



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 11:32 AM EDT

PDB ID : 5FYQ / pdb_00005fyq
Title : Sirt2 in complex with a 13-mer trifluoroacetylated Ran peptide
Authors : Knyphausen, P.; de Boor, S.; Scislowski, L.; Extra, A.; Baldus, L.; Schacherl, M.; Baumann, U.; Neundorf, I.; Lammers, M.
Deposited on : 2016-03-09
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

<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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (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

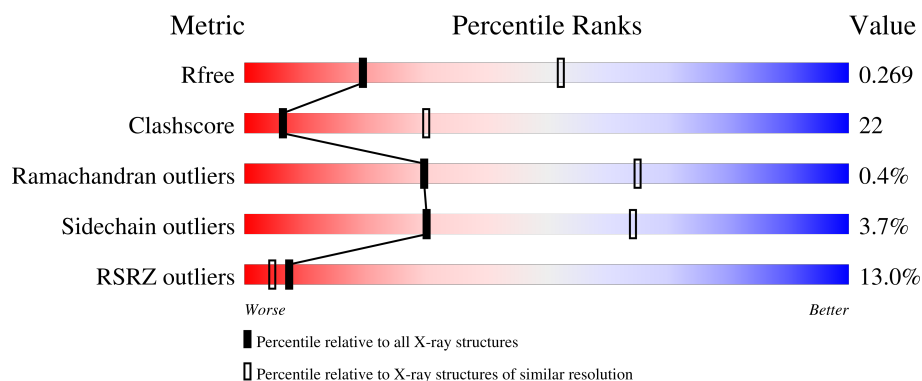
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	360	6% 55% 21% • 22%
1	B	360	14% 51% 21% • 26%
2	C	13	8% 31% 15% 46%
2	D	13	15% 23% 15% 23% 38%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	1357	-	-	X	-
3	SO4	B	1357	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4605 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-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	0	0
			2250	1445	372	417	16			
1	B	266	Total	C	N	O	S	0	0	0
			2019	1287	345	374	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q8IXJ6
A	-2	SER	-	expression tag	UNP Q8IXJ6
A	-1	GLY	-	expression tag	UNP Q8IXJ6
A	0	MET	-	expression tag	UNP Q8IXJ6
B	-3	GLY	-	expression tag	UNP Q8IXJ6
B	-2	SER	-	expression tag	UNP Q8IXJ6
B	-1	GLY	-	expression tag	UNP Q8IXJ6
B	0	MET	-	expression tag	UNP Q8IXJ6

- Molecule 2 is a protein called RAN AA 31-43.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	7	Total	C	F	N	O	0	0	0
			72	47	3	9	13			
2	D	8	Total	C	F	N	O	0	0	0
			76	49	3	10	14			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



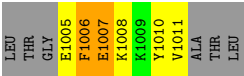
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

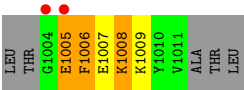
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	96	Total	O	0	0
			96	96		
5	B	79	Total	O	0	0
			79	79		
5	D	1	Total	O	0	0
			1	1		



● Molecule 2: RAN AA 31-43



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	114.95Å 114.95Å 206.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	56.61 – 3.00 56.61 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (56.61-3.00) 100.0 (56.61-3.00)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.46 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.232 , 0.271 0.234 , 0.269	Depositor DCC
R_{free} test set	856 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4605	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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, SO4, FAK

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	0.72	0/2300	1.00	7/3101 (0.2%)
1	B	0.69	0/2057	0.98	4/2777 (0.1%)
2	C	0.68	0/57	0.96	0/73
2	D	0.84	0/61	1.13	0/78
All	All	0.70	0/4475	0.99	11/6029 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	127	HIS	CA-C-N	7.15	126.78	119.56
1	B	127	HIS	C-N-CA	7.15	126.78	119.56
1	A	121	ILE	N-CA-C	7.00	117.76	110.62
1	B	205	PRO	N-CA-CB	6.69	110.27	103.25
1	B	140	PRO	N-CA-CB	6.19	109.41	102.60
1	A	209	MET	N-CA-C	5.44	116.89	111.07
1	A	207	SER	N-CA-C	-5.36	98.51	107.99
1	A	136	LYS	N-CA-C	-5.29	106.96	113.41
1	A	204	TYR	CA-C-N	5.25	126.52	120.85
1	A	204	TYR	C-N-CA	5.25	126.52	120.85
1	A	262	THR	N-CA-C	5.25	117.23	108.99

