



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:17 PM UTC

PDB ID : 8BBK / pdb_00008bbk
Title : Crystal structure of human Sirt3 in complex with a fragment of the human AROS protein
Authors : Steegborn, C.; Weiss, S.
Deposited on : 2022-10-13
Resolution : 3.27 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

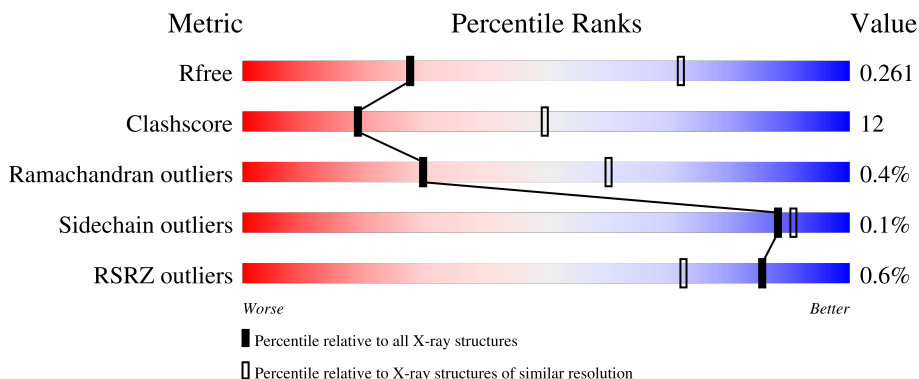
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.27 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}	180053	1303 (3.30-3.26)
Clashscore	190562	1354 (3.30-3.26)
Ramachandran outliers	187476	1334 (3.30-3.26)
Sidechain outliers	187428	1333 (3.30-3.26)
RSRZ outliers	180081	1303 (3.30-3.26)

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	399	
1	B	399	
1	C	399	
1	D	399	
1	E	399	

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Mol	Chain	Length	Quality of chain
1	F	399	 <p>% 51% 17% 31%</p>
2	G	136	 <p>98%</p>
2	H	136	 <p>98%</p>
2	I	136	 <p>98%</p>
2	J	136	 <p>98%</p>
2	K	136	 <p>98%</p>
2	L	136	 <p>98%</p>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13135 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 NAD-dependent protein deacetylase sirtuin-3, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	274	Total 2148	C 1384	N 370	O 385	S 9	0	0	0
1	B	274	Total 2159	C 1393	N 371	O 386	S 9	0	1	0
1	C	274	Total 2159	C 1393	N 371	O 386	S 9	0	1	0
1	D	274	Total 2159	C 1393	N 371	O 386	S 9	0	1	0
1	E	274	Total 2159	C 1393	N 371	O 386	S 9	0	1	0
1	F	274	Total 2159	C 1393	N 371	O 386	S 9	0	1	0

- Molecule 2 is a protein called Active regulator of SIRT1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	G	3	Total 31	C 18	N 10	O 3	0	0	0
2	H	3	Total 31	C 18	N 10	O 3	0	0	0
2	I	3	Total 31	C 18	N 10	O 3	0	0	0
2	J	3	Total 31	C 18	N 10	O 3	0	0	0
2	K	3	Total 31	C 18	N 10	O 3	0	0	0
2	L	3	Total 31	C 18	N 10	O 3	0	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Zn 1	0	0
3	B	1	Total 1	Zn 1	0	0
3	C	1	Total 1	Zn 1	0	0
3	D	1	Total 1	Zn 1	0	0
3	E	1	Total 1	Zn 1	0	0
3	F	1	Total 1	Zn 1	0	0

PHE
THR
GLU
GLU
ASP
PHE
GLN
LYS
PHE
GLN
GLN
GLU
TYR
PHE
GLY
SER

- Molecule 2: Active regulator of SIRT1

Chain J: ... 98%

MET
SER
ALA
ALA
LEU
LEU
ARG
ARG
GLY
PHE
LEU
LEU
GLU
GLU
ALA
ALA
SER
GLU
LEU
PHE
LEU
LEU
PRO
ARG
ASP
THR
PRO
PRO
ARG
GLY
GLN
ALA
ALA
LYS
PRO
ARG
GLY
GLY
PRO
VAL
GLN
ILE
LYS
ARG
ARG
PRO
ARG
GLN
LYS
THR
LYS
ALA
ILE
LYS
ARG
ASN
GLN
ASN
ARG
THR
LYS
GLY
LYS
LYS
GLY
LYS
VAL
VAL
ALA
PRO
LYS
SER
GLY
ALA
VAL

PHE
THR
GLU
GLU
ASP
PHE
GLN
LYS
PHE
GLN
GLN
GLU
TYR
PHE
GLY
SER

- Molecule 2: Active regulator of SIRT1

Chain K: .. 98%

MET
SER
ALA
ALA
LEU
LEU
ARG
ARG
GLY
PHE
LEU
LEU
GLU
GLU
ALA
ALA
SER
GLU
LEU
PHE
LEU
LEU
PRO
ARG
ASP
THR
PRO
PRO
ARG
GLY
GLN
ALA
ALA
LYS
PRO
ARG
GLY
GLY
PRO
VAL
GLN
ILE
LYS
ARG
ARG
PRO
ARG
GLN
LYS
THR
LYS
ALA
ILE
LYS
ARG
ASN
GLN
ASN
ARG
THR
LYS
GLY
LYS
LYS
GLY
LYS
VAL
VAL
ALA
PRO
LYS
SER
GLY
ALA
VAL

