



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 04:50 PM UTC

PDB ID : 1PP8 / pdb_00001pp8
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

<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

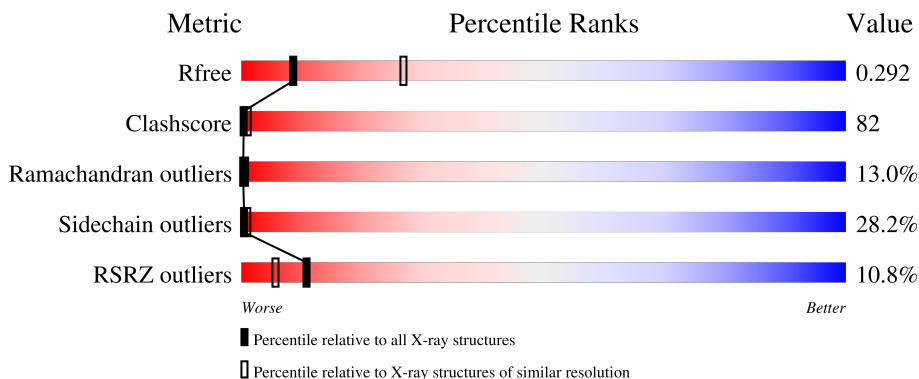
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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.



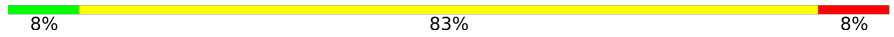
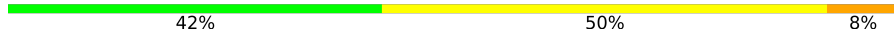




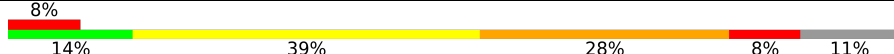
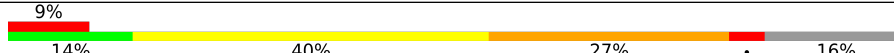

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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 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	E	12	
1	I	12	
1	K	12	
1	Y	12	
2	G	12	

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Mol	Chain	Length	Quality of chain
2	J	12	 8% 83% 8%
2	R	12	 42% 50% 8%
2	T	12	 8% 67% 17% 8%
3	F	132	 11% 17% 38% 27% 14%
3	M	132	 7% 17% 39% 28% 6% 11%
3	O	132	 18% 8% 39% 20% 6% 27%
3	P	132	 8% 14% 39% 28% 8% 11%
3	U	132	 9% 14% 40% 27% 16%
3	V	132	 9% 9% 33% 29% 26%

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:

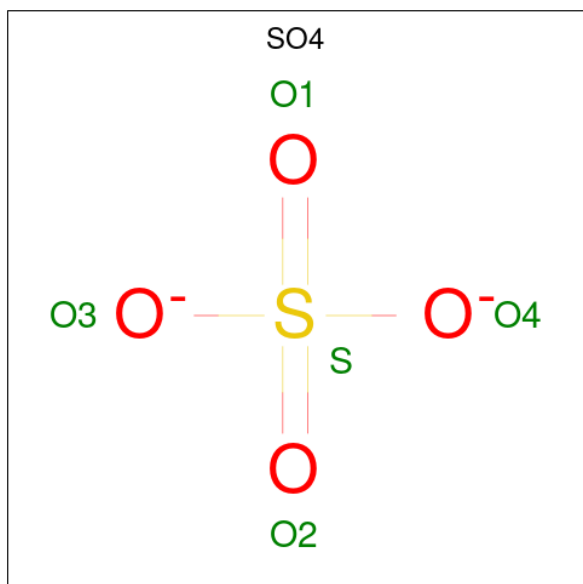
Chain	Residue	Modelled	Actual	Comment	Reference
U	127	HIS	-	expression tag	UNP Q95VR4
U	128	HIS	-	expression tag	UNP Q95VR4
U	129	HIS	-	expression tag	UNP Q95VR4
U	130	HIS	-	expression tag	UNP Q95VR4
U	131	HIS	-	expression tag	UNP Q95VR4
U	132	HIS	-	expression tag	UNP Q95VR4
P	127	HIS	-	expression tag	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 (CCD ID: 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, 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: ALPHA-SCS INR



