



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 04:54 PM EDT

PDB ID : 6F08  
Title : 14-3-3 zeta in complex with the human Son of sevenless homolog 1 (SOS1)  
Authors : Ballone, A.; Centorrino, F.; Ottmann, C.; Guo, S.; Leysen, S.  
Deposited on : 2017-11-17  
Resolution : 1.90 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.37.1  
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) : 2.37.1

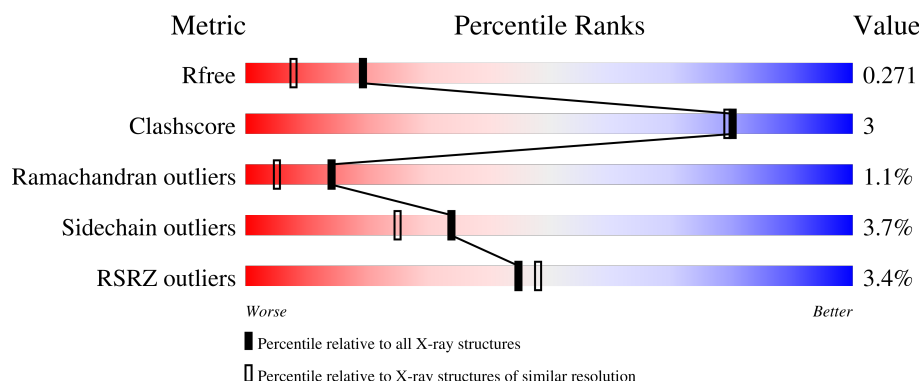
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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  $\geq 3$ , 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	230	<div> <div>88%</div> <div>9%</div> <div>.</div> </div>
1	B	230	<div> <div>6%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>
1	I	230	<div> <div>2%</div> <div>87%</div> <div>9%</div> <div>.</div> <div>.</div> </div>
1	J	230	<div> <div>4%</div> <div>84%</div> <div>7%</div> <div>.</div> <div>6%</div> </div>
2	D	13	<div> <div>8%</div> <div>54%</div> <div>15%</div> <div>31%</div> </div>

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Mol	Chain	Length	Quality of chain
2	K	13	<div><div>8%</div><div>62%</div><div>8%</div><div>8%</div><div>23%</div></div>
2	N	13	<div><div>62%</div><div>38%</div></div>
2	Q	13	<div><div>69%</div><div>8%</div><div>23%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7819 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.

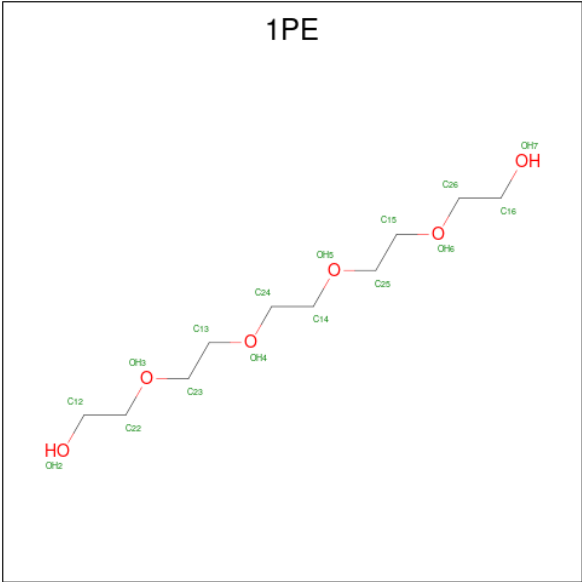
- Molecule 1 is a protein called 14-3-3 protein zeta/delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1745	1100	286	350	9			
1	B	225	Total	C	N	O	S	0	0	1
			1708	1075	286	338	9			
1	I	224	Total	C	N	O	S	0	0	1
			1722	1089	287	337	9			
1	J	217	Total	C	N	O	S	0	0	1
			1656	1042	280	325	9			

- Molecule 2 is a protein called Son of sevenless homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	9	Total	C	N	O	P	0	0	0
			74	41	15	17	1			
2	K	10	Total	C	N	O	P	0	0	0
			70	41	14	14	1			
2	N	8	Total	C	N	O	P	0	0	0
			61	35	11	14	1			
2	Q	10	Total	C	N	O	P	0	0	0
			74	41	13	19	1			

