



wwPDB X-ray Structure Validation Summary Report

Aug 20, 2023 – 04:01 AM EDT

PDB ID : 2H47
Title : Crystal Structure of an Electron Transfer Complex Between Aromatic Amine Dehydrogenase and Azurin from *Alcaligenes Faecalis* (Form 1)
Authors : Sukumar, N.; Chen, Z.; Leys, D.; Scrutton, N.S.; Ferrati, D.; Merli, A.; Rossi, G.L.; Bellamy, H.D.; Chistoserdov, A.; Davidson, V.L.; Mathews, F.S.
Deposited on : 2006-05-23
Resolution : 2.60 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

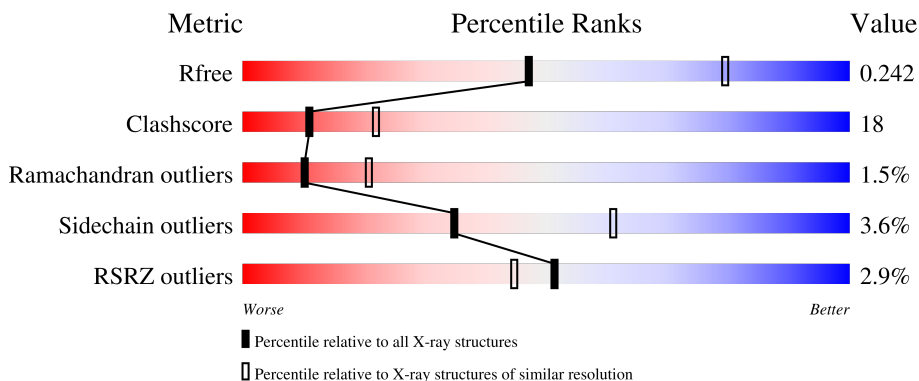
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	390	68% 23% 8%
1	D	390	66% 25% 7%
1	F	390	66% 25% 7%
1	H	390	67% 25% 7%
2	B	135	47% 43% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	135	<p>%</p> <p>56% 33% 7%</p>
2	G	135	<p>7%</p> <p>53% 35% 7%</p>
2	I	135	<p>4%</p> <p>47% 41% 8%</p>
3	C	128	<p>23%</p> <p>47% 49%</p>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 16799 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 Aromatic Amine Dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	360	2814	1776	491	534	13	0	0	0
1	D	361	2813	1774	491	535	13	0	0	0
1	F	362	2821	1779	492	537	13	0	0	0
1	H	362	2822	1780	493	536	13	0	0	0

- Molecule 2 is a protein called Aromatic Amine Dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	124	952	579	168	190	15	0	0	0
2	E	125	960	583	169	193	15	0	0	0
2	G	126	960	584	169	192	15	0	0	0
2	I	124	951	579	167	190	15	0	0	0

- Molecule 3 is a protein called Azurin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	128	958	596	160	195	7	0	0	0

