



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 08:21 PM BST

PDB ID : 6GVW
Title : Crystal structure of the BRCA1-A complex
Authors : Bunker, R.D.; Rabl, J.; Thoma, N.H.
Deposited on : 2018-06-21
Resolution : 3.75 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 : 2.13.1
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) : 2.13.1

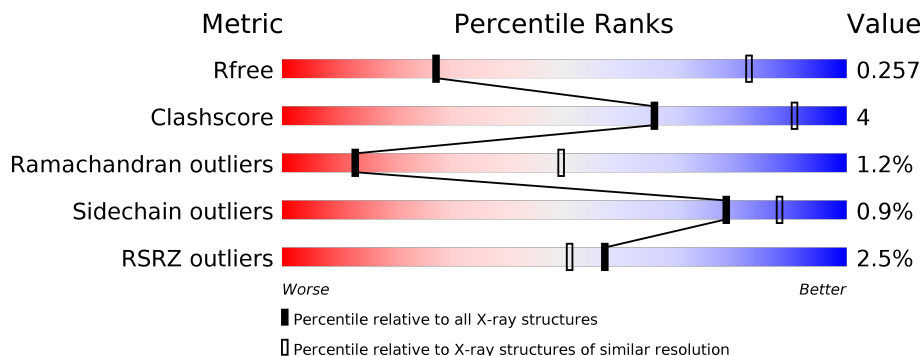
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.75 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.



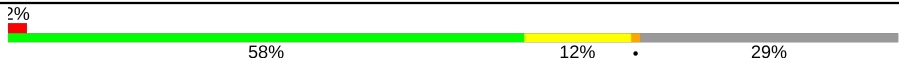



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1039 (3.94-3.58)
Clashscore	141614	1051 (3.92-3.60)
Ramachandran outliers	138981	1015 (3.92-3.60)
Sidechain outliers	138945	1011 (3.92-3.60)
RSRZ outliers	127900	1050 (3.96-3.56)

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	411	 2% 66% 9% 24%
1	F	411	 2% 70% 7% 22%
2	B	295	 80% 9% 11%
2	G	295	 2% 83% 6% 11%
3	C	387	 % 89% 10% ..
3	H	387	 3% 89% 10% .

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Mol	Chain	Length	Quality of chain
4	D	337	
4	I	337	
5	E	64	
5	J	64	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 40106 atoms, of which 19968 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 BRCA1-A complex subunit Abraxas 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	312	Total	C	H	N	O	S	160	0	0
			4992	1566	2500	440	472	14			
1	F	320	Total	C	H	N	O	S	162	0	0
			5122	1611	2561	448	486	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q8BPZ8
A	-2	GLY	-	expression tag	UNP Q8BPZ8
A	-1	GLY	-	expression tag	UNP Q8BPZ8
A	0	ARG	-	expression tag	UNP Q8BPZ8
F	-3	GLY	-	expression tag	UNP Q8BPZ8
F	-2	GLY	-	expression tag	UNP Q8BPZ8
F	-1	GLY	-	expression tag	UNP Q8BPZ8
F	0	ARG	-	expression tag	UNP Q8BPZ8

- Molecule 2 is a protein called Lys-63-specific deubiquitinase BRCC36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	B	262	Total	C	H	N	O	S	120	0	0
			4202	1316	2101	370	401	14			
2	G	262	Total	C	H	N	O	S	120	0	0
			4202	1316	2101	370	401	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P46737
B	-2	GLY	-	expression tag	UNP P46737
B	-1	GLY	-	expression tag	UNP P46737
B	0	ARG	-	expression tag	UNP P46737

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	GLY	-	expression tag	UNP P46737
G	-2	GLY	-	expression tag	UNP P46737
G	-1	GLY	-	expression tag	UNP P46737
G	0	ARG	-	expression tag	UNP P46737

