



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:01 AM GMT

PDB ID : 2P1N
Title : Mechanism of Auxin Perception by the TIR1 Ubiquitin Ligase
Authors : Tan, X.; Calderon-Villalobos, L.I.A.; Sharon, M.; Robinson, C.V.; Estelle, M.;
Zheng, C.; Zheng, N.
Deposited on : 2007-03-06
Resolution : 2.50 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

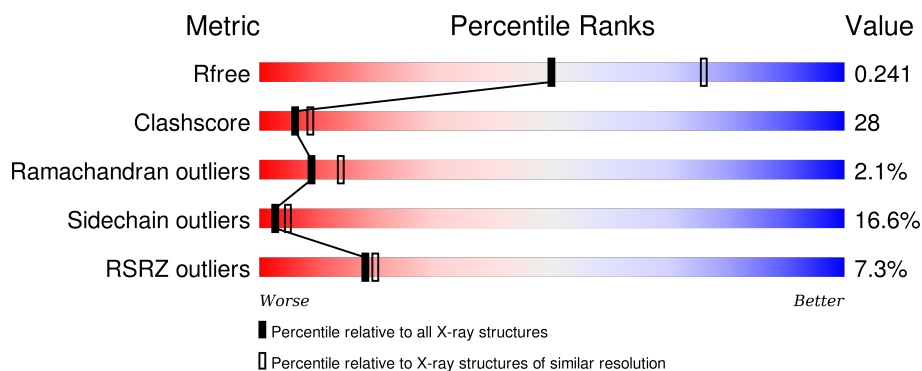
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.



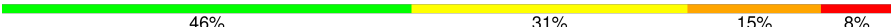
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	A	160	<div> <div>29%</div> <div>36% 31% 10% 21%</div> </div>
1	D	160	<div> <div>27%</div> <div>35% 29% 13% 21%</div> </div>
2	B	594	<div> <div>0%</div> <div>55% 31% 8%</div> </div>
2	E	594	<div> <div>2%</div> <div>53% 32% 9%</div> </div>
3	C	13	<div> <div>8%</div> <div>15% 38% 38% 8%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	13	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: green (46%), yellow (31%), orange (15%), and red (8%).

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11872 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 SKP1-like protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	126	Total	C	N	O	S	0	0	0
			1009	638	165	201	5			
1	D	127	Total	C	N	O	S	0	0	0
			1023	649	167	202	5			

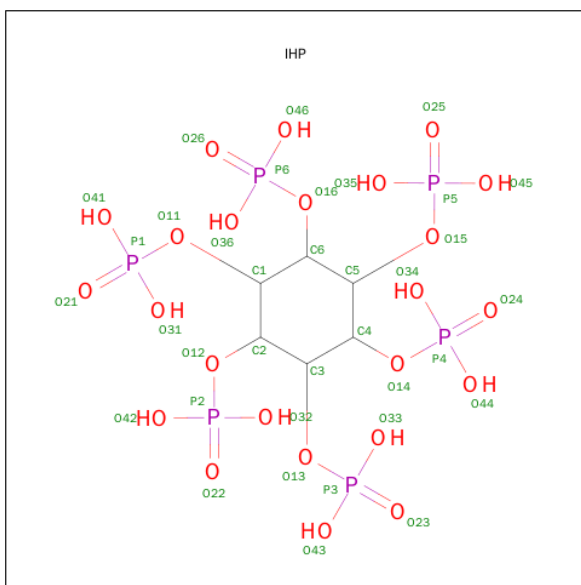
- Molecule 2 is a protein called TRANSPORT INHIBITOR RESPONSE 1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	571	Total	C	N	O	S	0	0	0
			4495	2871	759	828	37			
2	E	571	Total	C	N	O	S	0	0	0
			4495	2871	759	828	37			

- Molecule 3 is a protein called Auxin-responsive protein IAA7.

