



wwPDB X-ray Structure Validation Summary Report

Feb 14, 2017 – 07:07 am GMT

PDB ID : 1PP8
Title : crystal structure of the *T. vaginalis* IBP39 Initiator binding domain (IBD) bound to the alpha-SCS Inr element
Authors : Schumacher, M.A.; Lau, A.O.T.; Johnson, P.J.
Deposited on : 2003-06-16
Resolution : 3.05 Å (reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the  symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
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) : recalc28949

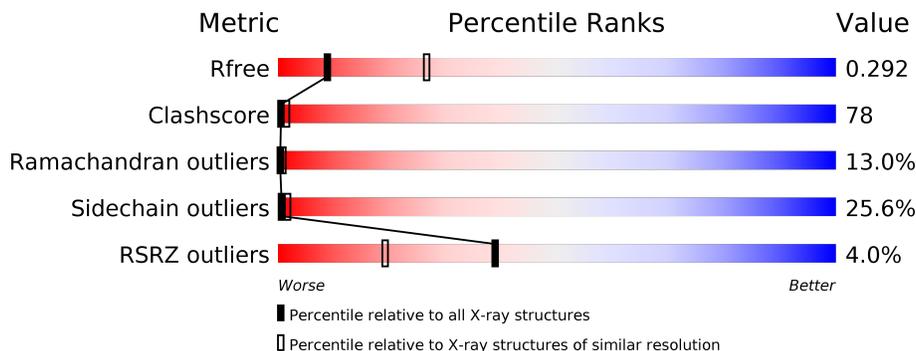
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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.



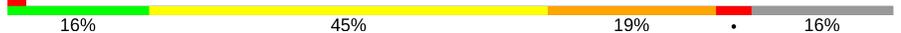
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1348 (3.10-3.02)
Clashscore	112137	1462 (3.10-3.02)
Ramachandran outliers	110173	1410 (3.10-3.02)
Sidechain outliers	110143	1410 (3.10-3.02)
RSRZ outliers	101464	1355 (3.10-3.02)

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 $\leq 5\%$. 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	E	12	
1	I	12	
1	K	12	
1	Y	12	
2	G	12	
2	J	12	

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Mol	Chain	Length	Quality of chain
2	R	12	
2	T	12	
3	F	132	
3	M	132	
3	O	132	
3	P	132	
3	U	132	
3	V	132	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7268 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 DNA chain called ALPHA-SCS INR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	E	12	Total 238	C 116	N 40	O 71	P 11	0	0	0
1	I	12	Total 238	C 116	N 40	O 71	P 11	0	0	0
1	Y	12	Total 238	C 116	N 40	O 71	P 11	0	0	0
1	K	12	Total 238	C 116	N 40	O 71	P 11	0	0	0

- Molecule 2 is a DNA chain called ALPHA-SCS INR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	T	12	Total 248	C 119	N 49	O 69	P 11	0	0	0
2	R	12	Total 248	C 119	N 49	O 69	P 11	0	0	0
2	J	12	Total 248	C 119	N 49	O 69	P 11	0	0	0
2	G	12	Total 248	C 119	N 49	O 69	P 11	0	0	0

- Molecule 3 is a protein called 39 kDa initiator binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	U	111	Total 901	C 570	N 163	O 165	S 3	0	0	0
3	P	118	Total 958	C 605	N 171	O 178	S 4	0	0	0
3	F	113	Total 915	C 577	N 166	O 169	S 3	0	0	0
3	V	98	Total 794	C 511	N 141	O 139	S 3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	118	958	605	171	178	4	0	0	0
3	O	97	788	508	140	137	3	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

