



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 24, 2026 – 04:13 PM EDT

PDB ID : 11VK / pdb_000011vk
Title : Effector BcTde1 in complex with BcTdi1 mutant G156R
Authors : Bosch, D.E.
Deposited on : 2026-03-13
Resolution : 2.41 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

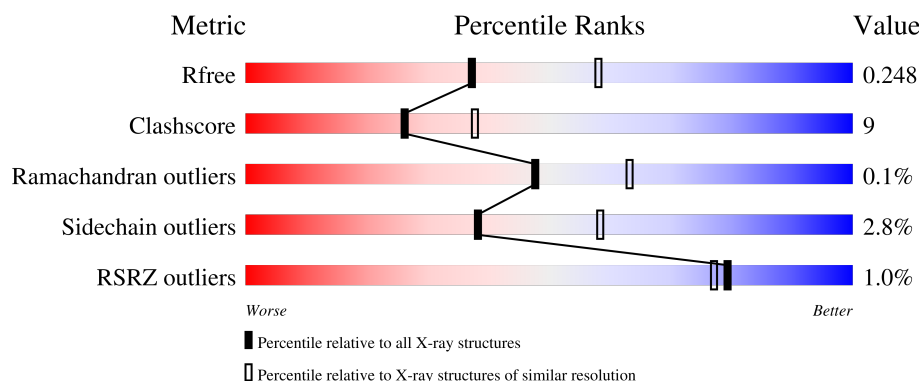
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	A	170	57% 15% 28%
1	C	170	64% 10% 26%
1	E	170	51% 15% • 32%
1	G	170	49% 14% • 36%
2	B	185	75% 22% ••

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Mol	Chain	Length	Quality of chain
2	D	185	76% 21% 2% ..
2	F	185	74% 24% 2% ..
2	H	185	72% 24% 2% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10163 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 Novel toxin 15 domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	123	Total	C	N	O	S	0	0	0
			1039	652	178	207	2			
1	C	125	Total	C	N	O	S	0	0	0
			1052	659	180	211	2			
1	E	115	Total	C	N	O	S	0	0	0
			960	601	162	195	2			
1	G	108	Total	C	N	O	S	0	0	0
			911	573	156	180	2			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A9X7BBB2
A	2	ALA	PRO	conflict	UNP A0A9X7BBB2
A	88	GLU	GLY	conflict	UNP A0A9X7BBB2
A	116	SER	GLY	conflict	UNP A0A9X7BBB2
A	165	HIS	-	expression tag	UNP A0A9X7BBB2
A	166	HIS	-	expression tag	UNP A0A9X7BBB2
A	167	HIS	-	expression tag	UNP A0A9X7BBB2
A	168	HIS	-	expression tag	UNP A0A9X7BBB2
A	169	HIS	-	expression tag	UNP A0A9X7BBB2
A	170	HIS	-	expression tag	UNP A0A9X7BBB2
C	1	MET	-	initiating methionine	UNP A0A9X7BBB2
C	2	ALA	PRO	conflict	UNP A0A9X7BBB2
C	88	GLU	GLY	conflict	UNP A0A9X7BBB2
C	116	SER	GLY	conflict	UNP A0A9X7BBB2
C	165	HIS	-	expression tag	UNP A0A9X7BBB2
C	166	HIS	-	expression tag	UNP A0A9X7BBB2
C	167	HIS	-	expression tag	UNP A0A9X7BBB2
C	168	HIS	-	expression tag	UNP A0A9X7BBB2
C	169	HIS	-	expression tag	UNP A0A9X7BBB2
C	170	HIS	-	expression tag	UNP A0A9X7BBB2
E	1	MET	-	initiating methionine	UNP A0A9X7BBB2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	2	ALA	PRO	conflict	UNP A0A9X7BBB2
E	88	GLU	GLY	conflict	UNP A0A9X7BBB2
E	116	SER	GLY	conflict	UNP A0A9X7BBB2
E	165	HIS	-	expression tag	UNP A0A9X7BBB2
E	166	HIS	-	expression tag	UNP A0A9X7BBB2
E	167	HIS	-	expression tag	UNP A0A9X7BBB2
E	168	HIS	-	expression tag	UNP A0A9X7BBB2
E	169	HIS	-	expression tag	UNP A0A9X7BBB2
E	170	HIS	-	expression tag	UNP A0A9X7BBB2
G	1	MET	-	initiating methionine	UNP A0A9X7BBB2
G	2	ALA	PRO	conflict	UNP A0A9X7BBB2
G	88	GLU	GLY	conflict	UNP A0A9X7BBB2
G	116	SER	GLY	conflict	UNP A0A9X7BBB2
G	165	HIS	-	expression tag	UNP A0A9X7BBB2
G	166	HIS	-	expression tag	UNP A0A9X7BBB2
G	167	HIS	-	expression tag	UNP A0A9X7BBB2
G	168	HIS	-	expression tag	UNP A0A9X7BBB2
G	169	HIS	-	expression tag	UNP A0A9X7BBB2
G	170	HIS	-	expression tag	UNP A0A9X7BBB2