PHE
THR
GLU
GLU
ASP
PHE
GLN
LYS
PHE
GLN
GLN
GLU
TYR
PHE
GLY
SER

- Molecule 2: Active regulator of SIRT1

Chain L: .. 98%

MET
SER
ALA
ALA
LEU
LEU
ARG
ARG
GLY
PHE
LEU
LEU
GLU
GLU
ALA
ALA
SER
GLU
LEU
PHE
LEU
LEU
PRO
ARG
ASP
THR
PRO
PRO
ARG
GLY
GLN
ALA
ALA
LYS
PRO
ARG
GLY
GLY
PRO
VAL
GLN
ILE
LYS
ARG
ARG
PRO
ARG
GLN
LYS
THR
LYS
ALA
ILE
LYS
ARG
ASN
GLN
ASN
ARG
THR
LYS
GLY
LYS
LYS
GLY
LYS
VAL
VAL
ALA
PRO
LYS
SER
GLY
ALA
VAL

PHE
THR
GLU
GLU
ASP
PHE
GLN
LYS
PHE
GLN
GLN
GLU
TYR
PHE
GLY
SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	110.22Å 110.22Å 344.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.19 – 3.27 49.19 – 3.27	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.19-3.27) 99.8 (49.19-3.27)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 3.25Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.202 , 0.261 0.205 , 0.261	Depositor DCC
R_{free} test set	1929 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	103.0	Xtrriage
Anisotropy	0.294	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13135	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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	0.54	0/2203	0.80	2/3001 (0.1%)
1	B	0.49	0/2215	0.79	0/3017
1	C	0.47	0/2215	0.76	0/3017
1	D	0.48	0/2215	0.77	0/3017
1	E	0.51	0/2215	0.79	1/3017 (0.0%)
1	F	0.51	0/2215	0.82	2/3017 (0.1%)
2	G	0.76	0/30	1.22	0/36
2	H	0.58	0/30	1.13	0/36
2	I	1.09	0/30	1.39	0/36
2	J	0.95	0/30	2.03	1/36 (2.8%)
2	K	0.73	0/30	1.10	0/36
2	L	0.77	0/30	1.77	0/36
All	All	0.51	0/13458	0.80	6/18302 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ARG	CD-NE-CZ	7.62	135.07	124.40
1	A	139	ARG	CG-CD-NE	-6.22	98.32	112.00
1	F	293	PHE	CA-C-N	5.87	132.75	121.54
1	F	293	PHE	C-N-CA	5.87	132.75	121.54
2	J	65	LYS	CD-CE-NZ	5.87	130.67	111.90
1	E	235	ARG	CB-CG-CD	-5.36	98.98	111.30

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	2148	0	2163	57	0
1	B	2159	0	2171	50	1
1	C	2159	0	2171	49	0
1	D	2159	0	2171	51	0
1	E	2159	0	2171	48	1
1	F	2159	0	2171	60	0
2	G	31	0	38	4	0
2	H	31	0	38	4	0
2	I	31	0	38	1	0
2	J	31	0	38	3	0
2	K	31	0	38	4	0
2	L	31	0	38	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
All	All	13135	0	13246	311	1

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 12.