- Molecule 3 is a protein called BRISC and BRCA1-A complex member 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	C	383	6085	1994	3008	505	564	14	161	0	0
			Total	C	H	N	O	S			
3	H	383	6085	1994	3008	505	564	14	161	0	0
			Total	C	H	N	O	S			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP Q8K3W0
C	-2	GLY	-	expression tag	UNP Q8K3W0
C	-1	GLY	-	expression tag	UNP Q8K3W0
C	0	ARG	-	expression tag	UNP Q8K3W0
H	-3	GLY	-	expression tag	UNP Q8K3W0
H	-2	GLY	-	expression tag	UNP Q8K3W0
H	-1	GLY	-	expression tag	UNP Q8K3W0
H	0	ARG	-	expression tag	UNP Q8K3W0

- Molecule 4 is a protein called BRISC and BRCA1-A complex member 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	D	239	3765	1206	1873	307	361	18	103	0	0
			Total	C	H	N	O	S			
4	I	238	3755	1203	1868	306	360	18	103	0	0
			Total	C	H	N	O	S			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	expression tag	UNP Q3UI43
D	-2	GLY	-	expression tag	UNP Q3UI43
D	-1	GLY	-	expression tag	UNP Q3UI43
D	0	ARG	-	expression tag	UNP Q3UI43
I	-3	GLY	-	expression tag	UNP Q3UI43
I	-2	GLY	-	expression tag	UNP Q3UI43

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-1	GLY	-	expression tag	UNP Q3UI43
I	0	ARG	-	expression tag	UNP Q3UI43

- Molecule 5 is a protein called BRCA1-A complex subunit RAP80.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
5	E	59	Total	C	H	N	O	S	25	0	0
			947	310	474	82	78	3			
5	J	59	Total	C	H	N	O	S	25	0	0
			947	310	474	82	78	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	271	GLY	-	expression tag	UNP Q5U5Q9
E	272	GLY	-	expression tag	UNP Q5U5Q9
E	273	GLY	-	expression tag	UNP Q5U5Q9
E	274	ARG	-	expression tag	UNP Q5U5Q9
J	271	GLY	-	expression tag	UNP Q5U5Q9
J	272	GLY	-	expression tag	UNP Q5U5Q9
J	273	GLY	-	expression tag	UNP Q5U5Q9
J	274	ARG	-	expression tag	UNP Q5U5Q9

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

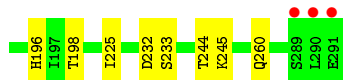
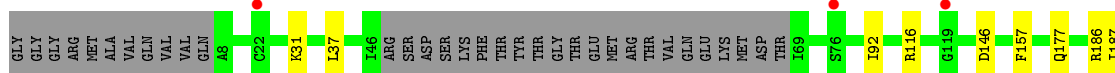
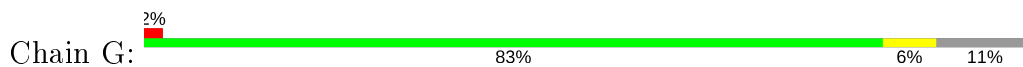
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total	Zn	0	0
			1	1		
6	B	1	Total	Zn	0	0
			1	1		

- Molecule 7 is water.

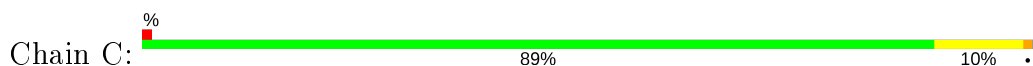
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	O	0	0
			1	1		
7	G	1	Total	O	0	0
			1	1		



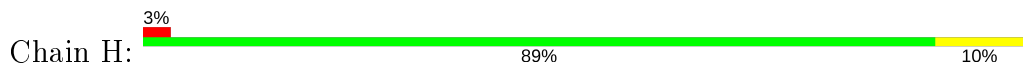
- Molecule 2: Lys-63-specific deubiquitinase BRCC36



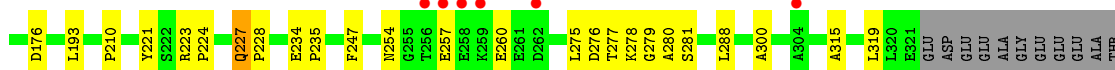
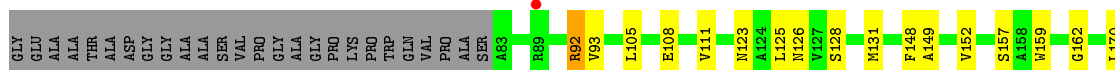
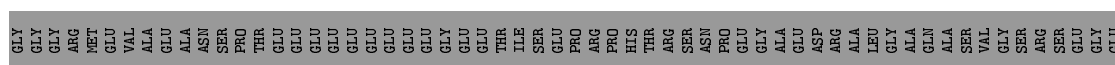
- Molecule 3: BRISC and BRCA1-A complex member 2