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	206	LEU	Peptide

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	2250	0	2234	90	0
1	B	2019	0	1937	92	0
2	C	72	0	61	14	0
2	D	76	0	64	10	0
3	A	5	0	0	2	0
3	B	5	0	0	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	96	0	0	44	0
5	B	79	0	0	38	0
5	D	1	0	0	0	0
All	All	4605	0	4296	193	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 22.

All (193) 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:B:147:ILE:HB	5:B:2030:HOH:O	1.18	1.29
1:A:148:CYS:HB2	5:A:2041:HOH:O	1.51	1.07
1:A:307:MET:HB2	5:A:2083:HOH:O	1.54	1.06
1:A:212:LYS:HB2	5:A:2059:HOH:O	1.59	1.00
1:A:155:LEU:HA	5:A:2043:HOH:O	1.59	0.99
1:A:276:ALA:HA	5:A:2074:HOH:O	1.63	0.97
1:A:219:PRO:HD2	5:A:2062:HOH:O	1.63	0.97
1:B:154:LEU:HB3	5:B:2031:HOH:O	1.65	0.96
1:A:108:GLU:HG2	5:A:2019:HOH:O	1.66	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:MET:HA	5:A:2059:HOH:O	1.69	0.92
1:A:222:GLU:HA	5:A:2064:HOH:O	1.69	0.92
1:A:106:ASN:HB3	5:A:2019:HOH:O	1.70	0.91
1:A:144:LYS:HE2	5:A:2040:HOH:O	1.68	0.90
1:A:99:PRO:C	1:A:104:TYR:HE1	1.79	0.90
1:B:116:GLU:HG2	2:C:1010:TYR:HE2	1.35	0.89
1:A:132:PHE:CD2	5:A:2062:HOH:O	2.25	0.87
1:B:267:GLN:HG2	2:C:1011:VAL:CG1	2.05	0.85
1:A:132:PHE:CE2	5:A:2062:HOH:O	2.29	0.85
1:B:136:LYS:O	1:B:139:TYR:N	2.11	0.83
1:B:267:GLN:HG2	2:C:1011:VAL:HG13	1.59	0.82
1:A:183:LEU:O	1:A:242:ARG:NH1	2.12	0.81
1:A:238:SER:HB2	5:A:2070:HOH:O	1.82	0.79
2:D:1005:GLU:HG2	2:D:1006:PHE:N	1.96	0.79
1:B:97:ARG:NH1	3:B:1357:SO4:S	2.56	0.79
1:A:307:MET:CB	5:A:2083:HOH:O	2.22	0.78
1:B:151:PHE:CG	5:B:2067:HOH:O	2.35	0.77
1:B:139:TYR:N	1:B:140:PRO:HA	1.99	0.77
1:A:107:LEU:H	1:A:107:LEU:HD23	1.50	0.77
1:B:151:PHE:CD1	5:B:2067:HOH:O	2.40	0.74
1:A:99:PRO:C	1:A:104:TYR:CE1	2.65	0.73
1:A:77:ARG:HD2	5:A:2008:HOH:O	1.88	0.73
1:B:195:CYS:SG	1:B:200:CYS:CB	2.77	0.72
2:D:1005:GLU:HG2	2:D:1006:PHE:H	1.54	0.72
1:B:118:ILE:HD11	1:B:119:PHE:CE2	2.25	0.72
1:A:251:PHE:HB3	5:A:2074:HOH:O	1.90	0.71
1:A:108:GLU:O	1:A:108:GLU:HG3	1.89	0.71
1:A:138:LEU:HB2	5:A:2035:HOH:O	1.90	0.71
1:B:116:GLU:HG2	2:C:1010:TYR:CE2	2.24	0.71
1:B:195:CYS:HB3	1:B:228:VAL:HG22	1.74	0.68
1:B:56:GLU:HG2	5:B:2001:HOH:O	1.93	0.68
2:D:1007:GLU:O	2:D:1009:LYS:HE2	1.94	0.67
