21	1:E:225:LYS:NZ	2.35	0.41
3:G:11:ILE:C	3:G:11:ILE:CD1	2.85	0.41
3:C:11:ILE:HD12	3:C:11:ILE:C	2.41	0.41
1:E:301:ASP:HA	1:E:302:PRO:HD2	1.87	0.41
1:E:108:LEU:HD13	1:E:118:TRP:CG	2.56	0.41
1:E:3:ILE:CG2	1:E:106:ILE:HD11	2.51	0.41
1:A:103:ILE:CG2	1:A:106:ILE:HD12	2.51	0.41
1:E:411:TYR:HB3	1:E:465:TYR:HB3	2.03	0.41
1:E:54:SER:HB3	1:E:68:CYS:HB2	2.03	0.41
1:A:283:LEU:HD23	1:A:283:LEU:HA	1.81	0.41
2:B:73:VAL:HG22	2:B:78:ARG:NH1	2.36	0.41
1:E:183:PHE:O	1:E:186:ALA:HB3	2.21	0.41
1:E:382:PHE:HA	1:E:383:PRO:HD3	1.98	0.41
1:E:53:ASN:O	3:G:18:ASN:HB3	2.20	0.41
4:H:11:ILE:HG23	4:H:15:VAL:HG22	2.02	0.41
1:A:460:ALA:CB	1:A:463:LEU:HD21	2.51	0.41
1:E:374:ARG:HD2	1:E:375:LYS:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ASN:HB3	1:A:213:GLN:HB2	2.02	0.40
1:A:216:PHE:HB2	1:E:139:LEU:HD22	2.04	0.40
1:E:158:ASN:HA	1:E:159:PRO:HD3	1.85	0.40
1:E:81:ILE:O	1:E:81:ILE:HG23	2.19	0.40
1:A:21:LEU:HD11	1:A:108:LEU:HG	2.04	0.40
1:A:148:MET:CE	1:A:220:LEU:CD2	2.98	0.40
1:A:467:ILE:O	1:A:467:ILE:HG23	2.22	0.40
2:F:49:GLU:HG3	2:F:64:THR:HG23	2.03	0.40
4:H:76:ARG:HB2	4:H:90:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	442/476 (93%)	418 (95%)	22 (5%)	2 (0%)	29	52
1	E	433/476 (91%)	408 (94%)	22 (5%)	3 (1%)	22	44
2	B	88/96 (92%)	86 (98%)	2 (2%)	0	100	100
2	F	89/96 (93%)	81 (91%)	7 (8%)	1 (1%)	14	31
3	C	39/72 (54%)	38 (97%)	1 (3%)	0	100	100
3	G	41/72 (57%)	39 (95%)	1 (2%)	1 (2%)	6	13
4	D	82/96 (85%)	78 (95%)	3 (4%)	1 (1%)	13	29
4	H	79/96 (82%)	75 (95%)	3 (4%)	1 (1%)	12	27
All	All	1293/1480 (87%)	1223 (95%)	61 (5%)	9 (1%)	22	44

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	371	GLY

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Mol	Chain	Res	Type
4	H	16	ILE
1	A	293	GLN
1	A	332	PHE
4	D	31	SER
1	E	72	SER
1	E	339	CYS
2	F	9	LYS
3	G	6	ILE

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	410/429 (96%)	380 (93%)	30 (7%)	14	30
1	E	403/429 (94%)	384 (95%)	19 (5%)	26	50
2	B	85/91 (93%)	78 (92%)	7 (8%)	11	24
2	F	86/91 (94%)	77 (90%)	9 (10%)	7	14
3	C	39/68 (57%)	34 (87%)	5 (13%)	4	9
3	G	41/68 (60%)	37 (90%)	4 (10%)	8	17
4	D	79/86 (92%)	74 (94%)	5 (6%)	18	37
4	H	76/86 (88%)	72 (95%)	4 (5%)	22	45
All	All	1219/1348 (90%)	1136 (93%)	83 (7%)	16	33

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	17	LYS
1	A	142	MET
1	A	178	SER
1	A	182	CYS
1	A	220	LEU
1	A	240	GLU

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Mol	Chain	Res	Type
1	A	252	SER
1	A	259	ASN
1	A	261	LYS
1	A	267	ASN
1	A	269	LYS
1	A	278	VAL
1	A	293	GLN
1	A	297	LYS
1	A	305	ASP
1	A	310	ILE
1	A	314	LYS
1	A	322	SER
1	A	323	PHE
1	A	325	LYS
1	A	332	PHE
1	A	339	CYS
1	A	369	LEU
1	A	378	ASP
1	A	393	SER
1	A	441	LYS
1	A	446	MET
1	A	453	GLU
1	A	470	VAL
2	B	7	GLN
2	B	8	LEU
2	B	12	ILE
2	B	28	GLU
2	B	41	LYS
2	B	51	ASN
2	B	76	SER
3	C	5	THR
3	C	7	THR
3	C	11	ILE
3	C	18	ASN
3	C	45	LEU
4	D	5	ASP
4	D	21	LEU
4	D	37	SER
4	D	47	ASP
4	D	80	LYS
1	E	15	LYS
1	E	81	ILE

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Mol	Chain	Res	Type
1	E	141	ASN
1	E	142	MET
1	E	145	THR
1	E	180	ASP
1	E	182	CYS
1	E	198	LEU
1	E	268	ASN
1	E	299	THR
1	E	320	LEU
1	E	324	HIS
1	E	330	LYS
1	E	369	LEU
1	E	370	ASN
1	E	394	THR
1	E	418	SER
1	E	433	LYS
1	E	459	GLN
2	F	7	GLN
2	F	8	LEU
2	F	9	LYS
2	F	24	LEU
2	F	41	LYS
2	F	44	ASP
2	F	52	ILE
2	F	53	ASN
2	F	75	ASP
3	G	8	ILE
3	G	11	ILE
3	G	35	GLN
3	G	40	THR
4	H	31	SER
4	H	37	SER
4	H	61	ASN
4	H	73	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	32	ASN
1	A	42	ASN
1	A	70	ASN