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C O	0	0
			16	10 6		

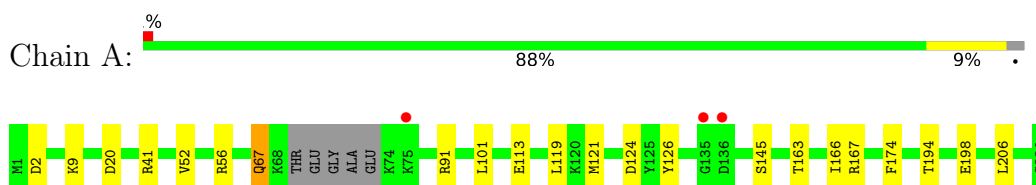
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	201	Total	O	0	0
			201	201		
4	B	124	Total	O	0	0
			124	124		
4	D	14	Total	O	0	0
			14	14		
4	I	158	Total	O	0	0
			158	158		
4	J	151	Total	O	0	0
			151	151		
4	K	19	Total	O	0	0
			19	19		
4	N	14	Total	O	0	0
			14	14		
4	Q	12	Total	O	0	0
			12	12		

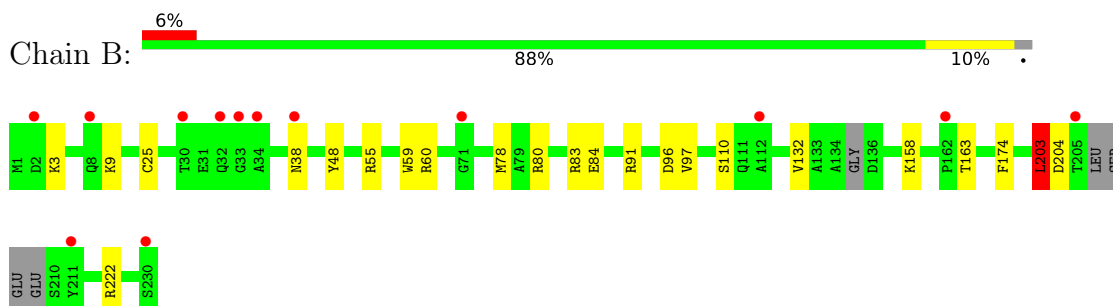
### 3 Residue-property plots

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

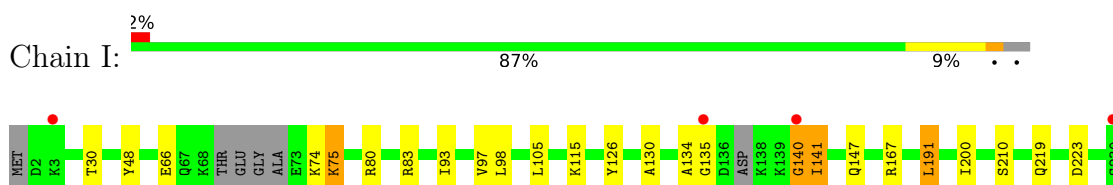
- Molecule 1: 14-3-3 protein zeta/delta



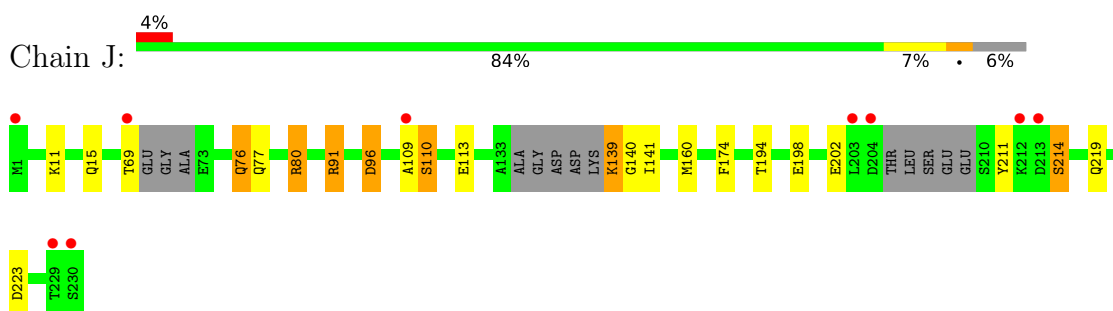
- Molecule 1: 14-3-3 protein zeta/delta



- Molecule 1: 14-3-3 protein zeta/delta



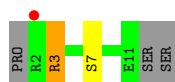
- Molecule 1: 14-3-3 protein zeta/delta



- Molecule 2: Son of sevenless homolog 1



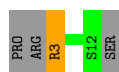
- Molecule 2: Son of sevenless homolog 1