- Molecule 3: BRISC and BRCA1-A complex member 2

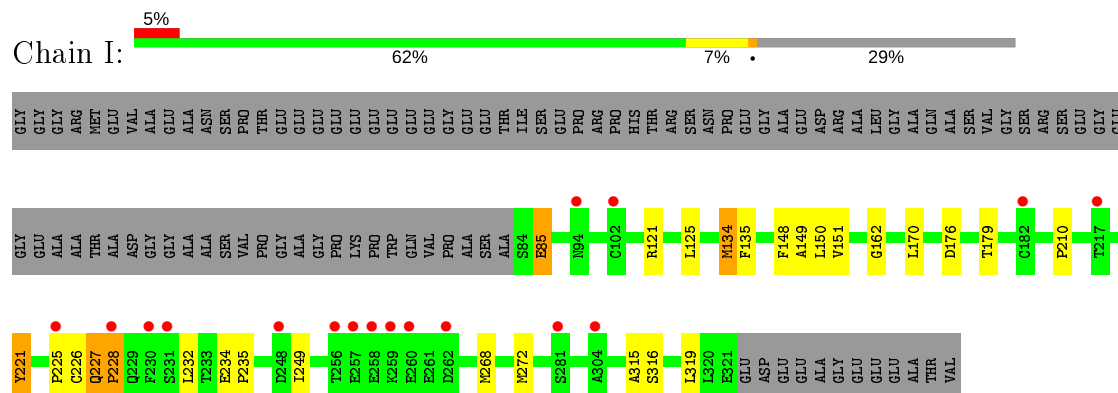


- Molecule 4: BRISC and BRCA1-A complex member 1

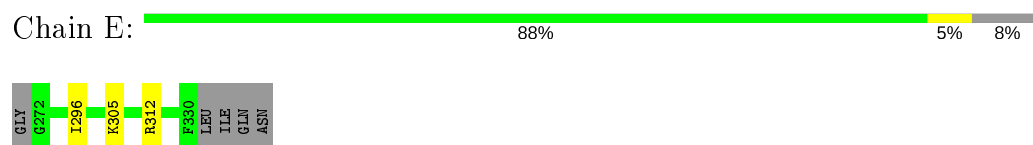


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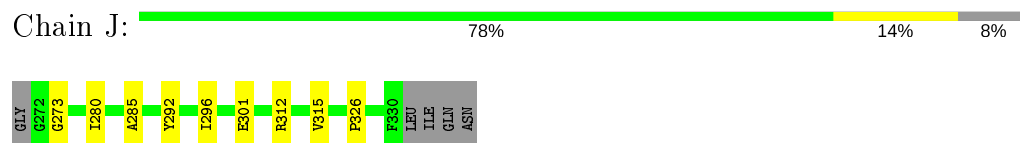
- Molecule 4: BRISC and BRCA1-A complex member 1



- Molecule 5: BRCA1-A complex subunit RAP80



- Molecule 5: BRCA1-A complex subunit RAP80



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.10Å 122.64Å 431.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.99 – 3.75 29.99 – 3.75	Depositor EDS
% Data completeness (in resolution range)	82.3 (29.99-3.75) 82.6 (29.99-3.75)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 3.75Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.227 , 0.259 0.226 , 0.257	Depositor DCC
R_{free} test set	2214 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	187.4	Xtrriage
Anisotropy	0.049	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 160.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	40106	wwPDB-VP
Average B, all atoms (Å ²)	223.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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	0.62	0/2538	0.65	0/3429
1	F	0.62	0/2608	0.64	0/3523
2	B	0.62	0/2138	0.61	0/2890
2	G	0.62	0/2138	0.61	0/2890
3	C	0.59	0/3169	0.64	0/4311
3	H	0.58	0/3169	0.59	0/4311
4	D	0.60	0/1937	0.64	0/2629
4	I	0.61	0/1932	0.61	0/2622
5	E	0.59	0/489	0.63	0/664
5	J	0.60	0/489	0.61	0/664
All	All	0.61	0/20607	0.62	0/27933