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Mol	Chain	Res	Type
1	A	77	HIS
1	A	90	ASN
1	A	110	ASN
1	A	144	ASN
1	A	153	GLN
1	A	168	GLN
1	A	213	GLN
1	A	236	GLN
1	A	250	HIS
1	A	267	ASN
1	A	276	HIS
1	A	324	HIS
1	A	459	GLN
1	A	469	GLN
2	B	7	GLN
2	B	21	ASN
2	B	57	ASN
2	B	84	GLN
3	C	18	ASN
3	C	25	GLN
1	E	33	HIS
1	E	90	ASN
1	E	105	ASN
1	E	110	ASN
1	E	141	ASN
1	E	170	HIS
1	E	192	HIS
1	E	259	ASN
1	E	276	HIS
1	E	335	HIS
1	E	340	ASN
1	E	348	GLN
2	F	11	GLN
2	F	13	GLN
2	F	27	ASN
3	G	18	ASN
3	G	25	GLN
3	G	34	GLN
4	H	48	HIS
4	H	96	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 14 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 [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	450/476 (94%)	0.07	22 (4%) 29 27	25, 42, 90, 126	0
1	E	441/476 (92%)	-0.07	7 (1%) 72 73	29, 49, 79, 113	0
2	B	90/96 (93%)	0.11	5 (5%) 24 22	30, 50, 91, 104	0
2	F	90/96 (93%)	0.36	4 (4%) 34 32	37, 59, 104, 116	0
3	C	41/72 (56%)	0.05	2 (4%) 29 27	27, 38, 77, 91	0
3	G	43/72 (59%)	0.25	4 (9%) 8 6	40, 51, 89, 100	0
4	D	88/96 (91%)	0.38	7 (7%) 12 10	27, 48, 98, 101	0
4	H	83/96 (86%)	0.38	11 (13%) 3 2	31, 48, 105, 118	1 (1%)
All	All	1326/1480 (89%)	0.09	62 (4%) 31 29	25, 47, 92, 126	1 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	95	THR	7.0
4	H	15	VAL	4.6
4	H	20	SER	4.4
4	H	13	PRO	4.2
2	B	95	THR	4.0
4	H	21	LEU	4.0
1	A	198	LEU	3.9
2	F	93	VAL	3.8
2	F	92	ILE	3.8
1	A	401	SER	3.6
1	A	0	ALA	3.6
4	H	9	LYS	3.6
1	A	258	PRO	3.5
3	C	45	LEU	3.5
4	D	15	VAL	3.4
4	D	19	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	327	GLU	3.3
1	E	268	ASN	3.2
4	H	11	ILE	3.2
2	B	15	TYR	3.1
4	H	8	ILE	3.1
1	A	287	ILE	2.9
1	A	210	THR	2.8
1	A	404	GLY	2.8
1	E	1	MET	2.8
1	A	332	PHE	2.8
4	D	16	ILE	2.8
1	A	260	ALA	2.8
1	A	288	VAL	2.7
1	A	259	ASN	2.7
3	C	44	ASP	2.7
1	E	369	LEU	2.6
1	A	394	THR	2.6
4	D	17	GLU	2.6
1	A	264	SER	2.6
1	E	259	ASN	2.6
2	F	94	ASP	2.6
3	G	44	ASP	2.5
1	E	367	HIS	2.5
1	A	261	LYS	2.5
4	H	14	LYS	2.5
1	A	175	LYS	2.4
3	G	45	LEU	2.4
4	H	10	GLY	2.4
3	G	3	GLU	2.4
2	B	92	ILE	2.3
2	B	93	VAL	2.3
1	E	14	GLU	2.3
4	D	14	LYS	2.3
1	A	403	ASN	2.3
4	H	6	ALA	2.3
1	E	371	GLY	2.2
2	B	94	ASP	2.2
1	A	340	ASN	2.2
1	A	286	SER	2.1
4	D	21	LEU	2.1
1	A	291	GLY	2.1
1	A	180	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
3	G	4	GLU	2.0
4	D	95	GLU	2.0
4	H	17	GLU	2.0
1	A	329	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 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. 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
5	ZN	D	101	1/1	0.97	0.12	47,47,47,47	0
5	ZN	A	506	1/1	0.98	0.04	80,80,80,80	0
5	ZN	A	502	1/1	0.99	0.12	41,41,41,41	0
5	ZN	E	505	1/1	0.99	0.08	59,59,59,59	0
5	ZN	A	501	1/1	0.99	0.13	39,39,39,39	0
5	ZN	A	505	1/1	0.99	0.10	56,56,56,56	0
5	ZN	A	504	1/1	0.99	0.11	42,42,42,42	0
5	ZN	H	101	1/1	0.99	0.11	45,45,45,45	0
5	ZN	E	503	1/1	0.99	0.10	61,61,61,61	0
5	ZN	E	502	1/1	0.99	0.14	39,39,39,39	0
5	ZN	E	506	1/1	1.00	0.07	59,59,59,59	0
5	ZN	E	501	1/1	1.00	0.11	55,55,55,55	0
5	ZN	E	504	1/1	1.00	0.06	43,43,43,43	0
5	ZN	A	503	1/1	1.00	0.11	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.