All (311) 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:248:HIS:HD2	2:G:65:LYS:HE3	1.06	1.11
1:A:248:HIS:CD2	2:G:65:LYS:HE3	1.88	1.07
1:F:293:PHE:N	1:F:296:GLU:OE1	2.01	0.92
1:D:248:HIS:CD2	2:J:65:LYS:HE2	2.07	0.88
1:F:292:VAL:HG12	2:L:65:LYS:HD2	1.55	0.86
1:F:296:GLU:HB3	1:F:297:PRO:HD2	1.57	0.85
1:A:145:GLY:HA3	1:A:320:THR:HB	1.62	0.82
1:A:154:ILE:HD13	1:A:204:TYR:CD2	2.20	0.77
1:A:296:GLU:O	2:G:64:ARG:N	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:LEU:HA	1:C:236:VAL:HG12	1.67	0.74
1:F:145:GLY:HA3	1:F:320:THR:HB	1.71	0.72
1:F:293:PHE:HB2	1:F:296:GLU:OE1	1.90	0.71
1:A:154:ILE:HD13	1:A:204:TYR:HD2	1.53	0.71
1:E:205:LYS:HG2	1:E:394:LEU:HD13	1.73	0.70
1:C:125:LEU:HD22	1:C:376:LEU:HD12	1.74	0.69
1:E:184[B]:PHE:HE1	1:E:191:PRO:HG2	1.59	0.67
1:F:256:CYS:SG	1:F:258:VAL:N	2.59	0.67
1:B:322:LEU:HD22	1:B:327:PHE:HB3	1.77	0.67
1:F:142:VAL:HG22	1:F:316:LEU:HB3	1.77	0.65
1:D:261:ARG:NH2	1:D:282:VAL:HG21	2.11	0.65
1:A:186:PHE:HD1	1:B:306:VAL:HG21	1.61	0.64
1:B:294:PHE:HE1	2:H:65:LYS:HZ2	1.45	0.64
1:B:184[B]:PHE:HE1	1:B:191:PRO:HG2	1.61	0.64
1:F:322:LEU:HD22	1:F:327:PHE:HB3	1.79	0.64
1:E:264:PRO:HD2	1:E:267:ASP:OD2	1.98	0.63
1:D:145:GLY:HA3	1:D:320:THR:HB	1.80	0.63
1:A:316:LEU:HG	1:A:318:LEU:HD21	1.81	0.63
1:A:154:ILE:HA	1:A:204:TYR:HE2	1.64	0.62
1:A:208:VAL:HG23	1:A:383:MET:HE2	1.82	0.62
1:F:348:VAL:HG12	1:F:349:GLY:H	1.64	0.61
1:D:184[B]:PHE:CE1	1:D:191:PRO:HG2	2.35	0.61
1:E:294:PHE:HD1	2:K:65:LYS:HG3	1.65	0.61
1:B:214:ARG:NH2	1:B:390:GLU:OE2	2.31	0.61
1:C:206:PRO:HG3	1:C:236:VAL:HG13	1.83	0.61
1:D:190:LYS:NZ	1:D:275:ASP:O	2.34	0.60
1:B:264:PRO:HD2	1:B:267:ASP:OD2	2.02	0.60
1:D:124:SER:O	1:D:127:ASP:HB2	2.02	0.60
1:D:200:TYR:CD2	1:D:201:PRO:HD2	2.37	0.60
1:F:293:PHE:CA	1:F:296:GLU:OE1	2.50	0.59
1:D:179:ILE:HG23	1:D:180:PHE:CD1	2.38	0.59
1:D:344:ASN:O	1:D:363:LEU:HA	2.03	0.59
1:A:374:VAL:HG11	1:A:383:MET:HG3	1.85	0.58
1:E:188:ASN:O	1:E:191:PRO:HD2	2.04	0.58
1:F:179:ILE:HD12	1:F:195:LEU:HD22	1.86	0.58
1:F:213:LEU:HD21	1:F:318:LEU:HD11	1.85	0.58
1:F:235:ARG:NH2	1:F:239:ILE:O	2.37	0.58
2:L:65:LYS:O	2:L:65:LYS:HG2	2.04	0.58
1:D:139:ARG:NH2	1:D:311:MET:O	2.36	0.58
1:E:184[B]:PHE:CE1	1:E:191:PRO:HG2	2.39	0.58
1:A:164:LEU:HD21	1:A:195:LEU:HD12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:296:GLU:HB3	1:F:297:PRO:CD	2.31	0.57
1:E:179:ILE:HD12	1:E:195:LEU:HD22	1.87	0.57
1:E:234:GLU:HB3	1:E:244:LEU:HD21	1.85	0.57
1:E:196:ALA:O	1:E:200:TYR:HB2	2.04	0.57
1:B:385:ASP:O	1:B:389:ARG:HG3	2.04	0.57
1:D:177:GLU:HB3	1:D:294:PHE:HE2	1.69	0.57
1:D:184[B]:PHE:HE1	1:D:191:PRO:HG2	1.69	0.57
1:F:293:PHE:C	1:F:295:GLY:H	2.12	0.57
2:G:64:ARG:HD2	2:G:64:ARG:O	2.05	0.57
1:C:214:ARG:NH2	1:C:390:GLU:OE2	2.27	0.57
1:D:248:HIS:HD2	2:J:65:LYS:HE2	1.67	0.57
1:C:318:LEU:HD23	1:C:343:ILE:HB	1.87	0.56
1:B:184[B]:PHE:CE1	1:B:191:PRO:HG2	2.40	0.56
1:B:261:ARG:NH2	1:B:282:VAL:HG11	2.21	0.56
1:E:248:HIS:ND1	2:K:65:LYS:HE2	2.20	0.56
1:F:188:ASN:O	1:F:191:PRO:HD2	2.06	0.56
1:A:131:LEU:HD23	1:A:136:ALA:HB3	1.88	0.56
1:A:124:SER:N	1:A:127:ASP:OD2	2.36	0.55
1:B:379:TRP:O	1:B:382:GLU:N	2.39	0.55
1:B:375:GLU:O	1:B:378:GLY:N	2.36	0.55
1:A:322:LEU:HD22	1:A:327:PHE:HB3	1.88	0.55
1:C:390:GLU:O	1:C:394:LEU:HD13	2.07	0.55
1:B:294:PHE:HD1	2:H:65:LYS:HD2	1.71	0.54
1:F:140:VAL:HG22	1:F:314:LEU:HB3	1.89	0.54
1:D:328:ALA:HB1	1:D:350:PRO:HG2	1.88	0.54
1:F:324:VAL:HG22	1:F:325:GLU:O	2.08	0.54
1:A:160:PRO:HA	1:A:165:TYR:CD2	2.43	0.54