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2492	2500	2483	24	0
1	F	2561	2561	2547	23	0
2	B	2101	2101	2087	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	2101	2101	2087	11	0
3	C	3077	3008	3000	29	0
3	H	3077	3008	3000	29	0
4	D	1892	1873	1864	26	0
4	I	1887	1868	1859	22	0
5	E	473	474	470	4	0
5	J	473	474	470	12	0
6	B	1	0	0	0	0
6	G	1	0	0	0	0
7	B	1	0	0	0	0
7	G	1	0	0	0	0
All	All	20138	19968	19867	158	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 4.

All (158) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:THR:HG22	2:G:260:GLN:OE1	1.82	0.78
4:I:148:PHE:HB2	4:I:170:LEU:HD11	1.65	0.77
4:D:276:ASP:O	4:D:277:THR:OG1	2.04	0.76
1:A:145:SER:OG	2:B:188:GLU:OE1	2.09	0.70
1:A:310:CYS:SG	1:A:311:ASN:N	2.66	0.67
1:F:298:ILE:HG13	5:J:280:ILE:HG21	1.78	0.65
3:C:40:LEU:HD21	3:C:53:CYS:CB	2.27	0.65
3:C:330:VAL:HG21	4:D:300:ALA:HB2	1.78	0.65
1:A:59:ILE:HG23	1:A:97:VAL:HG21	1.79	0.64
2:G:37:LEU:HD21	2:G:92:ILE:HD13	1.78	0.64
1:F:73:PHE:HB2	1:F:84:ALA:HB1	1.80	0.62
1:A:45:ILE:O	1:A:46:THR:OG1	2.16	0.62
4:D:247:PHE:O	4:D:281:SER:OG	2.11	0.61
2:B:111:THR:O	2:B:113:ARG:NH1	2.34	0.60
4:D:93:VAL:HG11	4:D:210:PRO:HB3	1.83	0.60
1:A:28:ASP:OD1	3:C:55:ARG:NH2	2.33	0.60
1:F:215:ILE:HG12	2:G:244:THR:HG23	1.84	0.60
4:I:149:ALA:HA	4:I:162:GLY:HA2	1.85	0.59
3:C:276:ALA:HB1	5:E:296:ILE:HG23	1.85	0.59
4:D:254:ASN:OD1	4:D:288:LEU:HD12	2.04	0.58
4:I:85:GLU:HB2	5:J:273:GLY:O	2.05	0.57
4:I:148:PHE:CB	4:I:170:LEU:HD11	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:221:TYR:CE2	4:I:249:ILE:HD11	2.40	0.56
1:F:315:HIS:O	1:F:316:VAL:HG12	2.05	0.56
1:F:303:ARG:O	5:J:285:ALA:N	2.29	0.56
4:D:223:ARG:N	4:D:224:PRO:CD	2.70	0.55
5:J:280:ILE:O	5:J:280:ILE:HD12	2.06	0.55
3:C:139:MET:SD	3:C:139:MET:N	2.78	0.55
3:C:165:TRP:O	3:C:166:THR:OG1	2.15	0.54
3:C:347:TYR:HB2	3:C:348:PRO:HD2	1.89	0.54
1:A:320:ASP:OD2	5:E:305:LYS:NZ	2.35	0.54
2:B:266:LEU:O	2:B:266:LEU:HD13	2.07	0.54
2:B:42:LEU:HD23	2:B:72:VAL:HG22	1.88	0.54
3:H:165:TRP:O	3:H:166:THR:OG1	2.16	0.54
1:A:85:LEU:O	1:A:88:VAL:HG22	2.08	0.54
3:H:284:THR:OG1	4:I:316:SER:N	2.40	0.53
2:B:129:VAL:HG22	2:B:171:THR:HG22	1.90	0.53
3:C:15:SER:N	3:C:16:PRO:HD2	2.25	0.52
4:I:227:GLN:HB2	4:I:228:PRO:HD3	1.91	0.52
4:D:92:ARG:HD3	4:D:92:ARG:H	1.74	0.52
1:A:77:LEU:HD11	3:C:103:ALA:HB2	1.89	0.52
3:C:182:SER:O	5:E:305:LYS:NZ	2.42	0.52
4:D:279:GLY:O	4:D:281:SER:N	2.43	0.52
1:F:298:ILE:CG1	5:J:280:ILE:HG21	2.40	0.51
3:C:155:MET:HE2	3:C:175:LEU:HD21	1.92	0.51
2:G:232:ASP:OD1	2:G:233:SER:N	2.42	0.51
3:H:334:THR:HG22	3:H:338:GLN:O	2.11	0.51
3:H:106:ASN:ND2	3:H:108:SER:OG	2.44	0.51
3:C:132:LEU:HG	3:C:139:MET:HE2	1.93	0.50