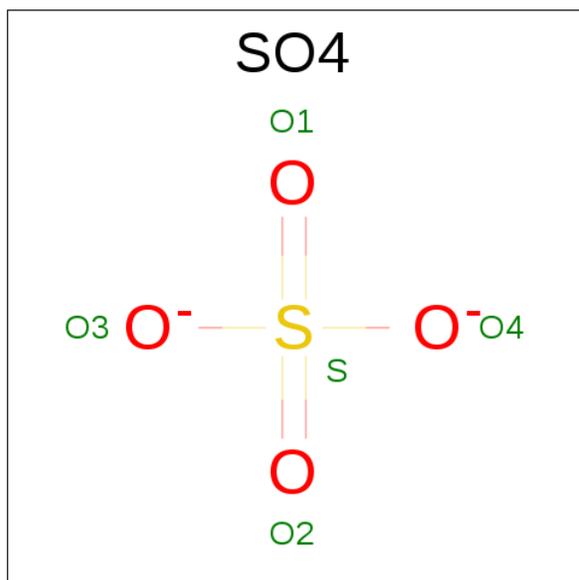
Chain	Residue	Modelled	Actual	Comment	Reference
U	127	HIS	-	EXPRESSION TAG	UNP Q95VR4
U	128	HIS	-	EXPRESSION TAG	UNP Q95VR4
U	129	HIS	-	EXPRESSION TAG	UNP Q95VR4
U	130	HIS	-	EXPRESSION TAG	UNP Q95VR4
U	131	HIS	-	EXPRESSION TAG	UNP Q95VR4
U	132	HIS	-	EXPRESSION TAG	UNP Q95VR4
P	127	HIS	-	EXPRESSION TAG	UNP Q95VR4
P	128	HIS	-	EXPRESSION TAG	UNP Q95VR4
P	129	HIS	-	EXPRESSION TAG	UNP Q95VR4
P	130	HIS	-	EXPRESSION TAG	UNP Q95VR4
P	131	HIS	-	EXPRESSION TAG	UNP Q95VR4
P	132	HIS	-	EXPRESSION TAG	UNP Q95VR4
F	127	HIS	-	EXPRESSION TAG	UNP Q95VR4
F	128	HIS	-	EXPRESSION TAG	UNP Q95VR4
F	129	HIS	-	EXPRESSION TAG	UNP Q95VR4
F	130	HIS	-	EXPRESSION TAG	UNP Q95VR4
F	131	HIS	-	EXPRESSION TAG	UNP Q95VR4
F	132	HIS	-	EXPRESSION TAG	UNP Q95VR4
V	127	HIS	-	EXPRESSION TAG	UNP Q95VR4
V	128	HIS	-	EXPRESSION TAG	UNP Q95VR4
V	129	HIS	-	EXPRESSION TAG	UNP Q95VR4
V	130	HIS	-	EXPRESSION TAG	UNP Q95VR4
V	131	HIS	-	EXPRESSION TAG	UNP Q95VR4
V	132	HIS	-	EXPRESSION TAG	UNP Q95VR4
M	127	HIS	-	EXPRESSION TAG	UNP Q95VR4
M	128	HIS	-	EXPRESSION TAG	UNP Q95VR4
M	129	HIS	-	EXPRESSION TAG	UNP Q95VR4
M	130	HIS	-	EXPRESSION TAG	UNP Q95VR4
M	131	HIS	-	EXPRESSION TAG	UNP Q95VR4
M	132	HIS	-	EXPRESSION TAG	UNP Q95VR4
O	127	HIS	-	EXPRESSION TAG	UNP Q95VR4
O	128	HIS	-	EXPRESSION TAG	UNP Q95VR4
O	129	HIS	-	EXPRESSION TAG	UNP Q95VR4
O	130	HIS	-	EXPRESSION TAG	UNP Q95VR4

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Chain	Residue	Modelled	Actual	Comment	Reference
O	131	HIS	-	EXPRESSION TAG	UNP Q95VR4
O	132	HIS	-	EXPRESSION TAG	UNP Q95VR4

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

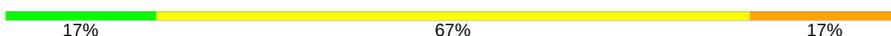


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	V	1	Total	O	S	0	0
			5	4	1		
4	O	1	Total	O	S	0	0
			5	4	1		

3 Residue-property plots [i](#)

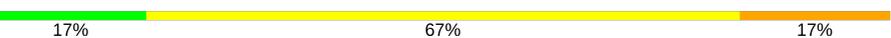
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: ALPHA-SCS INR

Chain E: 



- Molecule 1: ALPHA-SCS INR

Chain I: 



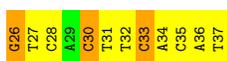
- Molecule 1: ALPHA-SCS INR

Chain Y: 



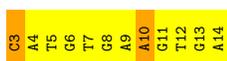
- Molecule 1: ALPHA-SCS INR

Chain K: 



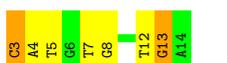
- Molecule 2: ALPHA-SCS INR

Chain T: 