- Molecule 2: Son of sevenless homolog 1



- Molecule 2: Son of sevenless homolog 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.06Å 93.14Å 74.52Å 90.00° 92.93° 90.00°	Depositor
Resolution (Å)	74.42 – 1.90 66.97 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (74.42-1.90) 99.9 (66.97-1.90)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.210 , 0.267 0.216 , 0.271	Depositor DCC
$R_{free}$ test set	3615 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.7	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7819	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.78% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, SEP

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	0.93	0/1764	0.97	7/2377 (0.3%)
1	B	0.85	0/1730	0.92	5/2338 (0.2%)
1	I	0.86	1/1745 (0.1%)	0.91	5/2354 (0.2%)
1	J	0.86	0/1677	0.93	3/2264 (0.1%)
2	D	0.99	0/64	0.86	0/84
2	K	0.87	0/60	0.89	0/79
2	N	0.71	0/51	1.02	0/67
2	Q	0.75	0/64	0.90	0/85
All	All	0.88	1/7155 (0.0%)	0.94	20/9648 (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	J	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	140	GLY	N-CA	7.00	1.56	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	91	ARG	NE-CZ-NH1	10.19	125.39	120.30
1	A	20	ASP	CB-CG-OD1	6.77	124.39	118.30
1	I	167	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	56	ARG	NE-CZ-NH2	-6.16	117.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	ASP	CB-CG-OD1	5.94	123.64	118.30
1	B	83	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	167	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	B	60	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	B	83	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	A	91	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	I	167	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	91	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	I	191	LEU	CA-CB-CG	5.37	127.64	115.30
1	J	96	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	A	41	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	B	55	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	I	191	LEU	CB-CG-CD1	5.06	119.60	111.00
1	I	80	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	B	203	LEU	CB-CG-CD1	5.01	119.52	111.00
1	J	80	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	139	LYS	Peptide

## 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	1745	0	1654	11	0
1	B	1708	0	1617	6	0
1	I	1722	0	1637	10	0
1	J	1656	0	1559	10	0
2	D	74	0	64	0	0
2	K	70	0	56	1	0
2	N	61	0	51	0	0
2	Q	74	0	58	1	0
3	A	16	0	22	3	0
4	A	201	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	124	0	0	0	1
4	D	14	0	0	0	0
4	I	158	0	0	0	0
4	J	151	0	0	1	1
4	K	19	0	0	0	0
4	N	14	0	0	0	0
4	Q	12	0	0	0	0
All	All	7819	0	6718	38	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 3.