5:J:280:ILE:HD12	5:J:292:TYR:OH	2.11	0.50
1:A:311:ASN:O	1:A:312:VAL:HG12	2.11	0.50
4:D:149:ALA:HA	4:D:162:GLY:HA2	1.93	0.50
4:I:227:GLN:CB	4:I:228:PRO:HD3	2.41	0.50
2:G:116:ARG:NH2	2:G:146:ASP:OD2	2.33	0.50
3:H:30:ASP:OD1	3:H:31:ALA:N	2.44	0.50
2:B:232:ASP:OD1	2:B:233:SER:N	2.45	0.50
1:F:192:SER:O	1:F:196:ARG:HB2	2.12	0.50
1:A:230:CYS:SG	2:B:204:LEU:HB3	2.51	0.50
4:D:148:PHE:CB	4:D:170:LEU:HD11	2.41	0.50
3:C:284:THR:O	4:D:315:ALA:HA	2.12	0.50
3:H:15:SER:N	3:H:16:PRO:HD2	2.27	0.50
3:C:30:ASP:OD1	3:C:31:ALA:N	2.45	0.49
1:F:172:GLY:O	2:G:31:LYS:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:302:ASN:OD1	1:F:303:ARG:N	2.44	0.49
2:B:210:LEU:HB3	2:B:211:PRO:HD3	1.95	0.49
1:A:291:GLU:O	1:A:292:VAL:HG22	2.13	0.49
4:D:123:ASN:ND2	4:D:126:ASN:OD1	2.42	0.49
1:F:34:LEU:CD2	1:F:96:VAL:HG12	2.43	0.48
1:F:179:TYR:CD2	2:G:225:ILE:HD11	2.47	0.48
3:C:25:GLY:O	3:C:26:LYS:HG2	2.13	0.48
1:F:70:LEU:H	1:F:70:LEU:HD22	1.78	0.48
3:C:40:LEU:HD21	3:C:53:CYS:HB2	1.96	0.48
1:F:179:TYR:CG	2:G:225:ILE:CD1	2.96	0.48
4:I:134:MET:SD	4:I:135:PHE:N	2.86	0.48
3:H:143:GLN:NE2	3:H:147:GLU:OE2	2.43	0.48
3:H:237:ILE:O	5:J:326:PRO:HA	2.15	0.47
3:H:188:LEU:HD13	4:I:210:PRO:HG2	1.96	0.47
1:F:322:LEU:O	3:H:272:ARG:NH2	2.48	0.47
1:A:311:ASN:OD1	1:A:314:HIS:N	2.46	0.47
3:H:284:THR:HG23	4:I:316:SER:O	2.15	0.47
3:C:155:MET:CE	3:C:175:LEU:HD21	2.45	0.46
3:H:276:ALA:HB1	5:J:296:ILE:HG23	1.97	0.46
3:C:34:CYS:SG	3:C:34:CYS:O	2.73	0.46
4:D:105:LEU:HD12	4:D:152:VAL:HG11	1.98	0.46
1:A:104:ARG:HB2	3:C:43:GLY:HA2	1.97	0.46
1:A:154:TYR:OH	1:A:163:ARG:NH1	2.49	0.46
1:F:158:ARG:C	1:F:160:LEU:H	2.18	0.46
1:F:321:GLN:O	5:J:301:GLU:OE2	2.33	0.46
2:G:196:HIS:ND1	2:G:198:THR:O	2.40	0.45
4:I:225:PRO:HD2	4:I:268:MET:SD	2.56	0.45
3:H:169:PHE:HB2	3:H:210:THR:HG22	1.99	0.45
3:C:199:ASP:N	3:C:199:ASP:OD1	2.46	0.45
3:H:3:PRO:HB2	5:J:315:VAL:HG11	1.98	0.45
2:B:196:HIS:ND1	2:B:198:THR:O	2.43	0.45
4:D:148:PHE:HB2	4:D:170:LEU:HD11	1.98	0.45
1:F:26:ASP:HB2	3:H:44:CYS:SG	2.57	0.45
3:H:55:ARG:NH1	3:H:73:PHE:O	2.49	0.45
3:H:284:THR:HG23	4:I:319:LEU:HD21	1.99	0.45
4:I:249:ILE:HD12	4:I:272:MET:CE	2.47	0.45
1:A:322:LEU:O	3:C:272:ARG:NH2	2.50	0.45
4:I:150:LEU:HD23	4:I:151:VAL:N	2.32	0.45
1:A:209:LEU:HD23	1:A:210:LYS:N	2.32	0.44
1:A:151:HIS:CE1	2:B:166:GLY:HA3	2.53	0.44
4:D:108:GLU:O	4:D:111:VAL:HG12	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:125:LEU:HD22	4:I:179:THR:CG2	2.48	0.44
4:I:226:CYS:O	4:I:228:PRO:CD	2.65	0.44
4:D:92:ARG:CD	4:D:92:ARG:H	2.31	0.44
3:C:55:ARG:NH1	3:C:73:PHE:O	2.51	0.44
1:A:35:GLY:HA3	1:A:60:ASP:O	2.18	0.44
4:D:193:LEU:HD23	4:D:193:LEU:O	2.18	0.44