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Cu	0	0
			1	1		

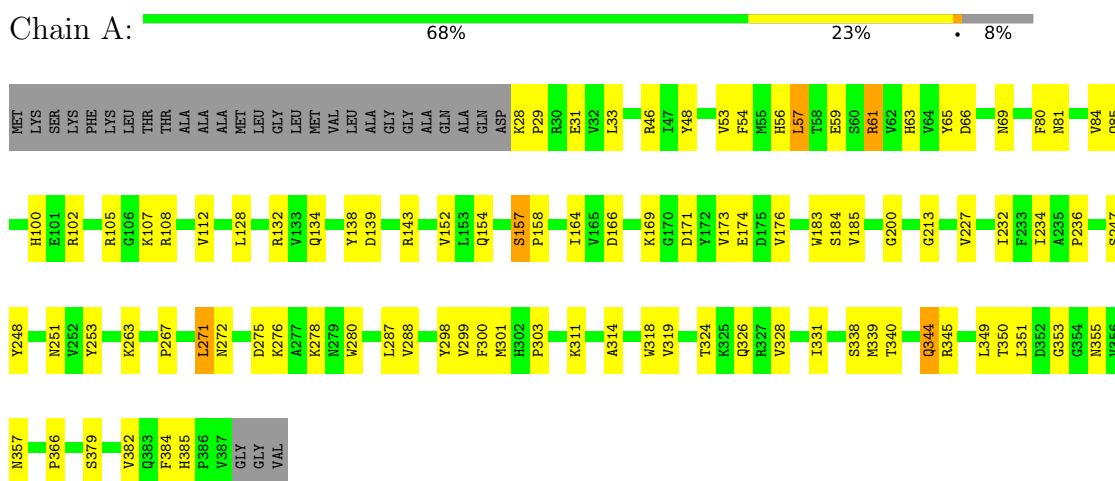
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	166	Total 166	O 166	0	0
5	B	34	Total 34	O 34	0	0
5	C	31	Total 31	O 31	0	0
5	D	133	Total 133	O 133	0	0
5	E	51	Total 51	O 51	0	0
5	F	109	Total 109	O 109	0	0
5	G	40	Total 40	O 40	0	0
5	H	146	Total 146	O 146	0	0
5	I	37	Total 37	O 37	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: Aromatic Amine Dehydrogenase