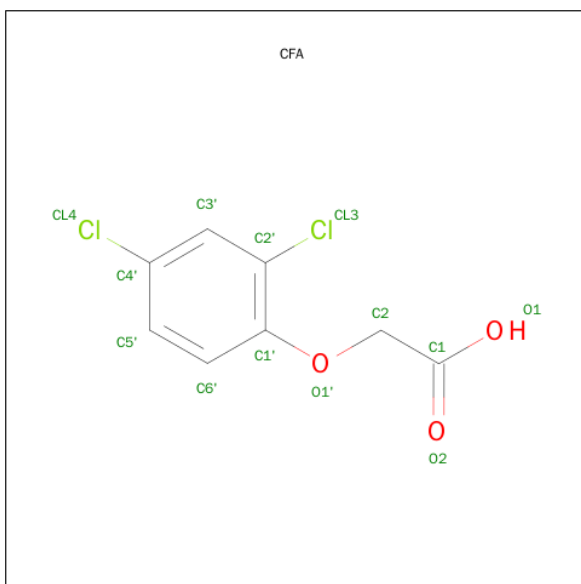
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	0	0	0
			114	74	23	17			
3	F	13	Total	C	N	O	0	0	0
			114	74	23	17			

- Molecule 4 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: C₆H₁₈O₂₄P₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	P	0	0
			36	6	24	6		
4	E	1	Total	C	O	P	0	0
			36	6	24	6		

- Molecule 5 is (2,4-DICHLOROPHENOXY)ACETIC ACID (three-letter code: CFA) (formula: $C_8H_6Cl_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	Cl	O	0	0
			13	8	2	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	1	Total	C	Cl	O	0	0
			13	8	2	3		

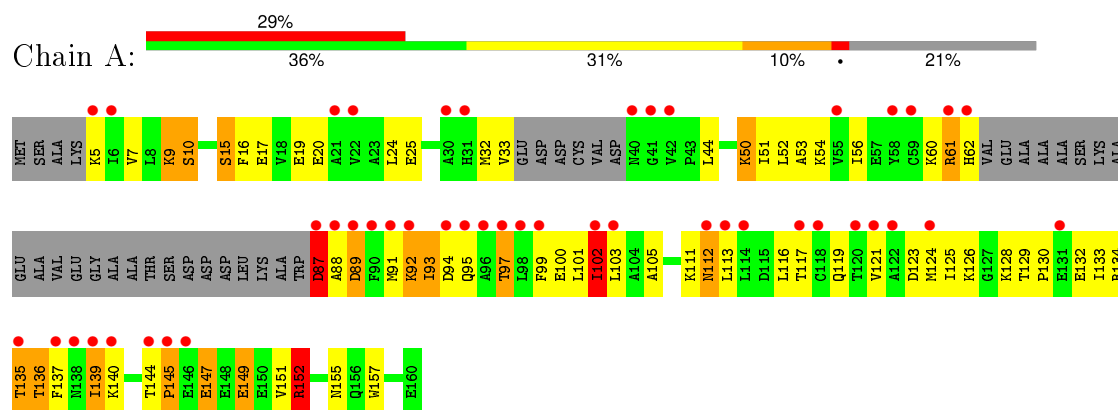
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	25	Total	O	0	0
			25	25		
6	B	217	Total	O	0	0
			217	217		
6	C	6	Total	O	0	0
			6	6		
6	D	32	Total	O	0	0
			32	32		
6	E	240	Total	O	0	0
			240	240		
6	F	4	Total	O	0	0
			4	4		