1:F:34:LEU:HD12	1:F:63:LYS:CE	2.48	0.43
1:F:103:ARG:NH2	1:F:107:ASP:O	2.51	0.43
3:H:237:ILE:HD12	3:H:238:PRO:HD2	2.01	0.43
4:I:134:MET:C	4:I:134:MET:SD	2.96	0.43
3:H:3:PRO:HB2	5:J:315:VAL:CG1	2.48	0.43
4:I:232:LEU:N	4:I:232:LEU:HD22	2.34	0.43
4:I:221:TYR:HE2	4:I:249:ILE:HD11	1.83	0.43
2:G:186:ARG:HG2	2:G:187:ILE:N	2.34	0.43
3:H:76:GLN:HA	3:H:76:GLN:OE1	2.19	0.43
3:H:284:THR:O	4:I:315:ALA:HA	2.17	0.42
4:D:148:PHE:HB3	4:D:170:LEU:HD11	2.01	0.42
1:A:17:ALA:HB1	2:B:261:TRP:CH2	2.54	0.42
3:C:34:CYS:SG	3:C:36:ARG:NH1	2.93	0.42
4:D:105:LEU:HD12	4:D:152:VAL:CG1	2.50	0.42
4:D:319:LEU:HD23	4:D:319:LEU:O	2.20	0.42
3:H:18:ILE:HD12	3:H:18:ILE:H	1.84	0.42
3:C:39:ASP:O	3:C:56:PHE:HA	2.20	0.42
1:A:238:ARG:HA	1:A:238:ARG:NE	2.35	0.42
2:B:39:ILE:HG22	2:B:115:MET:HB3	2.02	0.42
3:H:39:ASP:O	3:H:56:PHE:HA	2.20	0.42
3:H:195:ASP:OD2	5:J:312:ARG:HA	2.20	0.41
1:F:28:ASP:OD1	3:H:55:ARG:NH2	2.53	0.41
1:A:73:PHE:HB2	1:A:84:ALA:HB1	2.02	0.41
2:B:182:SER:O	2:B:183:GLU:C	2.59	0.41
4:I:234:GLU:N	4:I:235:PRO:HD2	2.35	0.41
4:D:227:GLN:HB3	4:D:228:PRO:CD	2.51	0.41
4:D:260:GLU:HA	4:D:260:GLU:OE1	2.21	0.41
1:F:196:ARG:CG	1:F:196:ARG:HH11	2.33	0.41
3:H:179:VAL:HB	3:H:181:PHE:CE2	2.55	0.41
1:A:63:LYS:HG2	1:A:64:TYR:N	2.34	0.41
2:B:266:LEU:C	2:B:266:LEU:HD13	2.40	0.41
4:D:125:LEU:C	4:D:125:LEU:HD13	2.41	0.41
2:B:263:GLU:OE1	1:F:190:VAL:HG23	2.20	0.41
3:C:28:GLY:HA3	3:C:156:GLU:OE2	2.21	0.41
3:H:150:GLN:OE1	3:H:150:GLN:N	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:GLU:O	1:A:293:LEU:N	2.47	0.41
3:C:252:GLN:O	3:C:256:LEU:HD13	2.21	0.41
3:H:330:VAL:O	3:H:330:VAL:HG12	2.21	0.41
3:C:30:ASP:HB2	3:C:61:PRO:HG2	2.02	0.41
4:D:234:GLU:N	4:D:235:PRO:HD2	2.36	0.41
3:C:150:GLN:N	3:C:150:GLN:OE1	2.45	0.41
3:C:195:ASP:OD2	5:E:312:ARG:HA	2.22	0.40
4:D:128:SER:HA	4:D:131:MET:HE2	2.03	0.40
4:D:159:TRP:CZ2	4:D:162:GLY:HA3	2.56	0.40
1:F:196:ARG:NH1	1:F:196:ARG:CG	2.83	0.40
2:G:177:GLN:OE1	2:G:177:GLN:HA	2.21	0.40
2:B:25:HIS:CE1	2:B:79:ILE:HG23	2.57	0.40
3:H:17:PHE:CE1	3:H:112:CYS:SG	3.15	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	308/411 (75%)	270 (88%)	31 (10%)	7 (2%)	6	38
1	F	316/411 (77%)	281 (89%)	30 (10%)	5 (2%)	9	44
2	B	258/295 (88%)	245 (95%)	10 (4%)	3 (1%)	13	49
2	G	258/295 (88%)	243 (94%)	14 (5%)	1 (0%)	34	69
3	C	381/387 (98%)	359 (94%)	20 (5%)	2 (0%)	29	65
3	H	381/387 (98%)	362 (95%)	18 (5%)	1 (0%)	41	74
4	D	237/337 (70%)	212 (90%)	20 (8%)	5 (2%)	7	40
4	I	236/337 (70%)	220 (93%)	11 (5%)	5 (2%)	7	40
5	E	57/64 (89%)	55 (96%)	2 (4%)	0	100	100
5	J	57/64 (89%)	55 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2489/2988 (83%)	2302 (92%)	158 (6%)	29 (1%)	13 49