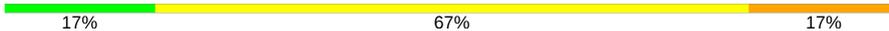


- Molecule 2: ALPHA-SCS INR

Chain R: 

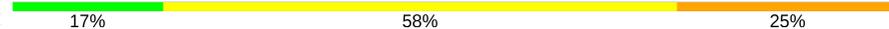


- Molecule 2: ALPHA-SCS INR

Chain J: 



- Molecule 2: ALPHA-SCS INR

Chain G: 



- Molecule 3: 39 kDa initiator binding protein

Chain U: 



- Molecule 3: 39 kDa initiator binding protein

Chain P: 



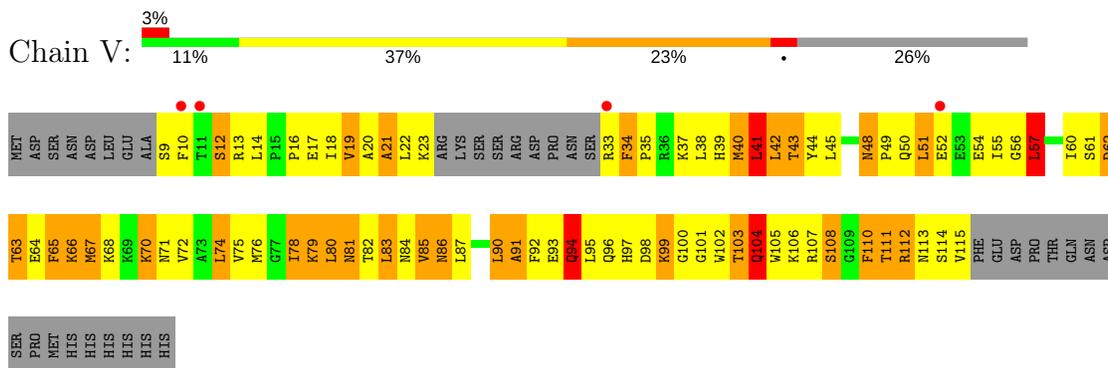
- Molecule 3: 39 kDa initiator binding protein

Chain F: 