1:B:129:GLU:HG3	5:B:2024:HOH:O	1.94	0.67
1:B:78:ARG:HD2	5:B:2012:HOH:O	1.95	0.66
1:B:136:LYS:O	1:B:139:TYR:CA	2.44	0.66
1:B:325:ASP:CB	5:B:2030:HOH:O	2.44	0.65
1:A:132:PHE:HE1	1:A:209:MET:HE3	1.61	0.65
1:A:56:GLU:N	5:A:2002:HOH:O	2.30	0.64
1:B:116:GLU:OE2	2:C:1010:TYR:OH	2.16	0.64
1:A:106:ASN:C	5:A:2019:HOH:O	2.40	0.64
1:A:77:ARG:NH2	1:B:89:THR:OG1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:GLU:HB2	5:B:2009:HOH:O	1.97	0.64
1:B:131:PHE:O	1:B:134:LEU:HG	1.98	0.64
1:B:204:TYR:CB	5:B:2042:HOH:O	2.46	0.63
1:A:209:MET:HE1	1:A:230:PRO:HD3	1.80	0.63
1:A:206:LEU:O	1:A:210:LYS:N	2.18	0.63
1:B:313:LYS:HA	5:B:2064:HOH:O	1.98	0.63
1:B:247:MET:HE1	1:B:275:LYS:HG3	1.81	0.62
1:B:278:LEU:HD23	5:B:2055:HOH:O	1.99	0.62
1:A:109:LYS:HA	1:A:110:TYR:C	2.24	0.62
1:B:279:SER:HB2	5:B:2056:HOH:O	1.99	0.62
1:A:207:SER:HA	1:A:208:TRP:C	2.24	0.62
1:A:111:HIS:CG	5:A:2024:HOH:O	2.52	0.62
1:B:116:GLU:CD	2:C:1010:TYR:OH	2.43	0.61
1:B:56:GLU:HG3	1:B:57:ARG:H	1.64	0.61
1:A:57:ARG:HD2	5:A:2003:HOH:O	2.01	0.61
1:A:134:LEU:O	1:A:135:ALA:HB3	2.01	0.60
1:B:135:ALA:HB3	1:B:136:LYS:C	2.26	0.59
1:B:267:GLN:CG	2:C:1011:VAL:CG1	2.79	0.59
1:A:238:SER:CB	5:A:2070:HOH:O	2.45	0.59
1:B:129:GLU:CG	5:B:2024:HOH:O	2.50	0.58
1:B:265:GLN:HB3	5:B:2051:HOH:O	2.03	0.58
1:B:116:GLU:CG	2:C:1010:TYR:HE2	2.14	0.58
1:A:237:GLU:O	2:D:1007:GLU:HB2	2.03	0.57
1:A:107:LEU:HD23	1:A:107:LEU:N	2.18	0.57
1:B:174:ARG:NE	1:B:180:GLN:OE1	2.38	0.56
1:B:213:ILE:CB	1:B:228:VAL:HB	2.35	0.56
1:B:133:ALA:O	1:B:134:LEU:HG	2.05	0.56
1:A:209:MET:HE2	1:A:213:ILE:HD11	1.88	0.56
1:B:97:ARG:NH1	3:B:1357:SO4:O1	2.39	0.56
1:A:139:TYR:HB3	1:A:140:PRO:C	2.32	0.55
1:B:325:ASP:CG	5:B:2030:HOH:O	2.49	0.55
1:B:264:LEU:HD22	5:B:2053:HOH:O	2.05	0.55
1:B:134:LEU:C	1:B:136:LYS:HA	2.31	0.55
2:C:1005:GLU:HG2	2:C:1007:GLU:HB2	1.88	0.55
1:A:259:VAL:HB	5:A:2080:HOH:O	2.05	0.54
1:B:84:GLY:HA3	1:B:262:THR:HB	1.90	0.54
1:B:328:CYS:CB	5:B:2067:HOH:O	2.55	0.54
1:A:140:PRO:HD2	1:A:143:PHE:CZ	2.42	0.54
1:B:118:ILE:HA	5:B:2022:HOH:O	2.08	0.53
1:A:134:LEU:O	1:A:135:ALA:CB	2.56	0.53
1:A:287:LYS:HB3	5:A:2089:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:LYS:HE3	5:A:2081:HOH:O	2.09	0.52
1:A:309:PHE:CE2	5:A:2083:HOH:O	2.54	0.52
1:A:132:PHE:CE1	1:A:209:MET:HE3	2.43	0.52