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	312	VAL
2	B	290	LEU
1	F	177	LEU
1	F	316	VAL
4	I	227	GLN
4	D	278	LYS
4	I	228	PRO
1	A	182	GLU
3	C	26	LYS
4	D	280	ALA
2	G	157	PHE
1	A	44	SER
1	A	290	SER
1	A	292	VAL
1	A	310	CYS
3	C	25	GLY
4	D	157	SER
4	D	176	ASP
1	F	182	GLU
4	I	85	GLU
4	I	121	ARG
4	I	176	ASP
1	A	179	TYR
3	H	245	CYS
2	B	183	GLU
1	F	91	ASN
1	F	202	PHE
2	B	114	PRO
4	D	227	GLN

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	287/371 (77%)	285 (99%)	2 (1%)	84	91
1	F	294/371 (79%)	291 (99%)	3 (1%)	76	86
2	B	239/267 (90%)	238 (100%)	1 (0%)	91	95
2	G	239/267 (90%)	238 (100%)	1 (0%)	91	95
3	C	336/337 (100%)	332 (99%)	4 (1%)	71	84
3	H	336/337 (100%)	333 (99%)	3 (1%)	78	88
4	D	218/288 (76%)	214 (98%)	4 (2%)	59	78
4	I	218/288 (76%)	216 (99%)	2 (1%)	78	88
5	E	50/55 (91%)	50 (100%)	0	100	100
5	J	50/55 (91%)	50 (100%)	0	100	100
All	All	2267/2636 (86%)	2247 (99%)	20 (1%)	78	88