- Molecule 2 is a protein called Tdi.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	183	Total	C	N	O	S	0	2	0
			1523	997	237	285	4			
2	D	183	Total	C	N	O	S	0	0	0
			1516	992	236	284	4			
2	F	183	Total	C	N	O	S	0	0	0
			1516	992	236	284	4			
2	H	183	Total	C	N	O	S	0	0	0
			1516	992	236	284	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	81	LEU	ILE	conflict	UNP A0A9X7CU01
B	156	ARG	GLY	engineered mutation	UNP A0A9X7CU01
B	185	PHE	-	expression tag	UNP A0A9X7CU01
D	81	LEU	ILE	conflict	UNP A0A9X7CU01
D	156	ARG	GLY	engineered mutation	UNP A0A9X7CU01
D	185	PHE	-	expression tag	UNP A0A9X7CU01
F	81	LEU	ILE	conflict	UNP A0A9X7CU01

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Chain	Residue	Modelled	Actual	Comment	Reference
F	156	ARG	GLY	engineered mutation	UNP A0A9X7CU01
F	185	PHE	-	expression tag	UNP A0A9X7CU01
H	81	LEU	ILE	conflict	UNP A0A9X7CU01
H	156	ARG	GLY	engineered mutation	UNP A0A9X7CU01
H	185	PHE	-	expression tag	UNP A0A9X7CU01

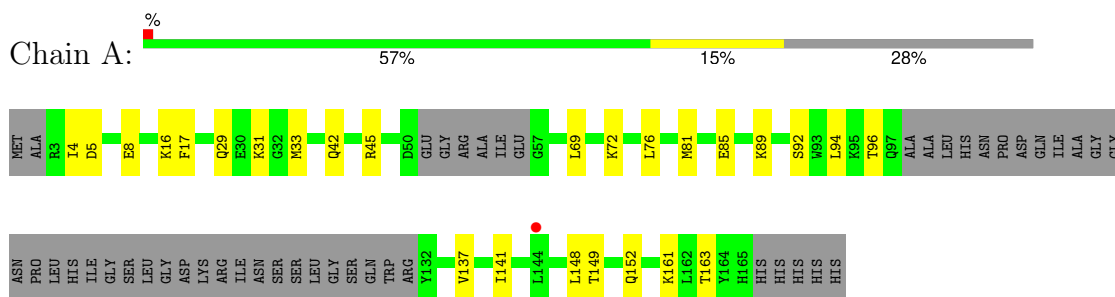
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	10	Total O 10 10	0	0
3	B	43	Total O 43 43	0	0
3	C	8	Total O 8 8	0	0
3	D	26	Total O 26 26	0	0
3	E	5	Total O 5 5	0	0
3	F	24	Total O 24 24	0	0
3	G	1	Total O 1 1	0	0
3	H	13	Total O 13 13	0	0

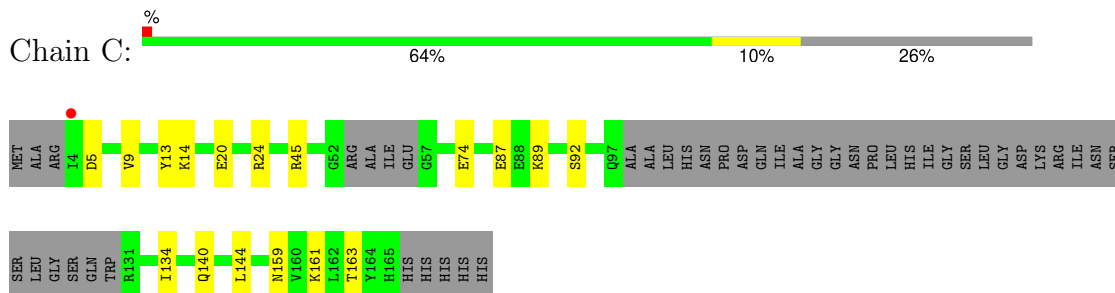
3 Residue-property plots [i](#)

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.