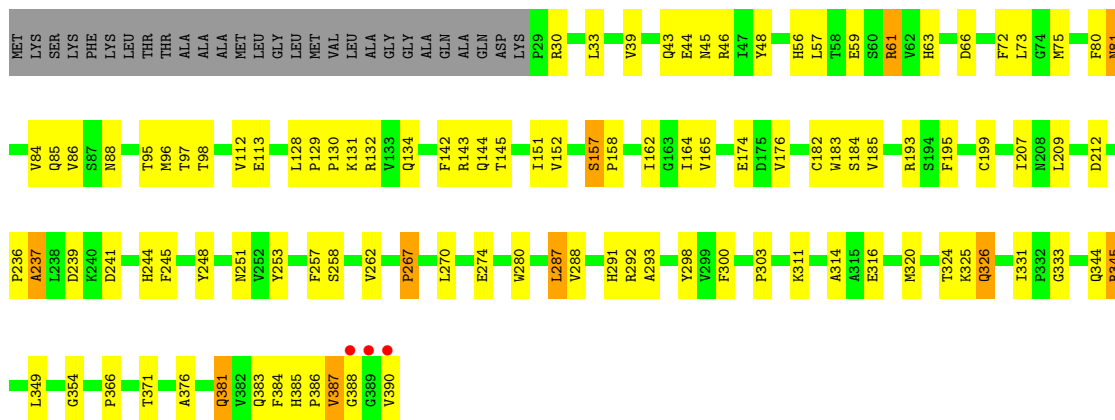


• Molecule 1: Aromatic Amine Dehydrogenase

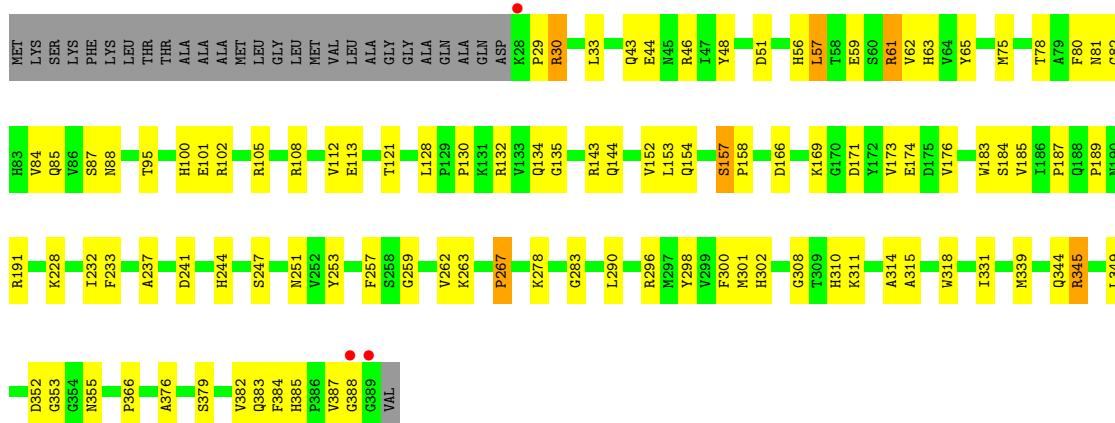


• Molecule 1: Aromatic Amine Dehydrogenase

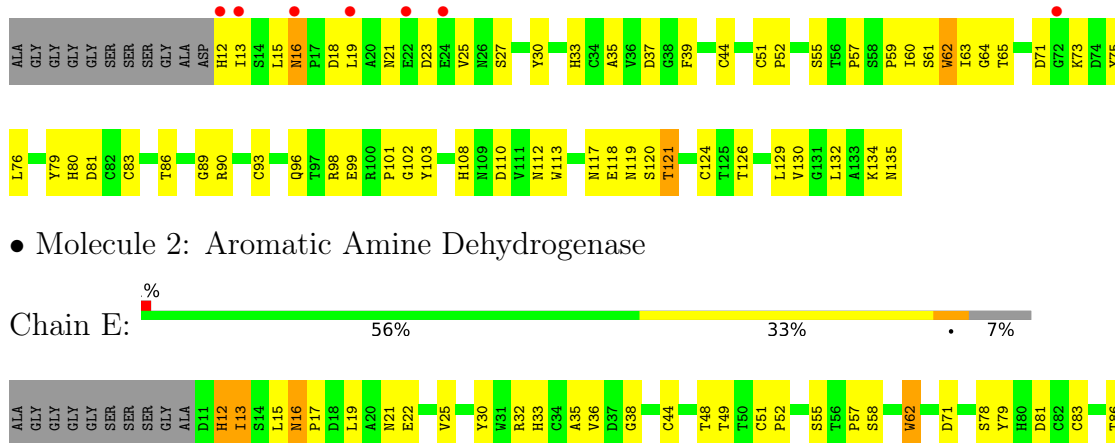




- Molecule 1: Aromatic Amine Dehydrogenase



- Molecule 2: Aromatic Amine Dehydrogenase

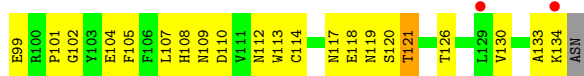


- Molecule 2: Aromatic Amine Dehydrogenase





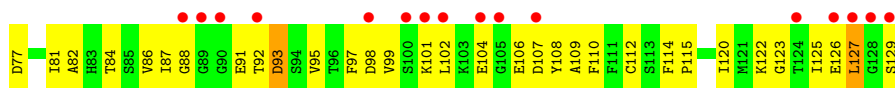
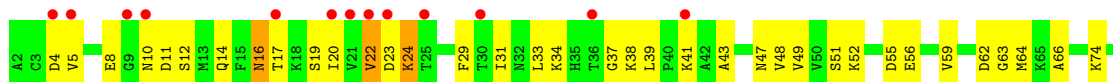
- Molecule 2: Aromatic Amine Dehydrogenase



- Molecule 2: Aromatic Amine Dehydrogenase



- Molecule 3: Azurin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.50Å 124.61Å 189.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.01 – 2.60 34.01 – 2.40	Depositor EDS
% Data completeness (in resolution range)	69.5 (34.01-2.60) 60.5 (34.01-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 2.39Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.188 , 0.249 0.180 , 0.242	Depositor DCC
R_{free} test set	5582 reflections (10.15%)	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtrriage
Anisotropy	0.580	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16799	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.94 % 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 1.2289e-04. 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, 0.333 respectively for untwinned datasets, and 0.375, 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: CU, TRQ

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	0.35	0/2879	0.66	0/3902
1	D	0.35	0/2878	0.67	1/3900 (0.0%)
1	F	0.35	0/2886	0.68	1/3910 (0.0%)
1	H	0.35	0/2887	0.66	0/3912
2	B	0.35	0/960	0.69	0/1306
2	E	0.36	0/968	0.69	0/1317
2	G	0.36	0/968	0.70	0/1318
2	I	0.35	0/959	0.70	0/1306
3	C	0.35	0/973	0.75	1/1307 (0.1%)
All	All	0.35	0/16358	0.68	3/22178 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	127	LEU	CA-CB-CG	10.75	140.03	115.30
1	F	237	ALA	N-CA-C	-5.32	96.64	111.00
1	D	237	ALA	N-CA-C	-5.17	97.05	111.00

There are no chirality outliers.