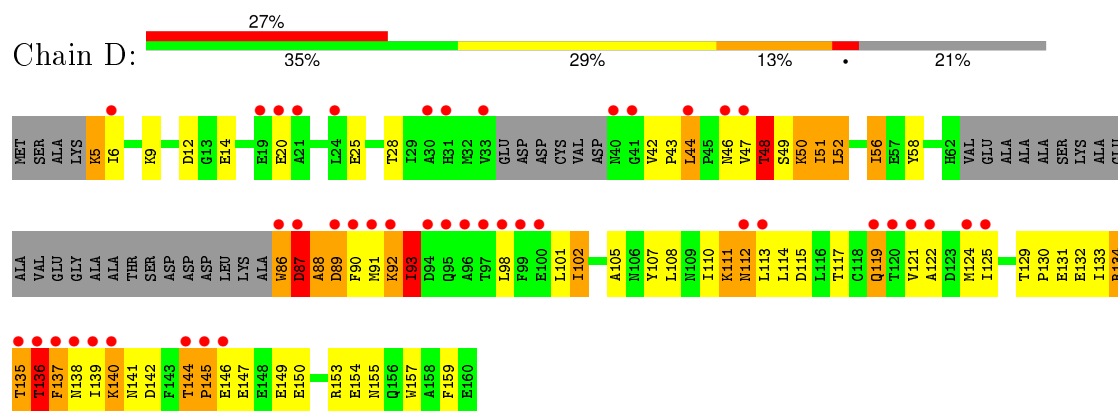
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