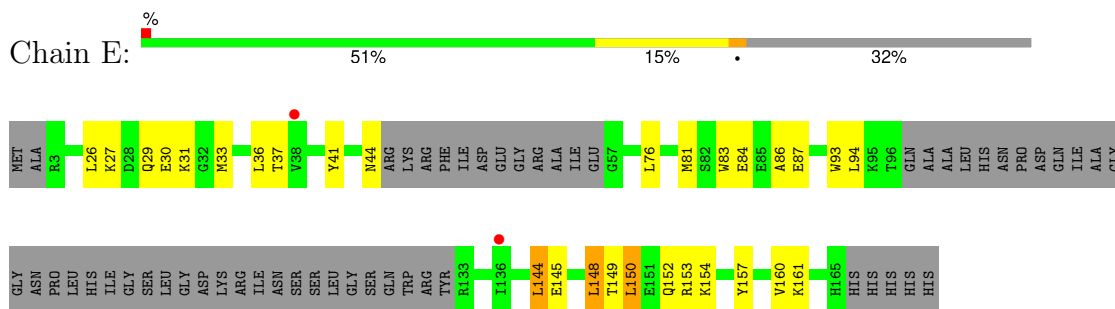
- Molecule 1: Novel toxin 15 domain-containing protein



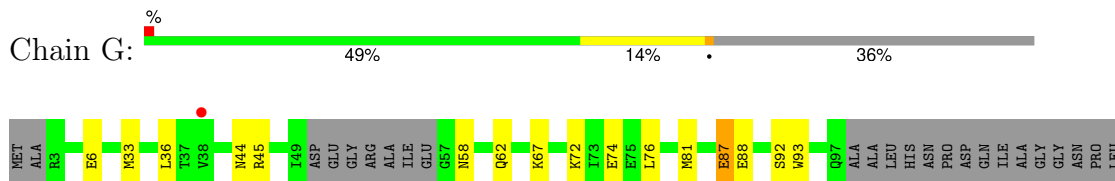
- Molecule 1: Novel toxin 15 domain-containing protein



- Molecule 1: Novel toxin 15 domain-containing protein



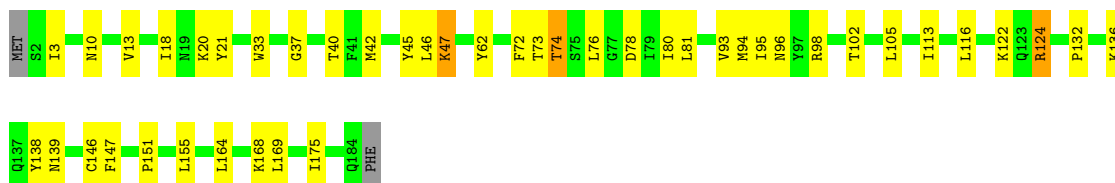
- Molecule 1: Novel toxin 15 domain-containing protein





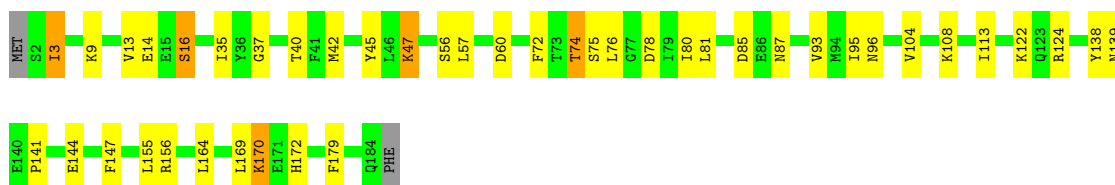
• Molecule 2: Tdi

Chain B: 75% 22% ..



• Molecule 2: Tdi

Chain D: 76% 21% ..



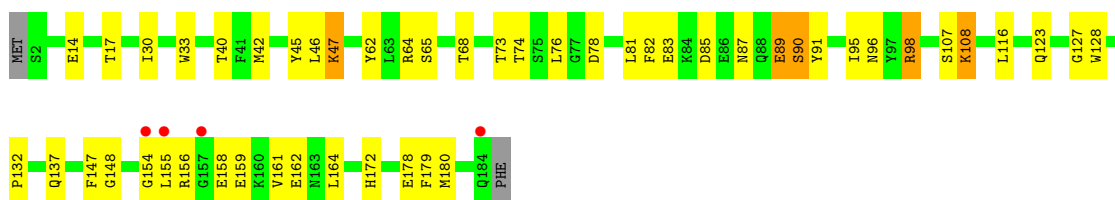
• Molecule 2: Tdi

Chain F: 2% 74% 24% ..