All (38) 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:9:LYS:CD	1:B:25:CYS:SG	2.70	0.79
1:A:113:GLU:CB	1:A:113:GLU:C	2.57	0.73
1:B:163:THR:HG21	1:B:203:LEU:HD13	1.72	0.71
1:A:113:GLU:OE1	1:A:166:ILE:HD12	1.91	0.70
1:J:11:LYS:O	1:J:15:GLN:HG3	1.98	0.62
1:I:130:ALA:HB2	1:I:141:ILE:HD11	1.84	0.60
1:I:48:TYR:CD1	1:I:97:VAL:HG22	2.37	0.59
1:J:139:LYS:O	1:J:141:ILE:N	2.34	0.59
1:A:113:GLU:CB	1:A:113:GLU:N	2.66	0.58
1:A:119:LEU:CD2	1:A:119:LEU:CB	2.81	0.57
1:I:66:GLU:OE1	1:I:83:ARG:NE	2.31	0.56
1:J:113:GLU:HA	1:J:160:MET:CE	2.39	0.53
1:I:219:GLN:NE2	1:I:223:ASP:OD1	2.38	0.52
1:J:219:GLN:O	1:J:223:ASP:N	2.39	0.50
1:B:59:TRP:CE2	1:B:132:VAL:HG12	2.48	0.49
1:I:130:ALA:N	1:I:141:ILE:HD11	2.28	0.48
1:A:119:LEU:CB	1:A:119:LEU:CD1	2.91	0.48
1:I:126:TYR:O	1:I:141:ILE:CD1	2.61	0.48
3:A:301:1PE:H131	1:B:78:MET:HG3	1.95	0.48
1:J:194:THR:O	1:J:198:GLU:HG3	2.15	0.46
2:K:3:ARG:HG2	2:Q:3:ARG:HG3	1.96	0.46
1:J:202:GLU:CG	1:J:202:GLU:O	2.64	0.45
1:A:9:LYS:HE2	3:A:301:1PE:OH7	2.17	0.45
1:I:93:ILE:O	1:I:97:VAL:HG23	2.17	0.45
1:A:194:THR:O	1:A:198:GLU:HG3	2.16	0.44
1:I:30:THR:HG23	1:I:105:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:TYR:CD1	1:B:97:VAL:CG2	3.00	0.44
1:A:9:LYS:HE2	3:A:301:1PE:OH6	2.18	0.44
1:A:126:TYR:HB3	1:A:145:SER:HB2	2.00	0.44
1:B:80:ARG:NH1	1:B:84:GLU:OE2	2.52	0.43
1:I:74:LYS:O	1:I:75:LYS:CB	2.67	0.42
1:J:76:GLN:HE22	1:J:80:ARG:NH1	2.17	0.42
1:I:98:LEU:HD22	1:I:126:TYR:CE2	2.55	0.42
1:J:109:ALA:O	1:J:110:SER:CB	2.69	0.41
1:J:211:TYR:HA	1:J:214:SER:HB2	2.02	0.41
1:A:101:LEU:HD11	1:A:121:MET:HG2	2.03	0.41
1:A:163:THR:HB	1:A:206:LEU:HD13	2.03	0.40
1:J:91:ARG:NH2	4:J:310:HOH:O	2.54	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)
4:B:418:HOH:O	4:J:428:HOH:O[1_456]	1.91	0.29

## 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	218/230 (95%)	211 (97%)	6 (3%)	1 (0%)	29	18
1	B	219/230 (95%)	212 (97%)	5 (2%)	2 (1%)	17	7
1	I	218/230 (95%)	212 (97%)	2 (1%)	4 (2%)	8	2
1	J	209/230 (91%)	199 (95%)	7 (3%)	3 (1%)	11	3
2	D	6/13 (46%)	5 (83%)	1 (17%)	0	100	100
2	K	7/13 (54%)	7 (100%)	0	0	100	100
2	N	5/13 (38%)	5 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Q	7/13 (54%)	7 (100%)	0	0	100	100
All	All	889/972 (92%)	858 (96%)	21 (2%)	10 (1%)	14	5

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3	LYS
1	I	75	LYS
1	I	140	GLY
1	J	77	GLN
1	J	140	GLY
1	A	67	GLN
1	I	134	ALA
1	B	110	SER
1	J	110	SER
1	I	135	GLY

### 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	175/200 (88%)	171 (98%)	4 (2%)	50	45
1	B	171/200 (86%)	163 (95%)	8 (5%)	26	16
1	I	171/200 (86%)	165 (96%)	6 (4%)	36	27
1	J	163/200 (82%)	158 (97%)	5 (3%)	40	32
2	D	6/10 (60%)	5 (83%)	1 (17%)	2	0
2	K	4/10 (40%)	3 (75%)	1 (25%)	0	0
2	N	4/10 (40%)	4 (100%)	0	100	100
2	Q	6/10 (60%)	5 (83%)	1 (17%)	2	0
All	All	700/840 (83%)	674 (96%)	26 (4%)	34	25