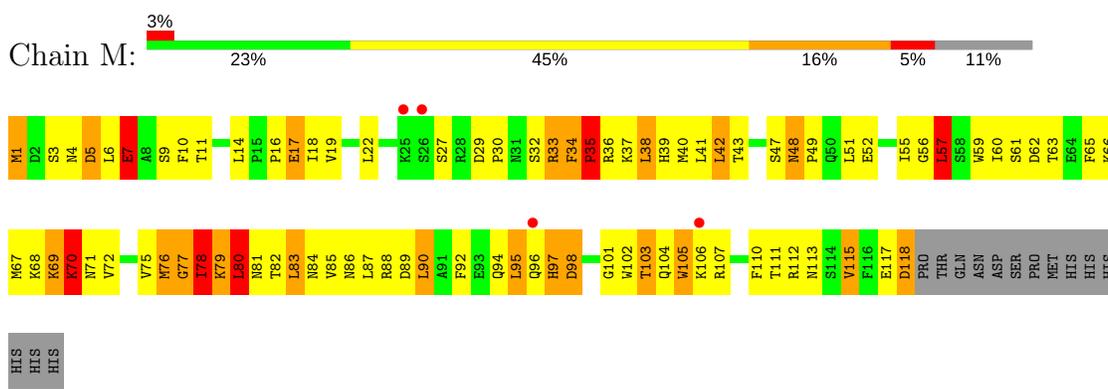


MET
HIS
HIS
HIS
HIS
HIS
HIS

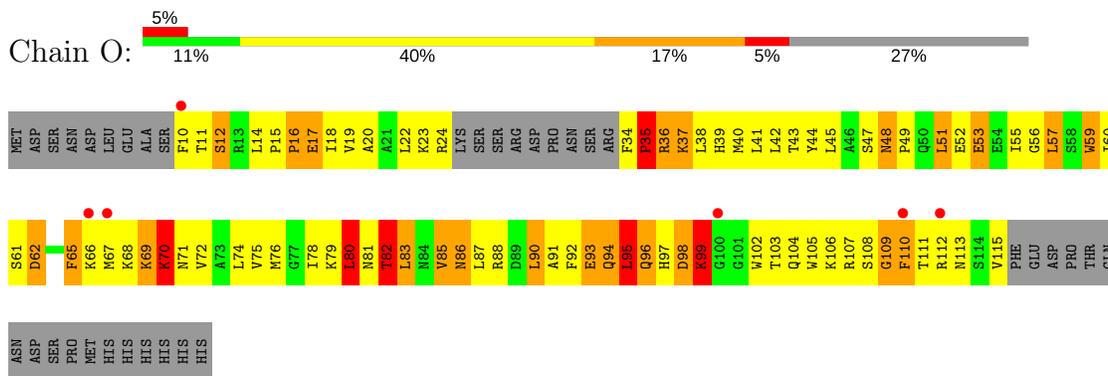
• Molecule 3: 39 kDa initiator binding protein



• Molecule 3: 39 kDa initiator binding protein



• Molecule 3: 39 kDa initiator binding protein



4 Data and refinement statistics i

Property	Value	Source
Space group	F 2 3	Depositor
Cell constants a, b, c, α , β , γ	292.00Å 292.00Å 292.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	146.00 – 3.05 146.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.2 (146.00-3.05) 91.9 (146.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 3.01Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.269 , 0.311 0.261 , 0.292	Depositor DCC
R_{free} test set	1836 reflections (4.97%)	DCC
Wilson B-factor (Å ²)	104.0	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 107.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.032 for k,h,-l	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7268	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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: SO4

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	E	1.07	0/265	1.33	1/406 (0.2%)
1	I	1.03	1/265 (0.4%)	1.50	5/406 (1.2%)
1	K	1.06	0/265	1.12	1/406 (0.2%)
1	Y	1.06	1/265 (0.4%)	1.16	0/406
2	G	1.30	1/279 (0.4%)	1.36	1/430 (0.2%)
2	J	1.27	1/279 (0.4%)	1.14	0/430
2	R	1.07	1/279 (0.4%)	1.15	0/430
2	T	1.18	1/279 (0.4%)	1.21	0/430
3	F	0.66	0/933	0.94	2/1256 (0.2%)
3	M	0.79	0/977	1.02	1/1315 (0.1%)
3	O	0.58	0/804	0.89	0/1081
3	P	0.90	0/977	1.07	2/1315 (0.2%)
3	U	0.88	2/919 (0.2%)	1.04	3/1237 (0.2%)
3	V	0.79	0/810	1.01	1/1089 (0.1%)
All	All	0.90	8/7596 (0.1%)	1.09	17/10637 (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	E	0	1
1	K	0	2
2	G	0	1
2	J	0	1
2	R	0	1
2	T	0	3
All	All	0	9

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	105	TRP	CB-CG	-6.32	1.38	1.50
1	Y	29	DA	C5-C6	-6.29	1.35	1.41
2	G	3	DC	C4-C5	6.09	1.47	1.43
2	R	3	DC	N1-C2	5.89	1.46	1.40
2	J	11	DG	C2-N3	5.77	1.37	1.32

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	35	DC	O4'-C1'-N1	10.44	115.31	108.00
1	I	35	DC	C1'-O4'-C4'	-9.46	100.64	110.10
1	I	35	DC	N1-C1'-C2'	8.73	129.19	112.60
3	P	14	LEU	CA-CB-CG	8.55	134.97	115.30
1	I	35	DC	C3'-C2'-C1'	-7.95	92.96	102.50

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	26	DG	Sidechain
1	K	26	DG	Sidechain
1	K	33	DC	Sidechain
2	T	3	DC	Sidechain
2	T	5	DT	Sidechain

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	E	238	0	138	24	0
1	I	238	0	138	11	0
1	K	238	0	138	32	0
1	Y	238	0	138	14	0
2	G	248	0	137	25	0
2	J	248	0	137	27	0
2	R	248	0	137	12	0
2	T	248	0	137	21	0
3	F	915	0	926	143	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	M	958	0	966	141	1
3	O	788	0	812	147	0
3	P	958	0	966	179	0
3	U	901	0	915	173	0
3	V	794	0	817	169	0
4	O	5	0	0	0	0
4	V	5	0	0	0	0
All	All	7268	0	6502	1062	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 78.