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	ARG
1	A	109	ILE
2	B	157	PHE
3	C	139	MET
3	C	236	HIS
3	C	333	PHE
3	C	361	ARG
4	D	92	ARG
4	D	221	TYR
4	D	257	GLU
4	D	275	LEU
1	F	51	ASP
1	F	196	ARG
1	F	209	LEU
2	G	245	LYS
3	H	218	LYS
3	H	227	HIS
3	H	281	HIS
4	I	134	MET
4	I	221	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	HIS
1	A	151	HIS
1	A	257	GLN
2	B	177	GLN
2	B	226	HIS
3	C	281	HIS
3	H	122	GLN
3	H	266	GLN

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	312/411 (75%)	-0.01	8 (2%) 56 49	149, 225, 297, 336	0
1	F	320/411 (77%)	0.11	8 (2%) 57 51	170, 239, 312, 350	0
2	B	262/295 (88%)	-0.09	1 (0%) 92 91	170, 221, 276, 299	0
2	G	262/295 (88%)	-0.08	6 (2%) 60 55	175, 223, 289, 353	0
3	C	383/387 (98%)	-0.21	3 (0%) 86 84	148, 196, 256, 294	0
3	H	383/387 (98%)	-0.05	13 (3%) 45 39	180, 234, 302, 362	0
4	D	239/337 (70%)	0.06	7 (2%) 51 44	151, 221, 318, 391	0
4	I	238/337 (70%)	0.10	17 (7%) 16 12	193, 249, 356, 397	0
5	E	59/64 (92%)	-0.18	0 100 100	166, 202, 246, 265	0
5	J	59/64 (92%)	-0.21	0 100 100	183, 223, 300, 313	0
All	All	2517/2988 (84%)	-0.04	63 (2%) 57 51	148, 224, 302, 397	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	1	MET	5.0
4	I	257	GLU	4.4
3	H	166	THR	3.9
4	I	256	THR	3.5
4	I	304	ALA	3.5
4	D	256	THR	3.5
3	H	164	ASN	3.3
1	F	1	MET	3.3
4	I	262	ASP	3.3
4	D	257	GLU	3.2
4	D	89	ARG	3.2
1	F	2	GLU	3.2
4	I	248	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
3	H	165	TRP	3.2
4	I	260	GLU	3.1
2	B	151	GLY	3.1
4	D	262	ASP	3.0
1	F	3	GLY	3.0
4	D	304	ALA	3.0
1	F	330	TYR	2.9
3	C	83	ASP	2.9
1	F	29	THR	2.9
1	A	314	HIS	2.9
1	A	179	TYR	2.8
1	A	315	HIS	2.7
1	A	288	PRO	2.7
3	H	83	ASP	2.6
3	H	214	GLN	2.6
4	I	231	SER	2.6
4	D	259	LYS	2.5
3	H	2	SER	2.5
3	H	290	ASP	2.5
4	I	259	LYS	2.5
1	F	328	TYR	2.5
2	G	22	CYS	2.4
4	I	182	CYS	2.4
4	I	230	PHE	2.4
3	H	308	PHE	2.3
4	I	102	CYS	2.3
2	G	290	LEU	2.3
1	F	326	VAL	2.3
3	C	2	SER	2.3
4	I	258	GLU	2.3
1	A	304	HIS	2.3
3	H	190	LYS	2.3
3	H	291	ALA	2.3
3	H	163	ASN	2.2
1	F	327	GLU	2.2
4	D	258	GLU	2.2
3	C	1	MET	2.2
2	G	289	SER	2.2
4	I	217	THR	2.1
4	I	228	PRO	2.1
4	I	94	ASN	2.1
1	A	300	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	290	SER	2.1
3	H	298	THR	2.1
4	I	225	PRO	2.1
2	G	291	GLU	2.1
2	G	119	GLY	2.1
2	G	76	SER	2.0
1	A	317	ASP	2.0
4	I	281	SER	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
6	ZN	B	301	1/1	0.96	0.22	192,192,192,192	0
6	ZN	G	301	1/1	0.99	0.18	192,192,192,192	0

6.5 Other polymers [i](#)

There are no such residues in this entry.