1:E:145:GLY:HA3	1:E:320:THR:HB	1.90	0.54
1:F:164:LEU:HD21	1:F:195:LEU:HD12	1.89	0.54
1:F:292:VAL:O	2:L:65:LYS:HE3	2.08	0.54
1:A:200:TYR:CD2	1:A:201:PRO:HD2	2.43	0.53
1:A:148:ILE:HB	1:A:209:THR:HG21	1.89	0.53
1:F:348:VAL:HG12	1:F:349:GLY:N	2.22	0.53
1:C:122:LYS:HG3	1:C:123:LEU:H	1.73	0.53
1:C:188:ASN:O	1:C:191:PRO:HD2	2.08	0.53
1:D:188:ASN:O	1:D:191:PRO:HD2	2.09	0.53
1:D:235:ARG:NH2	1:D:239:ILE:O	2.42	0.53
1:D:205:LYS:HG2	1:D:394:LEU:HD13	1.90	0.53
1:F:184[B]:PHE:HE1	1:F:191:PRO:HG2	1.74	0.53
1:D:374:VAL:HG11	1:D:383:MET:HG3	1.90	0.53
1:B:219:LYS:NZ	1:B:382:GLU:OE2	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:LEU:HD11	1:B:344:ASN:HB2	1.91	0.53
1:C:361:ALA:HB1	1:C:363:LEU:HD21	1.90	0.53
1:F:293:PHE:CB	1:F:296:GLU:OE1	2.56	0.53
1:C:343:ILE:HG12	1:C:362:GLN:HB3	1.90	0.52
1:B:385:ASP:O	1:B:388:GLN:HB3	2.10	0.52
1:C:196:ALA:O	1:C:200:TYR:HB2	2.08	0.52
1:B:200:TYR:CD2	1:B:201:PRO:HD2	2.45	0.52
1:A:200:TYR:CG	1:A:201:PRO:HD2	2.44	0.52
1:C:139:ARG:NH2	1:C:139:ARG:HB2	2.25	0.52
1:B:125:LEU:HD11	1:B:373:LEU:HB2	1.93	0.51
1:C:325:GLU:OE2	1:C:326:PRO:HA	2.09	0.51
1:B:139:ARG:HD2	1:B:311:MET:HE2	1.91	0.51
1:C:344:ASN:O	1:C:363:LEU:HA	2.10	0.51
1:A:325:GLU:OE2	1:A:326:PRO:HA	2.10	0.51
1:A:347:LEU:HB2	1:A:363:LEU:HD21	1.93	0.51
1:E:160:PRO:HA	1:E:165:TYR:CG	2.45	0.51
1:D:256:CYS:HB3	1:D:260:GLN:H	1.76	0.51
1:D:342:LEU:HD11	1:D:344:ASN:HB2	1.93	0.51
1:E:365:ASP:OD1	1:E:366:VAL:N	2.44	0.51
1:A:217:HIS:HB2	1:A:222:LEU:HD23	1.92	0.51
1:E:374:VAL:HG11	1:E:383:MET:HG3	1.93	0.51
1:C:164:LEU:HD22	1:C:198:GLU:HG2	1.93	0.50
1:B:386:LEU:HD13	1:B:389:ARG:HH21	1.76	0.50
1:C:288:LYS:HG2	1:C:289:PRO:O	2.12	0.50
1:E:200:TYR:CG	1:E:201:PRO:HD2	2.47	0.50
1:F:264:PRO:HD2	1:F:267:ASP:OD2	2.12	0.50
1:C:279:ARG:NH1	1:E:307:VAL:HB	2.27	0.50
1:E:294:PHE:CD1	2:K:65:LYS:HG3	2.47	0.50
1:D:385:ASP:O	1:D:389:ARG:HD2	2.12	0.50
1:E:124:SER:O	1:E:127:ASP:HB2	2.12	0.50
1:B:268:ILE:O	1:B:272:VAL:HG23	2.12	0.49
1:D:151:PRO:HB2	1:D:207:ASN:ND2	2.27	0.49
1:C:345:ARG:NH2	1:C:365:ASP:HA	2.27	0.49
1:F:292:VAL:CG1	2:L:65:LYS:HD2	2.36	0.49
1:B:160:PRO:HA	1:B:165:TYR:CD2	2.47	0.49
1:C:259:CYS:SG	1:C:261:ARG:HG3	2.53	0.49
1:A:302:PHE:CZ	1:A:326:PRO:HG2	2.47	0.49
1:C:208:VAL:HG11	1:C:367:VAL:HG13	1.95	0.49
1:B:167:ASN:O	1:B:170:GLN:HB3	2.13	0.49
1:A:149:SER:HB3	1:A:154:ILE:HG13	1.93	0.49
1:A:372:SER:O	1:A:376:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ARG:HG2	1:B:269:ARG:HH11	1.76	0.48
1:A:259:CYS:HB3	1:A:283:CYS:SG	2.53	0.48
1:B:279:ARG:HH21	1:B:284:THR:HB	1.79	0.48
1:F:200:TYR:CG	1:F:201:PRO:HD2	2.49	0.48
1:D:316:LEU:HD12	1:D:316:LEU:HA	1.53	0.48
1:E:173:LEU:HD22	1:E:178:ALA:HB3	1.96	0.48
1:F:184[B]:PHE:CE1	1:F:191:PRO:HG2	2.49	0.48
1:A:208:VAL:HG23	1:A:383:MET:CE	2.44	0.48
1:F:226:TYR:CE2	1:F:309:PHE:HE1	2.32	0.48
1:D:200:TYR:CG	1:D:201:PRO:HD2	2.49	0.48
1:E:342:LEU:HD11	1:E:344:ASN:HB2	1.95	0.48
1:B:288:LYS:HG2	1:B:289:PRO:O	2.14	0.47
1:C:303:LEU:HD13	1:D:257:THR:HG23	1.94	0.47
1:F:184[B]:PHE:O	1:F:187:HIS:HB3	2.13	0.47
1:D:383:MET:HE3	1:D:383:MET:HB3	1.78	0.47
1:B:296:GLU:O	2:H:65:LYS:HB2	2.13	0.47
1:A:203:ASN:O	1:A:204:TYR:HD1	1.98	0.47
1:C:124:SER:O	1:C:127:ASP:HB2	2.15	0.47
1:D:298:LEU:HG	2:J:64:ARG:O	2.15	0.47
1:A:132:ILE:HB	1:A:377:LEU:HD21	1.97	0.47
1:E:322:LEU:HD22	1:E:327:PHE:HB3	1.96	0.47
1:D:377:LEU:HD13	1:D:379:TRP:CZ3	2.50	0.47
1:D:288:LYS:HG2	1:D:289:PRO:O	2.15	0.46