1:A:131:PHE:O	1:A:134:LEU:O	2.28	0.52
1:B:354:ALA:HB3	5:B:2075:HOH:O	2.08	0.52
2:D:1005:GLU:HG2	2:D:1006:PHE:CD1	2.45	0.52
1:B:120:GLU:OE2	1:B:122:SER:OG	2.24	0.52
1:A:352:ILE:CG2	5:A:2040:HOH:O	2.56	0.52
1:A:139:TYR:CB	1:A:140:PRO:CA	2.88	0.51
1:B:325:ASP:HA	5:B:2030:HOH:O	2.11	0.51
1:A:312:LYS:CE	5:A:2086:HOH:O	2.59	0.51
2:C:1005:GLU:HG3	2:C:1007:GLU:H	1.76	0.51
2:D:1005:GLU:CG	2:D:1006:PHE:H	2.24	0.51
2:C:1006:PHE:N	2:C:1006:PHE:CD1	2.79	0.50
1:A:144:LYS:CE	5:A:2040:HOH:O	2.40	0.50
1:A:108:GLU:CG	5:A:2019:HOH:O	2.42	0.50
1:A:287:LYS:CE	5:A:2081:HOH:O	2.59	0.49
1:B:315:TYR:CE2	1:B:316:ARG:HG2	2.47	0.49
1:B:118:ILE:HB	5:B:2022:HOH:O	2.12	0.49
1:A:277:PRO:HD3	5:A:2074:HOH:O	2.12	0.49
1:A:110:TYR:CE1	1:A:129:GLU:HB3	2.47	0.49
1:A:352:ILE:HB	5:A:2040:HOH:O	2.12	0.49
1:B:83:VAL:HB	1:B:87:ILE:HD13	1.94	0.49
1:A:163:ARG:NH1	1:A:181:GLU:O	2.45	0.49
1:A:111:HIS:CB	5:A:2024:HOH:O	2.59	0.48
1:B:206:LEU:HA	1:B:207:SER:CB	2.42	0.48
1:B:97:ARG:NH1	3:B:1357:SO4:O3	2.46	0.48
1:A:160:LEU:HB2	5:A:2043:HOH:O	2.12	0.48
1:A:220:LYS:HG3	5:A:2063:HOH:O	2.13	0.48
1:A:235:PHE:HA	2:D:1008:FAK:H6	1.95	0.48
1:B:99:PRO:HG2	5:B:2020:HOH:O	2.12	0.48
1:A:139:TYR:HB2	1:A:140:PRO:HA	1.95	0.48
1:B:286:ASN:O	1:B:321:LEU:HA	2.14	0.48
1:B:136:LYS:O	1:B:139:TYR:HA	2.13	0.48
1:B:290:ALA:HB2	5:B:2052:HOH:O	2.12	0.48
1:B:140:PRO:N	1:B:141:GLY:CA	2.77	0.48
1:A:109:LYS:HA	1:A:110:TYR:O	2.14	0.47
1:A:229:LYS:HE3	1:A:234:PHE:CD1	2.49	0.47
1:B:126:LYS:C	1:B:128:PRO:HD3	2.39	0.47
1:B:169:ILE:HB	1:B:232:ILE:HD12	1.97	0.47
1:A:324:CYS:C	5:A:2041:HOH:O	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:PRO:N	1:B:141:GLY:HA2	2.29	0.47
1:A:263:SER:N	3:A:1357:SO4:O3	2.33	0.47
1:A:104:TYR:HA	1:A:107:LEU:HD11	1.97	0.46
1:B:292:GLN:C	5:B:2059:HOH:O	2.57	0.46
1:B:267:GLN:OE1	1:B:268:PRO:HA	2.15	0.46
1:A:132:PHE:HE1	1:A:209:MET:CE	2.24	0.46
1:A:139:TYR:CB	1:A:140:PRO:HA	2.46	0.46
1:B:118:ILE:HD11	1:B:119:PHE:CZ	2.50	0.46
1:B:114:TYR:CZ	1:B:117:ALA:HB2	2.50	0.45
2:C:1006:PHE:H	2:C:1006:PHE:HD1	1.64	0.45
1:B:60:ASP:C	1:B:60:ASP:OD1	2.59	0.45
1:B:98:SER:HB3	5:B:2019:HOH:O	2.16	0.45
1:A:312:LYS:HE3	5:A:2086:HOH:O	2.17	0.45
1:B:341:LEU:O	1:B:345:VAL:HG23	2.16	0.45
1:B:118:ILE:CA	5:B:2022:HOH:O	2.63	0.45