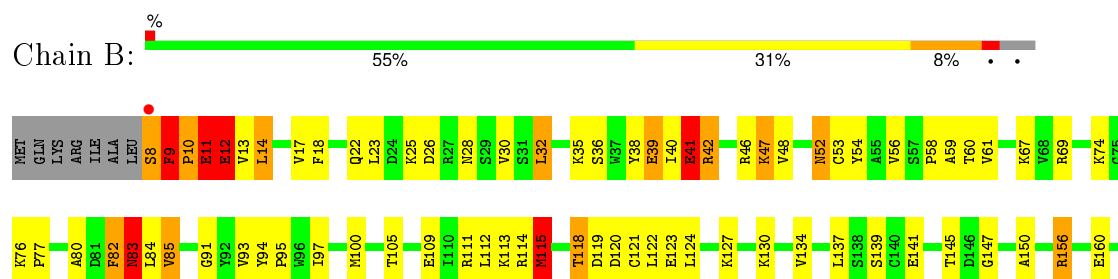
• Molecule 1: SKP1-like protein 1A

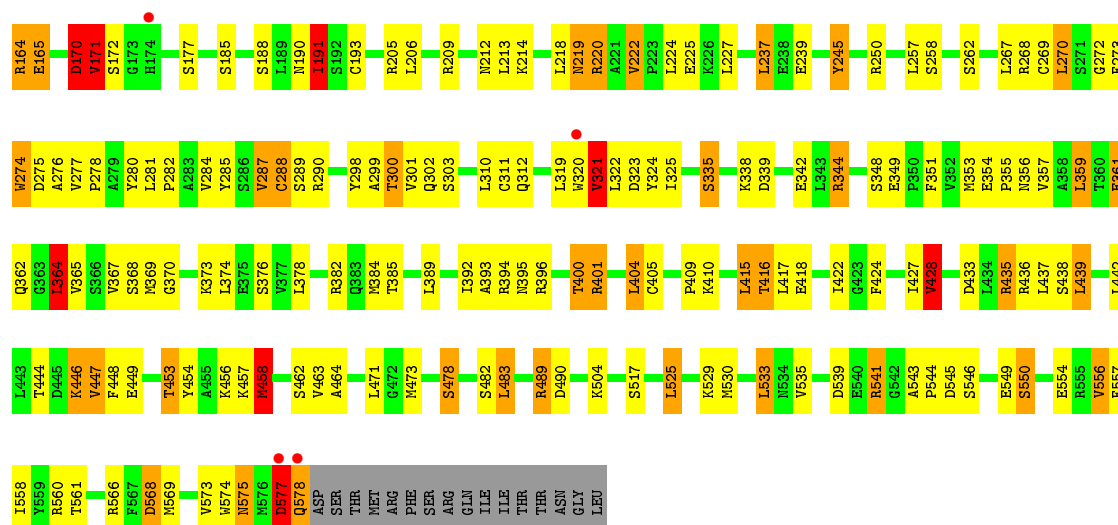


• Molecule 1: SKP1-like protein 1A

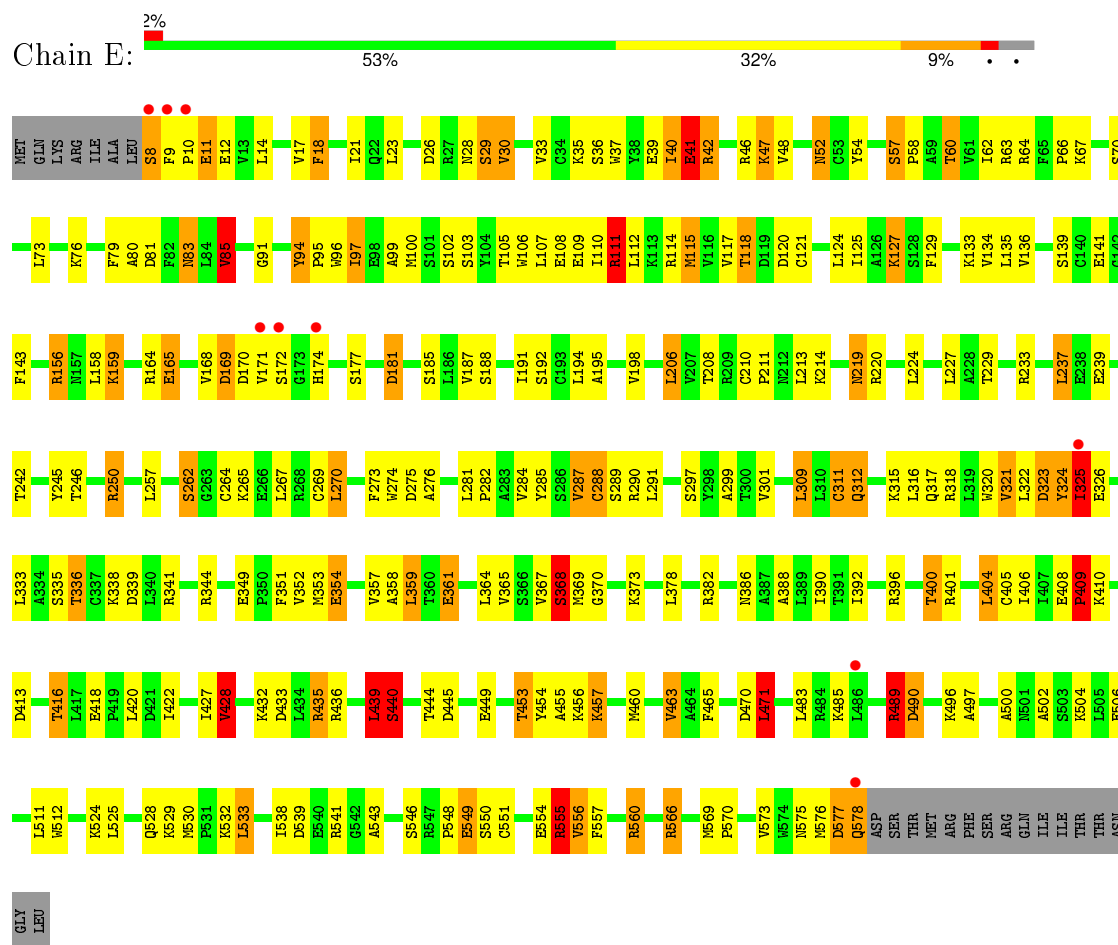


• Molecule 2: TRANSPORT INHIBITOR RESPONSE 1 protein



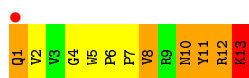


• Molecule 2: TRANSPORT INHIBITOR RESPONSE 1 protein



• Molecule 3: Auxin-responsive protein IAA7





● Molecule 3: Auxin-responsive protein IAA7

Chain F:
46% 31% 15% 8%

The overall validation bar for Chain F is divided into four segments: 46% green, 31% yellow, 15% orange, and 8% red.