1:A:279:ARG:HE	1:A:284:THR:HB	1.80	0.46
1:A:313:ASP:C	1:A:338:VAL:HG13	2.41	0.46
1:C:370:VAL:O	1:C:374:VAL:HG23	2.16	0.46
1:E:361:ALA:HB1	1:E:363:LEU:HD21	1.97	0.46
1:A:124:SER:O	1:A:127:ASP:HB2	2.16	0.46
1:A:125:LEU:HD11	1:A:373:LEU:HB2	1.97	0.46
1:C:141:VAL:HG23	1:C:223:LEU:HD23	1.97	0.46
1:D:271:ASP:HA	1:D:276:ARG:NH2	2.30	0.46
1:E:173:LEU:CD2	1:E:178:ALA:HB3	2.44	0.46
1:B:124:SER:H	1:B:127:ASP:HB2	1.80	0.46
1:E:313:ASP:C	1:E:338:VAL:HG13	2.41	0.46
1:A:344:ASN:OD1	1:A:345:ARG:N	2.48	0.46
1:D:154:ILE:HD13	1:D:204:TYR:CD2	2.51	0.46
1:E:228:GLN:HG2	1:E:327:PHE:CE2	2.51	0.46
1:F:196:ALA:O	1:F:200:TYR:HB2	2.16	0.46
1:F:375:GLU:O	1:F:378:GLY:N	2.37	0.46
1:A:375:GLU:O	1:A:378:GLY:N	2.35	0.46
1:B:344:ASN:O	1:B:363:LEU:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:LYS:HG3	1:F:123:LEU:H	1.80	0.46
1:C:266:GLU:OE1	1:C:266:GLU:N	2.45	0.46
1:C:279:ARG:HH21	1:C:284:THR:HB	1.81	0.46
1:D:124:SER:N	1:D:127:ASP:OD2	2.46	0.46
1:D:261:ARG:HH21	1:D:282:VAL:HG21	1.79	0.46
1:E:292:VAL:O	2:K:65:LYS:HE3	2.16	0.46
1:F:244:LEU:HD23	1:F:244:LEU:HA	1.74	0.46
1:A:149:SER:O	1:A:152:SER:N	2.49	0.45
1:B:303:LEU:HD23	1:B:303:LEU:HA	1.85	0.45
1:C:125:LEU:CD2	1:C:376:LEU:HD12	2.45	0.45
1:C:361:ALA:HB1	1:C:363:LEU:CD2	2.47	0.45
1:E:348:VAL:HG22	1:E:349:GLY:H	1.81	0.45
1:F:226:TYR:CE1	1:F:245:VAL:HG21	2.50	0.45
1:B:123:LEU:HD11	1:B:358:ARG:HE	1.81	0.45
1:D:320:THR:HG23	1:D:322:LEU:HG	1.98	0.45
1:A:173:LEU:HD22	1:A:178:ALA:HB3	1.98	0.45
1:A:279:ARG:HH21	1:A:284:THR:HB	1.82	0.45
1:B:322:LEU:HD23	1:B:322:LEU:HA	1.72	0.45
1:D:256:CYS:HB3	1:D:260:GLN:N	2.31	0.45
1:A:186:PHE:CD1	1:B:306:VAL:HG21	2.47	0.45
1:A:216:LEU:HD12	1:A:221:LEU:HD12	1.99	0.45
1:A:279:ARG:HA	1:A:285:GLY:O	2.17	0.45
1:A:228:GLN:HG2	1:A:327:PHE:CE2	2.52	0.45
1:B:122:LYS:HG2	1:B:123:LEU:H	1.81	0.45
1:E:224:ARG:NE	1:E:308:ASP:OD2	2.34	0.45
1:F:228:GLN:HG2	1:F:327:PHE:CE2	2.52	0.45
1:C:243:LYS:HD3	1:C:243:LYS:HA	1.75	0.45
1:D:164:LEU:O	1:D:168:LEU:HG	2.17	0.44
1:D:142:VAL:HG22	1:D:316:LEU:HB3	1.98	0.44
1:E:314:LEU:HD12	1:E:339:PRO:O	2.16	0.44
1:E:386:LEU:HD13	1:E:389:ARG:HH21	1.82	0.44
1:F:316:LEU:HG	1:F:318:LEU:HD21	1.99	0.44
1:F:379:TRP:O	1:F:382:GLU:N	2.50	0.44
1:A:154:ILE:HA	1:A:204:TYR:CE2	2.48	0.44
1:C:269:ARG:NH2	1:C:273:MET:HE2	2.32	0.44
1:F:279:ARG:HH21	1:F:284:THR:CB	2.31	0.44
1:D:246:GLU:OE1	1:D:250:THR:HB	2.17	0.44
1:A:214:ARG:HG3	1:A:386:LEU:HD21	1.99	0.44
1:A:325:GLU:OE1	1:A:328:ALA:HB3	2.16	0.44
1:B:248:HIS:C	1:B:292:VAL:HG23	2.42	0.44
1:D:182:LEU:HA	1:D:182:LEU:HD23	1.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:261:ARG:CZ	1:E:282:VAL:HG21	2.47	0.44
1:C:144:VAL:HB	1:C:148:ILE:HD13	1.99	0.44
1:A:322:LEU:HD22	1:A:327:PHE:CB	2.48	0.44
1:B:160:PRO:HA	1:B:165:TYR:CG	2.53	0.44
1:D:144:VAL:HG12	1:D:318:LEU:HB2	1.98	0.44
1:F:248:HIS:ND1	2:L:65:LYS:HE2	2.33	0.44
1:B:320:THR:HG23	1:B:322:LEU:HG	2.00	0.44
1:C:294:PHE:CD1	2:I:65:LYS:HG2	2.53	0.43
1:E:219:LYS:HD3	1:E:379:TRP:CZ2	2.52	0.43
1:C:184[B]:PHE:O	1:C:187:HIS:HB3	2.18	0.43
1:A:313:ASP:O	1:A:338:VAL:HG13	2.18	0.43
1:E:174:PRO:HG2	1:E:175:TYR:CE1	2.53	0.43
1:B:341:LEU:HD12	1:B:342:LEU:N	2.33	0.43
1:F:348:VAL:CG1	1:F:349:GLY:H	2.31	0.43
1:B:196:ALA:O	1:B:200:TYR:HB2	2.18	0.43
1:E:142:VAL:HB	1:E:225:LEU:HD13	2.00	0.43
1:C:145:GLY:HA3	1:C:320:THR:HB	2.01	0.43
1:C:268:ILE:HG22	1:C:278:PRO:HB2	2.00	0.43
1:F:134:ALA:O	1:F:135:ARG:HG3	2.18	0.43
1:F:235:ARG:HD2	1:F:235:ARG:HA	1.77	0.43