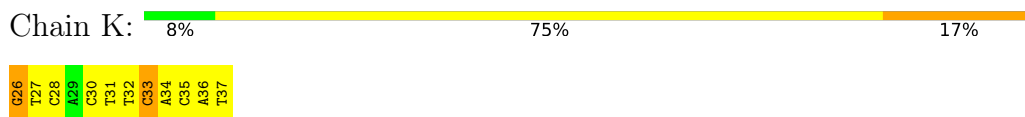
- Molecule 1: ALPHA-SCS INR



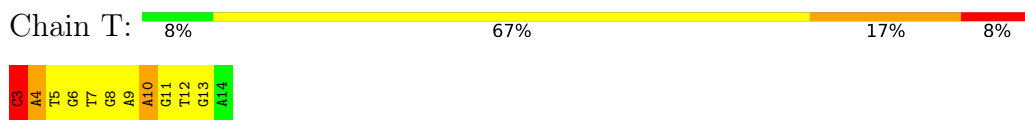
- Molecule 1: ALPHA-SCS INR



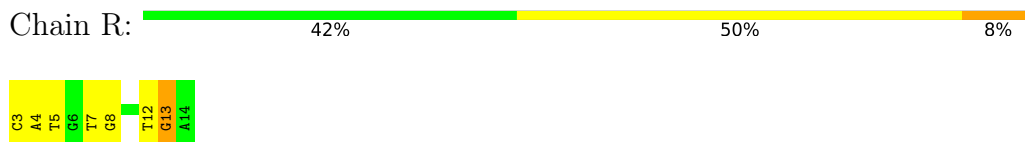
- Molecule 1: ALPHA-SCS INR



- Molecule 2: ALPHA-SCS INR



- Molecule 2: ALPHA-SCS INR



- Molecule 2: ALPHA-SCS INR

Chain J: 8% 83% 8%

C3 A4 A44 T5 T5 G6 G6 T7 T7 G8 G8 A9 A9 A10 A10 G11 G11 G12 G12 G13 G13 A14 A14

- Molecule 2: ALPHA-SCS INR

Chain G: 17% 67% 8% 8%

C3 A4 A4 T5 T5 G6 G6 T7 T7 G8 G8 A9 A9 A10 A10 G11 G11 G12 G12 G13 G13 A14 A14

- Molecule 3: 39 kDa initiator binding protein

Chain U: 9% 14% 40% 27% 16%

MET D2 S3 N4 D5 L6 E7 A8 S9 F10 T11 S12 R13 L14 P15 I18 V19 A20 A21 L22 K23 R24 K25 S26 S27 R28 D29 P30 R33 F34 P35 R36 K37 L38 H39 M40 L41 L42 T43 Y44 L45 A46 S47 M48 P49 Q50 L51 E52 E53 E54 I55 G56 L57 S58 W59 I60 D62

T63 E64 K66 M67 K68 K69 M70 N71 V72 A73 L74 W75 M76 G77 I78 K79 L80 N81 T82 L83 M84 W85 N86 L87 R88 D89 L90 A91 F92 L95 Q96 H97 D98 K99 M102 T103 Q104 M105 T43 K106 R107 S108 G109 F110 T111 R112 ASN SER VAL PHE GLU ASP PRO THR GLN ASN ASP SER

PRO MET HIS HIS HIS HIS HIS HIS

- Molecule 3: 39 kDa initiator binding protein

Chain P: 8% 14% 39% 28% 8% 11%

M1 D2 S3 N4 D5 L6 E7 A8 S9 F10 T11 S12 R13 L14 P15 I16 V17 I18 L19 V19 A20 A21 L22 K23 R24 K25 S26 S27 R28 D29 P30 N31 S32 R33 S34 P35 F36 R36 K37 L38 H39 M40 L41 L42 T43 Y44 L45 A46 S47 M48 P49 Q50 L51 E52 E53 E54 I55 G56 L57 S58 W59 I60