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.67Å 82.75Å 125.79Å 90.00° 100.40° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 49.55 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.5 (50.00-2.50) 90.5 (49.55-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.195 , 0.274 0.235 , 0.241	Depositor DCC
R_{free} test set	3305 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 34.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	8 of 65147 reflections (0.012%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11872	wwPDB-VP
Average B, all atoms (Å ²)	7.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.31 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.9529e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: IHP, CFA

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	1.01	2/1022 (0.2%)	1.03	5/1377 (0.4%)
1	D	0.92	2/1038 (0.2%)	1.14	5/1400 (0.4%)
2	B	1.31	11/4593 (0.2%)	1.36	53/6226 (0.9%)
2	E	1.29	13/4593 (0.3%)	1.34	39/6226 (0.6%)
3	C	4.02	1/118 (0.8%)	0.90	0/159
3	F	1.12	0/118	1.06	0/159
All	All	1.30	29/11482 (0.3%)	1.30	102/15547 (0.7%)

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	3	3
1	D	0	4
2	B	2	14
2	E	3	7
3	F	0	3
All	All	8	31

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	13	LYS	C-OXT	-41.90	0.43	1.23
2	E	440	SER	CB-OG	-8.13	1.31	1.42
1	A	20	GLU	CB-CG	7.43	1.66	1.52
1	A	20	GLU	CG-CD	7.25	1.62	1.51
2	E	408	GLU	CB-CG	7.25	1.66	1.52

The worst 5 of 102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	144	THR	C-N-CD	-19.80	77.03	120.60
2	B	220	ARG	N-CA-CB	-16.51	80.88	110.60
2	E	435	ARG	NE-CZ-NH2	-12.82	113.89	120.30
2	E	555	ARG	NE-CZ-NH1	12.14	126.37	120.30
2	B	339	ASP	CB-CG-OD1	10.63	127.86	118.30

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	99	PHE	CA
1	A	112	ASN	CA
1	A	153	ARG	CA
2	B	60	THR	CA
2	B	478	SER	CA

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	ARG	Peptide
1	A	87	ASP	Peptide
1	A	97	THR	Peptide
2	B	10	PRO	Peptide
2	B	9	PHE	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	1009	0	1003	71	3
1	D	1023	0	1013	114	0
2	B	4495	0	4529	219	0
2	E	4495	0	4529	220	0
3	C	114	0	118	24	3
3	F	114	0	118	17	0
4	B	36	0	6	1	0
4	E	36	0	6	2	0
5	B	13	0	5	1	0
5	E	13	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	25	0	0	3	0
6	B	217	0	0	21	0
6	C	6	0	0	1	0
6	D	32	0	0	6	0
6	E	240	0	0	22	0
6	F	4	0	0	1	0
All	All	11872	0	11332	642	3

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 28.

The worst 5 of 642 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)
2:B:351:PHE:CD2	3:C:13:LYS:HD2	1.56	1.40
1:D:144:THR:CB	1:D:145:PRO:CD	2.02	1.35
1:A:129:THR:HG23	1:A:132:GLU:OE1	1.14	1.31
1:D:144:THR:CB	1:D:145:PRO:HD2	1.40	1.26
2:B:11:GLU:N	2:B:12:GLU:HG3	1.55	1.21

All (3) 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)
1:A:15:SER:O	3:C:11:TYR:O[1_545]	0.76	1.44
1:A:15:SER:O	3:C:11:TYR:C[1_545]	1.98	0.22
1:A:15:SER:C	3:C:11:TYR:O[1_545]	1.98	0.22

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	120/160 (75%)	98 (82%)	15 (12%)	7 (6%)	2	2
1	D	121/160 (76%)	98 (81%)	18 (15%)	5 (4%)	3	4
2	B	569/594 (96%)	520 (91%)	41 (7%)	8 (1%)	14	24
2	E	569/594 (96%)	510 (90%)	50 (9%)	9 (2%)	12	21
3	C	11/13 (85%)	10 (91%)	1 (9%)	0	100	100
3	F	11/13 (85%)	8 (73%)	2 (18%)	1 (9%)	1	1
All	All	1401/1534 (91%)	1244 (89%)	127 (9%)	30 (2%)	9	14