1:D:160:PRO:HA	1:D:165:TYR:CD2	2.54	0.43
1:D:300:GLN:HB3	1:E:258:VAL:O	2.18	0.43
1:D:313:ASP:C	1:D:338:VAL:HG13	2.44	0.43
1:E:390:GLU:OE1	1:E:393:LYS:HD2	2.19	0.43
1:A:160:PRO:HA	1:A:165:TYR:CG	2.54	0.42
1:F:342:LEU:HD11	1:F:344:ASN:HB2	2.01	0.42
1:A:315:LEU:HB2	1:A:334:VAL:HG11	2.00	0.42
1:C:186:PHE:HD1	1:E:306:VAL:HG21	1.83	0.42
1:C:304:LEU:HG	1:D:258:VAL:HG21	2.01	0.42
1:D:164:LEU:HD21	1:D:195:LEU:HD12	2.00	0.42
1:F:126:GLN:HA	1:F:376:LEU:HD13	2.00	0.42
1:F:313:ASP:C	1:F:338:VAL:HG13	2.45	0.42
1:F:374:VAL:HG11	1:F:383:MET:HG3	2.01	0.42
2:L:66:ARG:HD2	2:L:66:ARG:HA	1.74	0.42
1:A:301:ARG:NH1	1:A:304:LEU:HD11	2.34	0.42
1:B:298:LEU:HD23	1:B:298:LEU:HA	1.88	0.42
1:C:320:THR:HG23	1:C:322:LEU:HG	2.01	0.42
1:F:139:ARG:NH2	1:F:139:ARG:HB2	2.34	0.42
1:B:315:LEU:CD2	1:B:317:ILE:HD11	2.50	0.42
1:C:122:LYS:HG3	1:C:123:LEU:N	2.33	0.42
1:C:279:ARG:HH21	1:C:284:THR:CB	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:LEU:HD23	1:C:322:LEU:HA	1.78	0.42
1:F:385:ASP:O	1:F:388:GLN:HB3	2.19	0.42
1:B:124:SER:N	1:B:127:ASP:OD2	2.52	0.42
1:B:269:ARG:NH2	1:B:273:MET:HE2	2.34	0.42
1:E:160:PRO:HB3	1:E:165:TYR:CE2	2.54	0.42
1:E:226:TYR:CE2	1:E:245:VAL:HG11	2.54	0.42
1:D:385:ASP:O	1:D:389:ARG:NH2	2.53	0.42
1:A:213:LEU:HD21	1:A:318:LEU:HD11	2.00	0.42
1:C:303:LEU:HD13	1:D:257:THR:CG2	2.50	0.42
1:F:298:LEU:HA	1:F:298:LEU:HD23	1.74	0.42
1:A:143:MET:HE2	1:A:143:MET:HB3	1.87	0.42
1:D:214:ARG:NH2	1:D:390:GLU:OE2	2.51	0.42
1:E:316:LEU:HD12	1:E:316:LEU:HA	1.85	0.42
1:A:174:PRO:HG2	1:A:175:TYR:CE2	2.55	0.42
1:C:209:THR:HG23	1:C:370:VAL:HG21	2.01	0.42
1:F:217:HIS:HB2	1:F:222:LEU:HD23	2.00	0.42
1:B:124:SER:O	1:B:127:ASP:HB2	2.20	0.41
1:B:279:ARG:HH21	1:B:284:THR:CB	2.33	0.41
1:E:261:ARG:NH2	1:E:282:VAL:HG11	2.35	0.41
1:B:168:LEU:HD23	1:B:168:LEU:HA	1.82	0.41
1:D:325:GLU:OE2	1:D:326:PRO:HA	2.20	0.41
1:E:184[B]:PHE:O	1:E:187:HIS:HB3	2.20	0.41
1:C:141:VAL:CG2	1:C:223:LEU:HD23	2.50	0.41
1:A:384:ARG:HD3	1:A:384:ARG:C	2.45	0.41
1:C:244:LEU:HD23	1:C:244:LEU:HA	1.85	0.41
1:C:362:GLN:O	1:C:362:GLN:HG3	2.19	0.41
1:F:217:HIS:HA	1:F:222:LEU:HB3	2.03	0.41
1:F:279:ARG:HH21	1:F:284:THR:HB	1.84	0.41
1:B:192:PHE:HE2	1:B:289:PRO:HD2	1.86	0.41
1:B:365:ASP:OD1	1:B:366:VAL:N	2.54	0.41
1:E:385:ASP:O	1:E:388:GLN:HB3	2.21	0.41
1:B:164:LEU:HD21	1:B:195:LEU:HD12	2.02	0.41
1:F:296:GLU:CB	1:F:297:PRO:CD	2.97	0.41
1:A:208:VAL:HG11	1:A:367:VAL:HG13	2.03	0.41
1:A:342:LEU:HD23	1:A:347:LEU:HD13	2.02	0.41
1:E:126:GLN:HB2	1:E:376:LEU:HD13	2.02	0.41
1:F:322:LEU:HD23	1:F:322:LEU:HA	1.86	0.41
1:F:374:VAL:CG1	1:F:383:MET:HG3	2.51	0.41
1:E:320:THR:HG23	1:E:322:LEU:HG	2.02	0.41
1:E:361:ALA:HB1	1:E:363:LEU:CD2	2.51	0.41
1:F:293:PHE:C	1:F:295:GLY:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:293:PHE:O	1:F:295:GLY:N	2.41	0.41
1:B:173:LEU:HD11	1:B:191:PRO:HB3	2.03	0.40
1:E:322:LEU:HD23	1:E:322:LEU:HA	1.84	0.40
2:H:64:ARG:O	2:H:64:ARG:HG3	2.21	0.40
1:E:170:GLN:O	1:E:170:GLN:HG2	2.21	0.40
1:F:344:ASN:O	1:F:363:LEU:HA	2.22	0.40
1:B:311:MET:HE2	1:B:311:MET:HB3	1.76	0.40
1:C:153:GLY:O	1:C:204:TYR:HE2	2.05	0.40
1:C:232:GLY:O	1:C:235:ARG:HB2	2.21	0.40
1:F:141:VAL:CG2	1:F:312:ALA:HB2	2.52	0.40
1:A:214:ARG:NE	1:A:218:ASP:OD2	2.50	0.40
1:C:125:LEU:HD21	1:C:373:LEU:HB2	2.03	0.40
1:D:347:LEU:HD23	1:D:352:ALA:HB2	2.04	0.40
1:F:256:CYS:SG	1:F:257:THR:N	2.95	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:SER:OG	1:E:130:GLU:OE1[6_554]	2.11	0.09

