W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Nov 16, 2017 – 10:21 AM EST

PDB ID	:	5LDE
Title	:	Crystal structure of a vFLIP-IKKgamma stapled peptide dimer
Authors	:	Barrett, T.
Deposited on	:	unknown
Resolution	:	3.38 Å(reported)

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

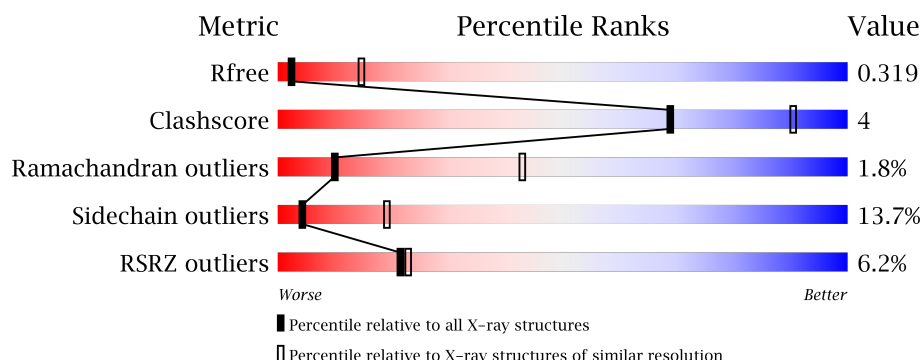|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

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 3.38 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}	100719	1241 (3.46-3.30)
Clashscore	112137	1319 (3.46-3.30)
Ramachandran outliers	110173	1298 (3.46-3.30)
Sidechain outliers	110143	1297 (3.46-3.30)
RSRZ outliers	101464	1251 (3.46-3.30)

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. 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 <=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	265	
1	B	265	
2	R	20	
2	S	20	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	6ZS	S	236	X	-	-	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3463 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 Immunoglobulin G-binding protein G,Viral FLICE protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total 1585	C 1011	N 265	O 302	S 7	0	0	0
1	B	225	Total 1575	C 998	N 271	O 299	S 7	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P19909
A	2	GLN	-	expression tag	UNP P19909
A	56	GLU	-	linker	UNP P19909
A	57	LEU	-	linker	UNP P19909
A	58	GLU	-	linker	UNP P19909
A	59	VAL	-	linker	UNP P19909
A	60	LEU	-	linker	UNP P19909
A	61	PHE	-	linker	UNP P19909
A	62	GLN	-	linker	UNP P19909
A	63	GLY	-	linker	UNP P19909
A	64	PRO	-	linker	UNP P19909
A	65	LEU	-	linker	UNP P19909
A	66	ASP	-	linker	UNP P19909
A	67	PRO	-	linker	UNP P19909
A	68	ASN	-	linker	UNP P19909
A	69	SER	-	linker	UNP P19909
A	289	LEU	-	expression tag	UNP F5HEZ4
A	290	GLU	-	expression tag	UNP F5HEZ4
A	291	HIS	-	expression tag	UNP F5HEZ4
A	292	HIS	-	expression tag	UNP F5HEZ4
A	293	HIS	-	expression tag	UNP F5HEZ4
A	294	HIS	-	expression tag	UNP F5HEZ4
A	295	HIS	-	expression tag	UNP F5HEZ4
A	296	HIS	-	expression tag	UNP F5HEZ4
B	1	MET	-	initiating methionine	UNP P19909

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2	GLN	-	expression tag	UNP P19909
B	56	GLU	-	linker	UNP P19909
B	57	LEU	-	linker	UNP P19909
B	58	GLU	-	linker	UNP P19909
B	59	VAL	-	linker	UNP P19909
B	60	LEU	-	linker	UNP P19909
B	61	PHE	-	linker	UNP P19909
B	62	GLN	-	linker	UNP P19909
B	63	GLY	-	linker	UNP P19909
B	64	PRO	-	linker	UNP P19909
B	65	LEU	-	linker	UNP P19909
B	66	ASP	-	linker	UNP P19909
B	67	PRO	-	linker	UNP P19909
B	68	ASN	-	linker	UNP P19909
B	69	SER	-	linker	UNP P19909
B	289	LEU	-	expression tag	UNP F5HEZ4
B	290	GLU	-	expression tag	UNP F5HEZ4
B	291	HIS	-	expression tag	UNP F5HEZ4
B	292	HIS	-	expression tag	UNP F5HEZ4
B	293	HIS	-	expression tag	UNP F5HEZ4
B	294	HIS	-	expression tag	UNP F5HEZ4
B	295	HIS	-	expression tag	UNP F5HEZ4
B	296	HIS	-	expression tag	UNP F5HEZ4

- Molecule 2 is a protein called Inhibitor of kappa light polypeptide gene enhancer in B-cells, kinase gamma, isoform CRA_a.