S61 D62 T63 E64 K66 M67 K68 K69 M70 N71 V72 A73 L74 W75 M76 G77 I78 K79 L80 N81 T82 L83 M84 W85 N86 L87 R88 D89 L90 A91 F92 L95 Q94 Q94 Q96 H97 D98 K99 M102 T103 Q104 M105 T43 K106 R107 S108 G109 F110 T111 R112 M113 M114 V115 F116 E117 D118 PRO THR GLN ASN ASP

SER PRO MET HIS HIS HIS HIS HIS

- Molecule 3: 39 kDa initiator binding protein

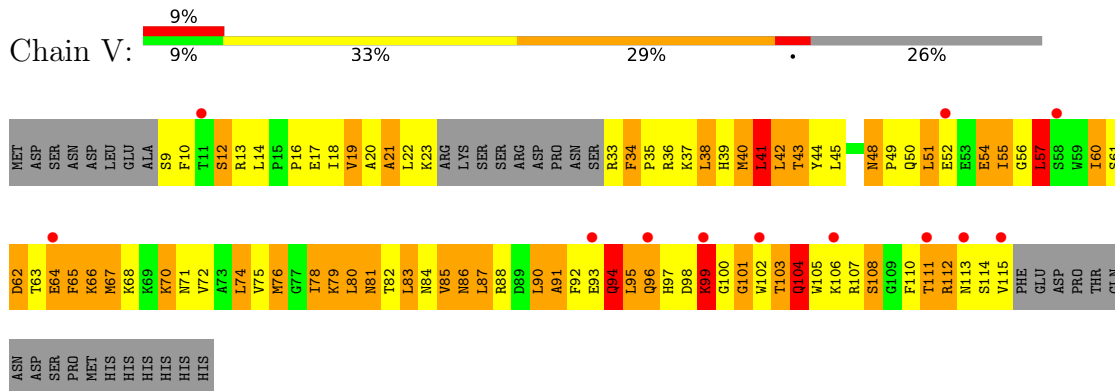
Chain F: 11% 17% 38% 27% 14%

MET D2 S3 N4 D5 L6 E7 A8 S9 F10 T11 S12 R13 L14 P15 I16 V17 I18 L19 V19 A20 A21 L22 K25 S26 S27 R28 D29 P30 N31 S32 R33 F34 P35 F36 R36 K37 L38 H39 M40 L41 L42 T43 Y44 L45 A46 S47 M48 P49 Q50 L51 E54 I55 G56 L57 S58 W59 I60 D62

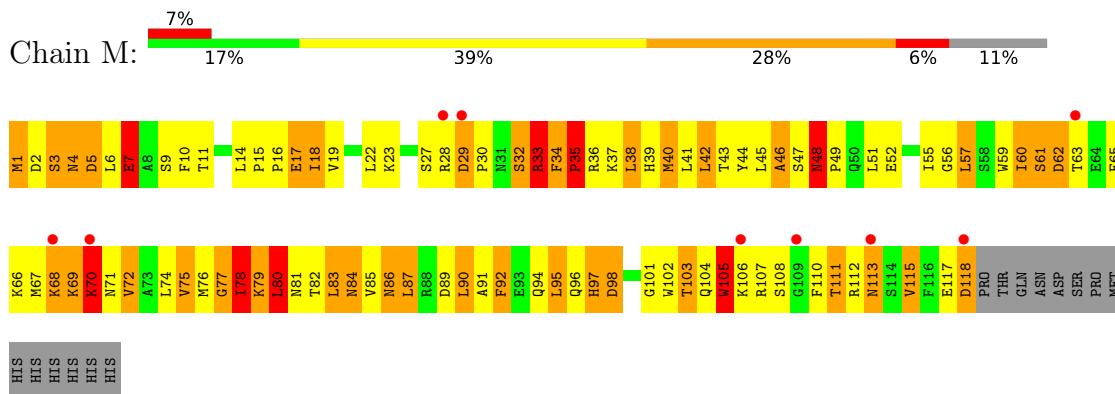
T63 E64 K66 M67 K68 K69 M70 N71 V72 A73 L74 W75 M76 G77 I78 K79 L80 N81 T82 L83 M84 W85 N86 L87 R88 D89 L90 A91 F92 L95 Q94 Q94 Q96 H97 D98 K99 M102 T103 Q104 M105 T43 K106 R107 S108 G109 F110 T111 R112 M113 M114 VAL PHE GLU ASP PRO THR GLN ASN ASP SER PRO