• Molecule 2: Tdi

Chain H: 2% 72% 24% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.87Å 81.12Å 99.09Å 75.77° 74.66° 84.57°	Depositor
Resolution (Å)	41.13 – 2.41 41.13 – 2.41	Depositor EDS
% Data completeness (in resolution range)	93.2 (41.13-2.41) 93.1 (41.13-2.41)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.21	Depositor
R, R_{free}	0.195 , 0.248 0.194 , 0.248	Depositor DCC
R_{free} test set	2000 reflections (3.08%)	wwPDB-VP
Wilson B-factor (Å ²)	56.1	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10163	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% 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](#)

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	0.43	0/1052	0.58	0/1404
1	C	0.39	0/1065	0.56	0/1421
1	E	0.42	0/971	0.60	0/1297
1	G	0.34	0/922	0.51	0/1228
2	B	0.49	0/1559	0.64	0/2100
2	D	0.45	0/1552	0.62	0/2090
2	F	0.42	0/1552	0.60	0/2090
2	H	0.45	0/1552	0.63	0/2090
All	All	0.43	0/10225	0.60	0/13720

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	H	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	98	ARG	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	A	1039	0	1015	19	0
1	C	1052	0	1024	16	0
1	E	960	0	935	27	0
1	G	911	0	884	20	0
2	B	1523	0	1530	31	0
2	D	1516	0	1523	30	0
2	F	1516	0	1523	32	0
2	H	1516	0	1523	42	0
3	A	10	0	0	0	0
3	B	43	0	0	0	0
3	C	8	0	0	0	0
3	D	26	0	0	1	0
3	E	5	0	0	0	0
3	F	24	0	0	0	0
3	G	1	0	0	0	0
3	H	13	0	0	0	0
All	All	10163	0	9957	187	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 9.

The worst 5 of 187 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:H:74:THR:HG22	2:H:76:LEU:H	1.27	0.97
2:F:74:THR:HG22	2:F:76:LEU:H	1.39	0.87
2:D:74:THR:HG22	2:D:76:LEU:H	1.45	0.81
1:A:4:ILE:HD12	1:E:144:LEU:HD13	1.64	0.79
2:F:42:MET:HE1	2:F:116:LEU:HD13	1.66	0.78

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	117/170 (69%)	114 (97%)	3 (3%)	0	100	100
1	C	119/170 (70%)	116 (98%)	3 (2%)	0	100	100
1	E	109/170 (64%)	103 (94%)	5 (5%)	1 (1%)	14	20
1	G	100/170 (59%)	96 (96%)	4 (4%)	0	100	100
2	B	182/185 (98%)	177 (97%)	5 (3%)	0	100	100
2	D	181/185 (98%)	175 (97%)	6 (3%)	0	100	100
2	F	181/185 (98%)	174 (96%)	7 (4%)	0	100	100
2	H	181/185 (98%)	172 (95%)	9 (5%)	0	100	100
All	All	1170/1420 (82%)	1127 (96%)	42 (4%)	1 (0%)	48	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	149	THR

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	111/147 (76%)	110 (99%)	1 (1%)	70	84
1	C	112/147 (76%)	111 (99%)	1 (1%)	70	84
1	E	103/147 (70%)	99 (96%)	4 (4%)	28	46
1	G	96/147 (65%)	93 (97%)	3 (3%)	35	55
2	B	168/169 (99%)	161 (96%)	7 (4%)	26	43
2	D	167/169 (99%)	160 (96%)	7 (4%)	26	43
2	F	167/169 (99%)	164 (98%)	3 (2%)	51	71
2	H	167/169 (99%)	162 (97%)	5 (3%)	36	56
All	All	1091/1264 (86%)	1060 (97%)	31 (3%)	38	58

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	169	LEU
2	H	89	GLU
1	E	148	LEU
2	H	108	LYS
1	G	87	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	96	ASN
2	H	10	ASN
1	E	43	GLN
1	G	159	ASN
1	E	42	GLN

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](#)

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(Å ²)	Q < 0.9
1	A	123/170 (72%)	0.06	1 (0%) 82 80	48, 71, 107, 119	0
1	C	125/170 (73%)	0.20	1 (0%) 82 80	59, 75, 102, 129	0
1	E	115/170 (67%)	0.30	2 (1%) 69 66	58, 78, 120, 150	0
1	G	108/170 (63%)	0.30	1 (0%) 81 79	65, 85, 128, 137	0
2	B	183/185 (98%)	-0.31	0 100 100	26, 57, 71, 118	1 (0%)
2	D	183/185 (98%)	-0.19	0 100 100	49, 61, 81, 110	0
2	F	183/185 (98%)	-0.12	3 (1%) 70 67	48, 64, 93, 117	0
2	H	183/185 (98%)	-0.03	4 (2%) 62 59	52, 66, 92, 127	0
All	All	1203/1420 (84%)	-0.02	12 (0%) 79 77	26, 67, 110, 150	1 (0%)

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	4	ILE	3.6
2	H	155	LEU	3.0
2	H	157	GLY	2.6
1	G	38	VAL	2.5
2	F	154	GLY	2.3

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.