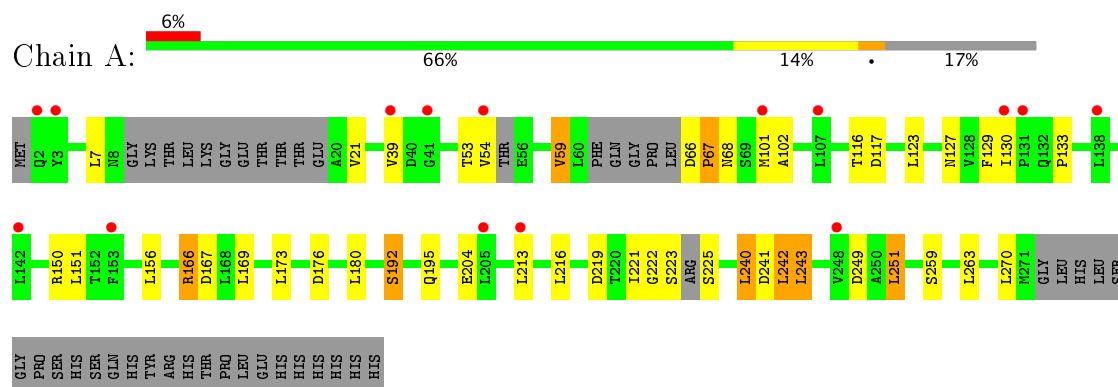| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	20	Total	C	N	O	S	0	0	0
			152	101	25	25	1			
2	S	20	Total	C	N	O	S	0	0	0
			151	100	25	25	1			

There are 6 discrepancies between the modelled and reference sequences:

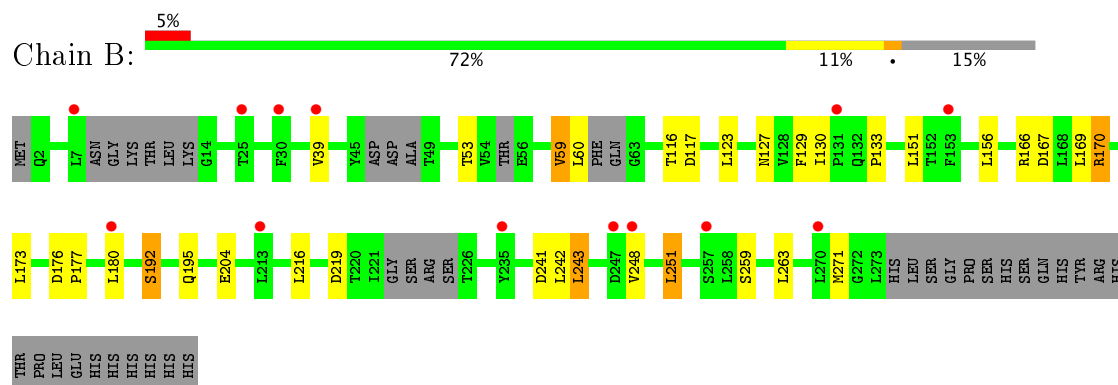| Chain	Residue	Modelled	Actual	Comment	Reference
R	236	6ZS	GLN	engineered mutation	UNP D3DWY2
R	240	6ZS	GLU	engineered mutation	UNP D3DWY2
R	249	CYS	VAL	engineered mutation	UNP D3DWY2
S	236	6ZS	GLN	engineered mutation	UNP D3DWY2
S	240	6ZS	GLU	engineered mutation	UNP D3DWY2
S	249	CYS	VAL	engineered mutation	UNP D3DWY2

3 Residue-property plots ⓘ

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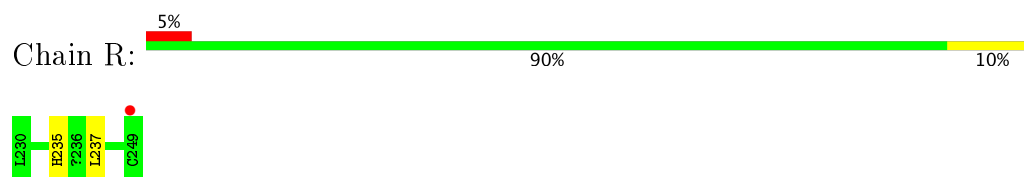
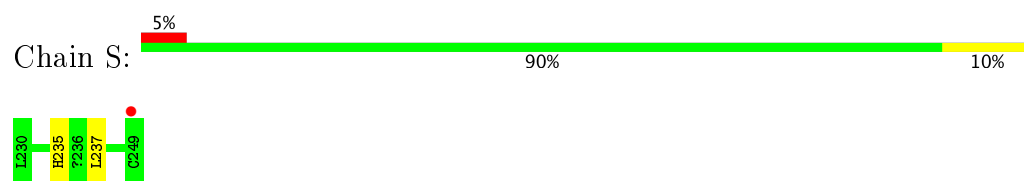• Molecule 1: Immunoglobulin G-binding protein G,Viral FLICE protein