MET
HIS
HIS
HIS
HIS
HIS
HIS

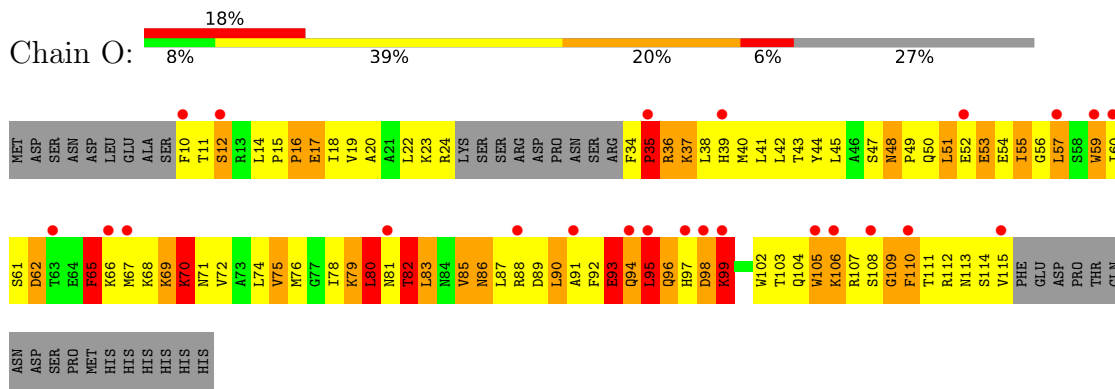
• Molecule 3: 39 kDa initiator binding protein



• Molecule 3: 39 kDa initiator binding protein



• Molecule 3: 39 kDa initiator binding protein



4 Data and refinement statistics

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 – 3.05	Depositor EDS
% Data completeness (in resolution range)	94.2 (146.00-3.05) 94.2 (146.00-3.05)	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 (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	104.0	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 196.2	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	0.91	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	0.61	0/265	1.30	1/406 (0.2%)
1	I	0.57	0/265	1.35	4/406 (1.0%)
1	K	0.59	0/265	0.98	0/406
1	Y	0.59	0/265	1.05	0/406
2	G	0.70	0/279	1.21	3/430 (0.7%)
2	J	0.63	0/279	1.11	2/430 (0.5%)
2	R	0.59	0/279	0.99	0/430
2	T	0.61	0/279	1.07	2/430 (0.5%)
3	F	0.83	0/933	1.41	14/1256 (1.1%)
3	M	1.06	4/977 (0.4%)	1.48	20/1315 (1.5%)
3	O	0.71	1/804 (0.1%)	1.24	7/1081 (0.6%)
3	P	1.16	5/977 (0.5%)	1.53	22/1315 (1.7%)
3	U	1.09	1/919 (0.1%)	1.60	23/1237 (1.9%)
3	V	1.05	1/810 (0.1%)	1.38	9/1089 (0.8%)
All	All	0.91	12/7596 (0.2%)	1.36	107/10637 (1.0%)

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 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	19	VAL	CA-CB	-7.39	1.46	1.54
3	M	40	MET	SD-CE	6.75	1.96	1.79
3	V	55	ILE	CA-CB	-6.41	1.46	1.54
3	P	105	TRP	C-N	5.85	1.40	1.33
3	M	15	PRO	CA-C	5.82	1.55	1.51