1:A:87:ILE:HD12	1:A:149:HIS:CE1	2.52	0.45
1:B:130:PRO:O	1:B:133:ALA:O	2.34	0.44
1:A:270:ALA:HB2	5:A:2050:HOH:O	2.18	0.44
1:B:124:PHE:CD1	1:B:124:PHE:C	2.95	0.44
1:B:148:CYS:SG	1:B:324:CYS:HB3	2.58	0.44
1:B:315:TYR:CZ	1:B:316:ARG:HG2	2.52	0.44
1:A:160:LEU:HD12	5:A:2043:HOH:O	2.17	0.44
1:A:204:TYR:OH	1:A:221:CYS:HA	2.17	0.44
1:A:225:GLN:HG3	5:A:2066:HOH:O	2.17	0.44
1:B:325:ASP:CA	5:B:2030:HOH:O	2.65	0.43
1:A:112:LEU:HD11	1:A:118:ILE:HG22	2.00	0.43
1:B:129:GLU:HB2	1:B:130:PRO:HD3	1.99	0.43
1:B:233:VAL:HG23	5:B:2038:HOH:O	2.18	0.43
1:B:244:PHE:HA	1:B:247:MET:HG2	1.99	0.43
1:A:107:LEU:C	5:A:2020:HOH:O	2.61	0.43
1:A:158:LYS:HE3	1:A:337:TRP:CE2	2.53	0.43
1:A:353:ASP:O	1:A:356:SER:N	2.51	0.43
1:B:99:PRO:HD3	5:B:2018:HOH:O	2.19	0.43
1:B:127:HIS:O	1:B:130:PRO:HD2	2.18	0.43
1:B:337:TRP:CZ3	5:B:2031:HOH:O	2.56	0.43
1:B:278:LEU:CD2	5:B:2055:HOH:O	2.64	0.43
1:A:174:ARG:HD2	1:A:185:GLU:OE2	2.19	0.43
1:B:56:GLU:CG	5:B:2001:HOH:O	2.62	0.42
1:B:118:ILE:CB	5:B:2022:HOH:O	2.65	0.42
1:B:288:GLU:HG3	5:B:2052:HOH:O	2.18	0.42
1:A:282:ARG:HB2	1:A:307:MET:HE3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:LYS:HD2	5:B:2031:HOH:O	2.19	0.42
1:B:247:MET:CE	1:B:275:LYS:HG3	2.48	0.42
1:B:263:SER:O	1:B:264:LEU:C	2.62	0.42
1:B:325:ASP:HB3	5:B:2030:HOH:O	2.15	0.42
1:A:309:PHE:CD1	1:A:319:ALA:HB2	2.54	0.42
1:A:144:LYS:HA	1:A:145:PRO:HD3	1.93	0.42
1:A:205:PRO:HG2	1:A:208:TRP:H	1.85	0.42
1:A:237:GLU:C	2:D:1007:GLU:HB2	2.44	0.42
1:B:135:ALA:HB3	1:B:137:GLU:HA	2.02	0.42
1:B:200:CYS:CB	5:B:2041:HOH:O	2.68	0.42
2:D:1006:PHE:CD1	2:D:1006:PHE:O	2.73	0.42
1:B:309:PHE:CE1	1:B:319:ALA:HB2	2.55	0.41
2:D:1006:PHE:O	2:D:1006:PHE:HD1	2.03	0.41
1:A:77:ARG:CD	5:A:2008:HOH:O	2.60	0.41
1:A:262:THR:HA	3:A:1357:SO4:O3	2.20	0.41
1:B:267:GLN:CG	2:C:1011:VAL:HG12	2.50	0.41
1:A:207:SER:HB2	1:A:210:LYS:HB3	2.02	0.41
1:A:247:MET:CE	1:A:275:LYS:HG3	2.51	0.40
1:A:129:GLU:O	1:A:130:PRO:C	2.61	0.40
2:C:1005:GLU:HG3	2:C:1006:PHE:N	2.37	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	274/360 (76%)	264 (96%)	10 (4%)	0	100	100
1	B	258/360 (72%)	243 (94%)	13 (5%)	2 (1%)	16	50
2	C	4/13 (31%)	4 (100%)	0	0	100	100
2	D	5/13 (38%)	3 (60%)	2 (40%)	0	100	100
All	All	541/746 (72%)	514 (95%)	25 (5%)	2 (0%)	30	65