• Molecule 1: Immunoglobulin G-binding protein G,Viral FLICE protein

• Molecule 2: Inhibitor of kappa light polypeptide gene enhancer in B-cells, kinase gamma, isoform CRA_a

• Molecule 2: Inhibitor of kappa light polypeptide gene enhancer in B-cells, kinase gamma, isoform CRA_a

Chain S:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	90.51Å 90.51Å 134.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 3.38 24.73 – 3.38	Depositor EDS
% Data completeness (in resolution range)	95.7 (25.00-3.38) 95.6 (24.73-3.38)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.32 (at 3.38Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.255 , 0.290 0.259 , 0.319	Depositor DCC
R_{free} test set	404 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	118.3	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 122.5	EDS
L-test for twinning[2]	$<|L|> = 0.48, <L^2> = 0.31$	Xtriage
Estimated twinning fraction	0.448 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3463	wwPDB-VP
Average B, all atoms (Å^2)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

Full wwPDB X-ray Structure Validation Report

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 6ZS

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	0.41	0/1608	0.62	0/2201
1	B	0.41	0/1594	0.62	0/2180
2	R	0.39	0/140	0.50	0/188
2	S	0.39	0/140	0.50	0/188
All	All	0.41	0/3482	0.61	0/4757

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
2	S	1	0

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	S	236	6ZS	CA

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1585	0	1466	16	0
1	B	1575	0	1423	12	0
2	R	152	0	112	1	0
2	S	151	0	112	2	0
All	All	3463	0	3113	28	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 (28) 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:59:VAL:HG12	1:B:60:LEU:H	1.23	1.02
1:B:59:VAL:CG1	1:B:60:LEU:H	2.01	0.71
1:B:59:VAL:HG12	1:B:60:LEU:N	2.01	0.69
1:A:7:LEU:HA	1:A:54:VAL:HG12	1.83	0.61
1:A:169:LEU:HD23	1:A:173:LEU:HD12	1.94	0.49
1:A:123:LEU:HB3	1:A:129:PHE:HA	1.95	0.49
1:B:123:LEU:HB3	1:B:129:PHE:HA	1.95	0.49
1:B:169:LEU:HD23	1:B:173:LEU:HD12	1.94	0.48
1:A:204:GLU:HB3	1:A:263:LEU:HD21	1.97	0.47
1:A:66:ASP:CB	1:A:67:PRO:HD3	2.44	0.47
1:B:204:GLU:HB3	1:B:263:LEU:HD21	1.97	0.46
1:A:223:SER:HA	1:A:225:SER:HA	1.98	0.46
1:A:240:LEU:HB3	1:A:242:LEU:HD12	1.98	0.46
1:B:170:ARG:HG2	1:B:177:PRO:HD3	1.99	0.45
1:A:68:ASN:HA	1:A:102:ALA:HB3	1.99	0.44
1:B:123:LEU:HD12	1:B:133:PRO:HG3	1.99	0.44
1:A:123:LEU:HD12	1:A:133:PRO:HG3	1.99	0.44
1:A:68:ASN:C	1:A:101:MET:H	2.21	0.43
1:A:221:ILE:HA	1:A:222:GLY:HA3	1.81	0.42
1:A:166:ARG:HA	1:A:169:LEU:HD12	2.01	0.42
1:A:176:ASP:H	2:S:235:HIS:CE1	2.37	0.42
1:A:176:ASP:H	2:S:235:HIS:HE1	1.68	0.42
1:B:166:ARG:HA	1:B:169:LEU:HD12	2.02	0.41
1:A:192:SER:H	1:A:195:GLN:HE21	1.69	0.41
1:A:243:LEU:HD21	1:A:251:LEU:HD12	2.02	0.41
1:B:192:SER:H	1:B:195:GLN:HE21	1.69	0.41
1:B:243:LEU:HD21	1:B:251:LEU:HD12	2.02	0.41
1:B:176:ASP:H	2:R:235:HIS:HE1	1.70	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	211/265 (80%)	199 (94%)	8 (4%)	4 (2%)	9	42
1	B	213/265 (80%)	204 (96%)	5 (2%)	4 (2%)	9	42
2	R	16/20 (80%)	15 (94%)	1 (6%)	0	100	100
2	S	16/20 (80%)	16 (100%)	0	0	100	100
All	All	456/570 (80%)	434 (95%)	14 (3%)	8 (2%)	10	43