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	272/399 (68%)	261 (96%)	11 (4%)	0	100 100
1	B	273/399 (68%)	264 (97%)	8 (3%)	1 (0%)	30 60
1	C	273/399 (68%)	259 (95%)	13 (5%)	1 (0%)	30 60
1	D	273/399 (68%)	264 (97%)	8 (3%)	1 (0%)	30 60
1	E	273/399 (68%)	264 (97%)	8 (3%)	1 (0%)	30 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	273/399 (68%)	261 (96%)	9 (3%)	3 (1%)	11	39
2	G	1/136 (1%)	1 (100%)	0	0	100	100
2	H	1/136 (1%)	0	1 (100%)	0	100	100
2	I	1/136 (1%)	1 (100%)	0	0	100	100
2	J	1/136 (1%)	0	1 (100%)	0	100	100
2	K	1/136 (1%)	1 (100%)	0	0	100	100
2	L	1/136 (1%)	1 (100%)	0	0	100	100
All	All	1643/3210 (51%)	1577 (96%)	59 (4%)	7 (0%)	30	60

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	294	PHE
1	F	183	PRO
1	C	183	PRO
1	D	183	PRO
1	E	183	PRO
1	F	295	GLY
1	B	183	PRO

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	237/327 (72%)	237 (100%)	0	100	100
1	B	238/327 (73%)	238 (100%)	0	100	100
1	C	238/327 (73%)	238 (100%)	0	100	100
1	D	238/327 (73%)	238 (100%)	0	100	100
1	E	238/327 (73%)	238 (100%)	0	100	100
1	F	238/327 (73%)	237 (100%)	1 (0%)	84	85
2	G	3/114 (3%)	3 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	3/114 (3%)	3 (100%)	0	100	100
2	I	3/114 (3%)	3 (100%)	0	100	100
2	J	3/114 (3%)	3 (100%)	0	100	100
2	K	3/114 (3%)	3 (100%)	0	100	100
2	L	3/114 (3%)	3 (100%)	0	100	100
All	All	1445/2646 (55%)	1444 (100%)	1 (0%)	88	91