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	205	PRO
1	B	133	ALA

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	247/307 (80%)	240 (97%)	7 (3%)	38	70
1	B	204/307 (66%)	198 (97%)	6 (3%)	37	70
2	C	6/10 (60%)	4 (67%)	2 (33%)	0	1
2	D	6/10 (60%)	4 (67%)	2 (33%)	0	1
All	All	463/634 (73%)	446 (96%)	17 (4%)	30	64

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	LEU
1	A	120	GLU
1	A	134	LEU
1	A	174	ARG
1	A	197	SER
1	A	265	GLN
1	A	326	GLN
1	B	98	SER
1	B	174	ARG
1	B	248	GLN
1	B	249	SER
1	B	266	VAL
1	B	279	SER
2	C	1006	PHE
2	C	1007	GLU
2	D	1005	GLU
2	D	1006	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	HIS
1	B	127	HIS
1	B	265	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	FAK	D	1008	2	13,14,15	1.74	3 (23%)	13,18,20	1.37	2 (15%)
2	FAK	C	1008	2	13,14,15	1.59	2 (15%)	13,18,20	1.24	2 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAK	D	1008	2	-	3/15/16/18	-
2	FAK	C	1008	2	-	0/15/16/18	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1008	FAK	FI2-CT	4.51	1.51	1.32
2	D	1008	FAK	CB-CA	-3.49	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1008	FAK	FI1-CT	3.41	1.46	1.32
2	D	1008	FAK	FI3-CT	-2.35	1.22	1.32
2	C	1008	FAK	FI1-CT	2.29	1.41	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1008	FAK	CD-CG-CB	-2.80	103.08	113.62
2	D	1008	FAK	CD-CE-NZ	-2.33	105.66	112.20
2	C	1008	FAK	CD-CG-CB	-2.26	105.10	113.62
2	C	1008	FAK	CD-CE-NZ	-2.17	106.10	112.20