The worst 5 of 107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	14	LEU	CA-C-N	12.93	133.69	120.38
3	U	14	LEU	C-N-CA	12.93	133.69	120.38
3	F	81	ASN	CA-CB-CG	11.09	123.69	112.60
1	I	35	DC	N1-C1'-C2'	10.46	129.19	113.50
1	E	37	DT	C2'-C3'-O3'	10.19	126.79	111.50

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	23	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	154	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	M	958	0	966	147	1
3	O	788	0	812	154	0
3	P	958	0	966	194	0
3	U	901	0	915	170	0
3	V	794	0	817	177	0
4	O	5	0	0	0	0
4	V	5	0	0	0	0
All	All	7268	0	6502	1107	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 82.

The worst 5 of 1107 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
3:U:21:ALA:HB3	3:U:40:MET:HE1	1.25	1.14
1:K:36:DA:H2''	1:K:37:DT:H5''	1.28	1.13

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	1
3	M	116/132 (88%)	76 (66%)	27 (23%)	13 (11%)	0	1
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	1
3	U	109/132 (83%)	64 (59%)	33 (30%)	12 (11%)	0	1
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	0

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%)	75 (74%)	27 (26%)	0	1
3	M	107/121 (88%)	79 (74%)	28 (26%)	0	2
3	O	86/121 (71%)	64 (74%)	22 (26%)	0	2
3	P	107/121 (88%)	76 (71%)	31 (29%)	0	1
3	U	100/121 (83%)	75 (75%)	25 (25%)	0	2
3	V	87/121 (72%)	54 (62%)	33 (38%)	0	0
All	All	589/726 (81%)	423 (72%)	166 (28%)	0	1

5 of 166 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	V	115	VAL

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Mol	Chain	Res	Type
3	M	118	ASP
3	M	7	GLU
3	M	72	VAL
3	O	51	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
3	V	104	GLN
3	O	104	GLN
3	M	94	GLN
3	O	86	ASN
3	M	71	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 oligosaccharides 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	V	599	-	4,4,4	0.40	0	6,6,6	0.13	0
4	SO4	O	299	-	4,4,4	0.38	0	6,6,6	0.13	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

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	E	12/12 (100%)	0.26	0 100 100	62, 80, 92, 93	0
1	I	12/12 (100%)	0.08	0 100 100	58, 78, 107, 118	0
1	K	12/12 (100%)	0.40	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%)	0.17	0 100 100	47, 79, 108, 114	0
2	J	12/12 (100%)	0.38	0 100 100	59, 82, 106, 111	0
2	R	12/12 (100%)	0.47	0 100 100	64, 76, 103, 107	0
2	T	12/12 (100%)	0.55	0 100 100	67, 81, 110, 118	0
3	F	113/132 (85%)	0.91	14 (12%) 8 5	70, 113, 159, 184	0
3	M	118/132 (89%)	0.44	9 (7%) 20 10	58, 91, 143, 163	0
3	O	97/132 (73%)	1.14	24 (24%) 2 1	89, 132, 186, 195	0
3	P	118/132 (89%)	0.41	10 (8%) 16 9	52, 82, 126, 156	0
3	U	111/132 (84%)	0.63	12 (10%) 11 5	51, 83, 142, 169	0
3	V	98/132 (74%)	0.74	12 (12%) 8 5	54, 101, 141, 168	0
All	All	751/888 (84%)	0.65	81 (10%) 11 5	47, 97, 158, 195	0

The worst 5 of 81 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	U	112	ARG	5.7
3	M	106	LYS	5.6
3	V	115	VAL	4.7
3	F	106	LYS	4.7
3	O	10	PHE	4.6

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 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(\AA^2)	Q<0.9
4	SO4	V	599	5/5	0.65	0.15	199,199,200,200	0
4	SO4	O	299	5/5	0.69	0.10	199,199,200,200	0

6.5 Other polymers [i](#)

There are no such residues in this entry.