The worst 5 of 1062 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:I:35:DC:N4	2:T:6:DG:H1	1.42	1.16
3:V:79:LYS:HG3	3:V:82:THR:HG21	1.25	1.15
1:E:30:DC:H2''	1:E:31:DT:H5''	1.26	1.15
1:K:36:DA:H2''	1:K:37:DT:H5''	1.28	1.13
3:U:83:LEU:CD2	3:U:87:LEU:HD11	1.78	1.12

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)
3:F:5:ASP:OD2	3:M:4:ASN:OD1[21_554]	2.19	0.01

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	
3	F	111/132 (84%)	70 (63%)	29 (26%)	12 (11%)	0	2
3	M	116/132 (88%)	76 (66%)	27 (23%)	13 (11%)	0	2
3	O	93/132 (70%)	51 (55%)	24 (26%)	18 (19%)	0	0
3	P	116/132 (88%)	70 (60%)	33 (28%)	13 (11%)	0	2
3	U	109/132 (83%)	64 (59%)	33 (30%)	12 (11%)	0	2
3	V	94/132 (71%)	59 (63%)	20 (21%)	15 (16%)	0	0
All	All	639/792 (81%)	390 (61%)	166 (26%)	83 (13%)	0	1

5 of 83 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	U	76	MET
3	P	34	PHE
3	P	98	ASP
3	F	8	ALA
3	F	35	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	
3	F	102/121 (84%)	79 (78%)	23 (22%)	1	3
3	M	107/121 (88%)	81 (76%)	26 (24%)	1	2
3	O	86/121 (71%)	67 (78%)	19 (22%)	1	4
3	P	107/121 (88%)	77 (72%)	30 (28%)	0	1
3	U	100/121 (83%)	76 (76%)	24 (24%)	1	2
3	V	87/121 (72%)	58 (67%)	29 (33%)	0	0
All	All	589/726 (81%)	438 (74%)	151 (26%)	0	2

5 of 151 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	80	LEU

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Mol	Chain	Res	Type
3	V	45	LEU
3	O	59	TRP
3	F	88	ARG
3	F	113	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
3	V	94	GLN
3	V	104	GLN
3	O	96	GLN
3	V	97	HIS
3	M	48	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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
4	SO4	O	299	-	4,4,4	0.34	0	6,6,6	0.11	0
4	SO4	V	599	-	4,4,4	0.37	0	6,6,6	0.15	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
4	SO4	O	299	-	-	0/0/0/0	0/0/0/0
4	SO4	V	599	-	-	0/0/0/0	0/0/0/0

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	E	12/12 (100%)	0.39	0 100 100	62, 80, 92, 93	0
1	I	12/12 (100%)	0.05	0 100 100	58, 78, 107, 118	0
1	K	12/12 (100%)	0.22	0 100 100	65, 86, 96, 103	0
1	Y	12/12 (100%)	0.36	0 100 100	57, 69, 109, 113	0
2	G	12/12 (100%)	0.15	0 100 100	47, 79, 108, 114	0
2	J	12/12 (100%)	0.05	0 100 100	59, 82, 106, 111	0
2	R	12/12 (100%)	0.00	0 100 100	64, 76, 103, 107	0
2	T	12/12 (100%)	0.16	0 100 100	67, 81, 110, 118	0
3	F	113/132 (85%)	0.69	10 (8%) 11 4	70, 113, 159, 184	0
3	M	118/132 (89%)	0.47	4 (3%) 46 23	58, 91, 143, 163	0
3	O	97/132 (73%)	0.56	6 (6%) 21 8	89, 132, 186, 195	0
3	P	118/132 (89%)	0.38	3 (2%) 58 33	52, 82, 126, 156	0
3	U	111/132 (84%)	0.42	3 (2%) 55 29	51, 83, 142, 169	0
3	V	98/132 (74%)	0.42	4 (4%) 38 18	54, 101, 141, 168	0
All	All	751/888 (84%)	0.45	30 (3%) 39 19	47, 97, 158, 195	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	28	ARG	8.0
3	F	27	SER	7.6
3	O	10	PHE	5.5
3	M	26	SER	3.7
3	V	10	PHE	3.6

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 carbohydrates 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. 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(\AA^2)	Q<0.9
4	SO4	V	599	5/5	0.33	0.29	-	199,199,200,200	0
4	SO4	O	299	5/5	0.84	0.13	-	199,199,200,200	0

6.5 Other polymers [i](#)

There are no such residues in this entry.