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1008	FAK	N-CA-CB-CG
2	D	1008	FAK	C-CA-CB-CG
2	D	1008	FAK	CE-CD-CG-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1008	FAK	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
3	SO4	B	1357	-	4,4,4	0.38	0	6,6,6	0.15	0
3	SO4	A	1357	-	4,4,4	0.39	0	6,6,6	0.45	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.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1357	SO4	3	0
3	A	1357	SO4	2	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	282/360 (78%)	0.31	21 (7%) 20 10	20, 39, 86, 109	0
1	B	266/360 (73%)	0.76	50 (18%) 3 2	24, 45, 108, 130	0
2	C	6/13 (46%)	0.10	0 100 100	22, 30, 36, 43	0
2	D	7/13 (53%)	1.39	2 (28%) 1 1	34, 35, 60, 69	0
All	All	561/746 (75%)	0.53	73 (13%) 7 4	20, 42, 99, 130	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	197	SER	6.2
1	B	202	HIS	5.5
1	B	196	VAL	5.4
1	B	216	GLU	4.9
1	B	113	PRO	4.9
1	B	137	GLU	4.9
1	B	207	SER	4.8
1	A	305	GLY	4.8
1	B	198	ALA	4.7
1	B	199	SER	4.6
1	B	209	MET	4.4
1	B	354	ALA	4.4
1	B	205	PRO	4.2
1	B	56	GLU	4.0
1	B	138	LEU	4.0
1	B	139	TYR	3.8
1	B	217	VAL	3.8
1	A	181	GLU	3.8
1	B	203	GLU	3.8
1	B	195	CYS	3.6
1	B	191	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	208	TRP	3.6
1	B	96	PHE	3.5
1	B	140	PRO	3.5
1	B	135	ALA	3.4
1	B	134	LEU	3.4
1	A	135	ALA	3.4
1	B	215	SER	3.3
1	A	223	ASP	3.1
1	B	305	GLY	3.0
1	B	353	ASP	2.9
1	A	198	ALA	2.9
1	A	138	LEU	2.9
1	B	212	LYS	2.9
1	A	142	GLN	2.8
1	B	136	LYS	2.8
1	B	206	LEU	2.8
1	B	99	PRO	2.8
1	A	224	CYS	2.7
1	A	110	TYR	2.7
1	B	142	GLN	2.7
1	A	180	GLN	2.6
2	D	1005	GLU	2.6
1	A	143	PHE	2.6
1	B	141	GLY	2.6
1	B	211	GLU	2.6
1	B	228	VAL	2.6
2	D	1004	GLY	2.6
1	A	225	GLN	2.5
1	B	356	SER	2.5
1	B	126	LYS	2.5
1	A	199	SER	2.4
1	A	139	TYR	2.4
1	B	194	HIS	2.4
1	B	180	GLN	2.4
1	A	109	LYS	2.4
1	A	352	ILE	2.3
1	A	107	LEU	2.3
1	B	114	TYR	2.3
1	B	238	SER	2.3
1	B	95	ASP	2.3
1	B	94	PRO	2.3
1	B	214	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	200	CYS	2.2
1	B	193	SER	2.2
1	B	192	THR	2.1
1	A	191	TYR	2.1
1	B	352	ILE	2.1
1	A	312	LYS	2.1
1	B	57	ARG	2.1
1	A	346	ARG	2.0
1	A	208	TRP	2.0
1	B	213	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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($\text{\AA}^2$)	Q<0.9
2	FAK	C	1008	15/16	0.92	0.10	27,29,47,49	0
2	FAK	D	1008	15/16	0.95	0.08	24,28,46,47	0

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($\text{\AA}^2$)	Q<0.9
3	SO4	A	1357	5/5	0.77	0.18	83,92,93,94	0
4	ZN	A	1358	1/1	0.92	0.09	100,100,100,100	0
4	ZN	B	1358	1/1	0.93	0.06	86,86,86,86	0
3	SO4	B	1357	5/5	0.95	0.10	48,51,54,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.