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	52	VAL
1	A	67	GLN
1	A	174	PHE
1	B	38	ASN
1	B	91	ARG
1	B	96	ASP
1	B	158	LYS
1	B	174	PHE
1	B	203	LEU
1	B	204	ASP
1	B	222	ARG
2	D	11	GLU
1	I	115	LYS
1	I	141	ILE
1	I	147	GLN
1	I	191	LEU
1	I	200	ILE
1	I	210	SER
1	J	69	THR
1	J	76	GLN
1	J	96	ASP
1	J	174	PHE
1	J	214	SER
2	K	3	ARG
2	Q	3	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	15	GLN
1	A	38	ASN
1	B	8	GLN
1	J	50	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	SEP	N	7	2	8,9,10	0.58	0	8,12,14	1.10	0
2	SEP	D	7	2	8,9,10	0.93	0	8,12,14	1.19	1 (12%)
2	SEP	K	7	2	8,9,10	0.65	0	8,12,14	2.80	3 (37%)
2	SEP	Q	7	2	8,9,10	1.03	0	8,12,14	0.84	0

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	SEP	N	7	2	-	0/5/8/10	-
2	SEP	D	7	2	-	0/5/8/10	-
2	SEP	K	7	2	-	0/5/8/10	-
2	SEP	Q	7	2	-	0/5/8/10	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	7	SEP	OG-CB-CA	6.35	114.32	108.14
2	K	7	SEP	O3P-P-OG	-2.98	98.80	106.73
2	K	7	SEP	O3P-P-O2P	2.82	118.43	107.64
2	D	7	SEP	OG-CB-CA	2.81	110.88	108.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

1 ligand is 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	$\# Z  > 2$
3	1PE	A	301	-	15,15,15	0.77	0	14,14,14	0.53	0

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
3	1PE	A	301	-	-	4/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	1PE	OH6-C15-C25-OH5
3	A	301	1PE	OH4-C13-C23-OH3
3	A	301	1PE	OH5-C14-C24-OH4
3	A	301	1PE	C24-C14-OH5-C25

There are no ring outliers.

1 monomer is involved in 3 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	1PE	3	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	225/230 (97%)	-0.03	3 (1%) 77 79	12, 21, 42, 63	0
1	B	225/230 (97%)	0.31	13 (5%) 23 25	14, 28, 56, 83	0
1	I	224/230 (97%)	0.03	4 (1%) 68 71	15, 27, 46, 71	0
1	J	217/230 (94%)	0.19	9 (4%) 37 40	16, 28, 56, 83	0
2	D	8/13 (61%)	0.74	1 (12%) 3 4	18, 24, 55, 81	0
2	K	9/13 (69%)	0.62	1 (11%) 5 6	19, 30, 62, 81	0
2	N	7/13 (53%)	0.33	0 100 100	23, 26, 37, 42	0
2	Q	9/13 (69%)	0.09	0 100 100	17, 27, 51, 53	0
All	All	924/972 (95%)	0.14	31 (3%) 45 48	12, 26, 53, 83	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	1	MET	6.7
2	K	2	ARG	4.5
1	B	205	THR	4.4
1	J	229	THR	3.3
1	J	204	ASP	3.2
1	J	69	THR	3.0
1	J	109	ALA	3.0
1	B	32	GLN	2.9
1	B	34	ALA	2.9
1	I	3	LYS	2.8
1	I	135	GLY	2.7
1	B	33	GLY	2.6
1	B	2	ASP	2.6
1	A	75	LYS	2.6
2	D	11	GLU	2.6
1	B	112	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	135	GLY	2.5
1	I	230	SER	2.4
1	J	230	SER	2.4
1	A	136	ASP	2.4
1	B	38	ASN	2.3
1	J	213	ASP	2.3
1	I	140	GLY	2.3
1	B	230	SER	2.3
1	J	212	LYS	2.3
1	B	71	GLY	2.2
1	J	203	LEU	2.2
1	B	162	PRO	2.1
1	B	30	THR	2.1
1	B	8	GLN	2.0
1	B	211	TYR	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	SEP	D	7	10/11	0.97	0.10	13,16,18,18	0
2	SEP	K	7	10/11	0.97	0.10	18,20,22,23	0
2	SEP	N	7	10/11	0.97	0.08	18,20,23,23	0
2	SEP	Q	7	10/11	0.99	0.08	15,17,18,18	0

## 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, 95<sup>th</sup> 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	1PE	A	301	16/16	0.84	0.18	41,47,60,61	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.