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	294	PHE

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

Mol	Chain	Res	Type
1	A	248	HIS
1	B	248	HIS
1	B	388	GLN
1	D	169	GLN
1	D	248	HIS
1	E	203	ASN
1	F	203	ASN
1	F	368	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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	274/399 (68%)	-0.53	2 (0%) 84 70	62, 92, 132, 155	0
1	B	274/399 (68%)	-0.46	3 (1%) 78 61	42, 91, 126, 142	1 (0%)
1	C	274/399 (68%)	-0.49	1 (0%) 88 78	41, 94, 126, 140	1 (0%)
1	D	274/399 (68%)	-0.41	1 (0%) 88 78	44, 99, 138, 162	1 (0%)
1	E	274/399 (68%)	-0.60	1 (0%) 88 78	42, 87, 112, 127	1 (0%)
1	F	274/399 (68%)	-0.53	2 (0%) 84 70	30, 92, 118, 146	1 (0%)
2	G	3/136 (2%)	-0.35	0 100 100	98, 98, 100, 114	0
2	H	3/136 (2%)	0.24	0 100 100	100, 100, 101, 115	0
2	I	3/136 (2%)	-0.07	0 100 100	95, 95, 95, 109	0
2	J	3/136 (2%)	-0.12	0 100 100	93, 93, 108, 122	0
2	K	3/136 (2%)	-0.62	0 100 100	100, 100, 112, 122	0
2	L	3/136 (2%)	-0.38	0 100 100	95, 95, 108, 119	0
All	All	1662/3210 (51%)	-0.50	10 (0%) 85 72	30, 92, 127, 162	5 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	184[A]	PHE	8.0
1	B	184[A]	PHE	7.1
1	E	184[A]	PHE	6.7
1	D	184[A]	PHE	6.5
1	C	184[A]	PHE	2.9
1	B	322	LEU	2.8
1	A	121	GLY	2.5
1	F	295	GLY	2.4
1	B	351	LEU	2.1
1	A	134	ALA	2.1

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 oligosaccharides 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
3	ZN	F	401	1/1	0.99	0.04	101,101,101,101	0
3	ZN	B	401	1/1	1.00	0.03	81,81,81,81	0
3	ZN	C	401	1/1	1.00	0.03	133,133,133,133	0
3	ZN	D	401	1/1	1.00	0.02	92,92,92,92	0
3	ZN	E	401	1/1	1.00	0.02	87,87,87,87	0
3	ZN	A	401	1/1	1.00	0.01	73,73,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.