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	92	LYS
2	B	42	ARG
2	B	83	ASN
2	B	219	ASN

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	113/137 (82%)	94 (83%)	19 (17%)	2	4
1	D	114/137 (83%)	88 (77%)	26 (23%)	1	1
2	B	504/525 (96%)	432 (86%)	72 (14%)	4	7
2	E	504/525 (96%)	420 (83%)	84 (17%)	3	5
3	C	12/12 (100%)	6 (50%)	6 (50%)	0	0
3	F	12/12 (100%)	10 (83%)	2 (17%)	3	5
All	All	1259/1348 (93%)	1050 (83%)	209 (17%)	3	5

5 of 209 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	11	TYR

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Mol	Chain	Res	Type
1	D	114	LEU
2	E	463	VAL
1	D	5	LYS
1	D	52	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	575	ASN
2	E	52	ASN
2	E	383	GLN
2	B	501	ASN
2	E	501	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](#)

4 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	IHP	B	601	-	36,36,36	2.37	10 (27%)	48,60,60	2.40	20 (41%)
5	CFA	B	602	-	10,13,13	1.22	1 (10%)	14,17,17	1.49	3 (21%)
4	IHP	E	601	-	36,36,36	2.71	13 (36%)	48,60,60	2.33	22 (45%)
5	CFA	E	602	-	10,13,13	1.68	2 (20%)	14,17,17	2.55	7 (50%)

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	IHP	B	601	-	-	0/30/54/54	0/1/1/1
5	CFA	B	602	-	-	0/3/5/5	0/1/1/1
4	IHP	E	601	-	-	0/30/54/54	0/1/1/1
5	CFA	E	602	-	-	0/3/5/5	0/1/1/1

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	IHP	O16-C6	-2.96	1.35	1.44
5	E	602	CFA	O1'-C1'	-2.95	1.31	1.37
5	E	602	CFA	C4'-CL4	-2.56	1.68	1.74
5	B	602	CFA	C4'-CL4	-2.02	1.69	1.74
4	E	601	IHP	P5-O45	2.01	1.61	1.54

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	IHP	P3-O13-C3	-6.54	105.87	121.56
4	B	601	IHP	O41-P1-O31	-5.32	87.11	107.38
5	E	602	CFA	C1'-C2'-CL3	-4.91	113.36	119.42
5	E	602	CFA	C2'-C3'-C4'	-4.76	113.40	118.69
4	E	601	IHP	P3-O13-C3	-4.27	111.33	121.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	601	IHP	1	0
5	B	602	CFA	1	0
4	E	601	IHP	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 [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	A	126/160 (78%)	1.69	46 (36%) 0 0	2, 6, 13, 22	0
1	D	127/160 (79%)	1.48	43 (33%) 0 0	2, 6, 13, 22	0
2	B	571/594 (96%)	-0.01	5 (0%) 85 88	2, 6, 18, 41	0
2	E	571/594 (96%)	0.10	9 (1%) 74 78	2, 6, 16, 32	0
3	C	13/13 (100%)	0.63	1 (7%) 16 18	5, 8, 13, 16	0
3	F	13/13 (100%)	0.58	0 100 100	2, 7, 11, 12	0
All	All	1421/1534 (92%)	0.33	104 (7%) 18 20	2, 6, 16, 41	0

The worst 5 of 104 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	ALA	5.8
1	D	137	PHE	5.4
1	A	90	PHE	4.6
1	A	97	THR	4.5
1	A	99	PHE	4.5

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(Å ²)	Q<0.9
4	IHP	B	601	36/36	0.96	0.16	-1.44	2,6,30,44	0
4	IHP	E	601	36/36	0.97	0.17	-1.77	2,7,25,32	0
5	CFA	B	602	13/13	0.97	0.16	-1.96	2,2,9,10	0
5	CFA	E	602	13/13	0.97	0.15	-4.16	2,2,10,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.