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	PRO
1	A	116	THR
1	B	116	THR
1	A	127	ASN
1	B	127	ASN
1	B	248	VAL
1	A	59	VAL
1	B	59	VAL

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	153/234 (65%)	129 (84%)	24 (16%)	3	14
1	B	144/234 (62%)	126 (88%)	18 (12%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	R	12/17 (71%)	11 (92%)	1 (8%)	13	44
2	S	12/17 (71%)	11 (92%)	1 (8%)	13	44
All	All	321/502 (64%)	277 (86%)	44 (14%)	4	19

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	39	VAL
1	A	53	THR
1	A	59	VAL
1	A	117	ASP
1	A	130	ILE
1	A	150	ARG
1	A	151	LEU
1	A	156	LEU
1	A	166	ARG
1	A	167	ASP
1	A	180	LEU
1	A	192	SER
1	A	213	LEU
1	A	216	LEU
1	A	219	ASP
1	A	240	LEU
1	A	241	ASP
1	A	242	LEU
1	A	243	LEU
1	A	249	ASP
1	A	251	LEU
1	A	259	SER
1	A	270	LEU
1	B	39	VAL
1	B	53	THR
1	B	117	ASP
1	B	130	ILE
1	B	151	LEU
1	B	156	LEU
1	B	167	ASP
1	B	170	ARG
1	B	180	LEU
1	B	192	SER

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Mol	Chain	Res	Type
1	B	216	LEU
1	B	219	ASP
1	B	241	ASP
1	B	242	LEU
1	B	243	LEU
1	B	251	LEU
1	B	259	SER
1	B	271	MET
2	R	237	LEU
2	S	237	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	GLN
1	B	132	GLN
1	B	195	GLN
1	B	232	HIS
2	R	235	HIS
2	S	235	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)

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	6ZS	R	236	2	3,6,7	0.69	0	3,8,10	1.47	0
2	6ZS	R	240	2	3,6,7	0.70	0	3,8,10	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	6ZS	S	236	2	2,5,7	0.80	0	0,7,10	0.00	-
2	6ZS	S	240	2	3,6,7	0.72	0	3,8,10	0.92	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	6ZS	R	236	2	-	0/3/6/9	0/0/0/0
2	6ZS	R	240	2	-	0/3/6/9	0/0/0/0
2	6ZS	S	236	2	1/1/1/2	0/2/3/9	0/0/0/0
2	6ZS	S	240	2	-	0/3/6/9	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	S	236	6ZS	CA

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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(Å²)	Q<0.9
1	A	221/265 (83%)	0.37	15 (6%)	18	20	75, 131, 245, 290	0
1	B	225/265 (84%)	0.23	13 (5%)	24	25	71, 128, 189, 260	0
2	R	18/20 (90%)	0.54	1 (5%)	25	26	111, 126, 136, 153	0
2	S	18/20 (90%)	0.33	1 (5%)	25	26	109, 126, 132, 141	0
All	All	482/570 (84%)	0.31	30 (6%)	21	23	71, 128, 205, 290	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	153	PHE	4.0
1	A	54	VAL	3.8
1	B	39	VAL	3.6
1	B	257	SER	3.6
1	B	153	PHE	3.5
1	A	205	LEU	3.3
1	B	7	LEU	3.3
1	A	101	MET	3.2
1	A	41	GLY	3.2
1	A	2	GLN	3.2
1	B	213	LEU	3.0
2	R	249	CYS	3.0
1	A	107	LEU	3.0
1	B	180	LEU	2.8
1	B	30	PHE	2.6
1	A	131	PRO	2.6
1	B	270	LEU	2.4
1	A	39	VAL	2.4
1	A	248	VAL	2.3
1	A	130	ILE	2.3
2	S	249	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	142	LEU	2.3
1	B	25	THR	2.2
1	A	213	LEU	2.2
1	B	248	VAL	2.1
1	B	247	ASP	2.1
1	A	3	TYR	2.1
1	B	235	TYR	2.1
1	B	131	PRO	2.0
1	A	138	LEU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors($Å^2$)	Q<0.9
2	6ZS	R	240	7/8	0.97	0.22	-	109,110,114,114	0
2	6ZS	R	236	7/8	0.95	0.18	-	112,113,113,114	0
2	6ZS	S	236	6/8	0.95	0.17	-	111,111,112,112	0
2	6ZS	S	240	7/8	0.96	0.15	-	108,109,113,113	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.