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	2814	0	2761	73	0
1	D	2813	0	2755	87	0
1	F	2821	0	2764	87	0
1	H	2822	0	2767	84	0
2	B	952	0	839	61	0
2	E	960	0	843	50	0
2	G	960	0	845	54	0
2	I	951	0	837	60	0
3	C	958	0	932	77	0
4	C	1	0	0	0	0
5	A	166	0	0	3	0
5	B	34	0	0	5	0
5	C	31	0	0	3	0
5	D	133	0	0	3	0
5	E	51	0	0	1	0
5	F	109	0	0	3	0
5	G	40	0	0	2	0
5	H	146	0	0	6	0
5	I	37	0	0	1	0
All	All	16799	0	15343	567	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 18.

The worst 5 of 567 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)
3:C:81:ILE:HG23	3:C:101:LYS:HD2	1.23	1.11
2:I:62:TRQ:HB2	2:I:113:TRP:NE1	1.70	1.05
2:B:62:TRQ:HB2	2:B:113:TRP:NE1	1.72	1.03
2:E:62:TRQ:HB2	2:E:113:TRP:NE1	1.73	1.03
2:G:62:TRQ:HB2	2:G:113:TRP:NE1	1.73	1.03

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	358/390 (92%)	328 (92%)	27 (8%)	3 (1%)	19	39
1	D	359/390 (92%)	325 (90%)	32 (9%)	2 (1%)	25	47
1	F	360/390 (92%)	324 (90%)	30 (8%)	6 (2%)	9	18
1	H	360/390 (92%)	317 (88%)	35 (10%)	8 (2%)	6	12
2	B	121/135 (90%)	108 (89%)	13 (11%)	0	100	100
2	E	122/135 (90%)	108 (88%)	12 (10%)	2 (2%)	9	19
2	G	123/135 (91%)	108 (88%)	11 (9%)	4 (3%)	4	6
2	I	121/135 (90%)	105 (87%)	12 (10%)	4 (3%)	4	6
3	C	126/128 (98%)	115 (91%)	9 (7%)	2 (2%)	9	19
All	All	2050/2228 (92%)	1838 (90%)	181 (9%)	31 (2%)	10	21

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	11	ASP
2	I	13	ILE
1	A	57	LEU
3	C	115	PRO
1	H	176	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	306/325 (94%)	300 (98%)	6 (2%)	55	78
1	D	305/325 (94%)	299 (98%)	6 (2%)	55	78
1	F	306/325 (94%)	296 (97%)	10 (3%)	38	64
1	H	306/325 (94%)	298 (97%)	8 (3%)	46	72
2	B	108/112 (96%)	103 (95%)	5 (5%)	27	51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	E	109/112 (97%)	104 (95%)	5 (5%)	27 51
2	G	108/112 (96%)	98 (91%)	10 (9%)	9 17
2	I	108/112 (96%)	103 (95%)	5 (5%)	27 51
3	C	106/106 (100%)	97 (92%)	9 (8%)	10 21
All	All	1762/1854 (95%)	1698 (96%)	64 (4%)	35 61

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	344	GLN
2	I	18	ASP
1	D	345	ARG
1	D	287	LEU
2	I	22	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	385	HIS
1	H	188	GLN
2	G	92	GLN
1	H	81	ASN
1	H	381	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](#)

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	TRQ	I	62	2	13,17,18	4.67	3 (23%)	14,24,26	2.52	5 (35%)
2	TRQ	E	62	2	13,17,18	4.75	3 (23%)	14,24,26	2.20	5 (35%)
2	TRQ	G	62	2	13,17,18	4.79	3 (23%)	14,24,26	4.83	6 (42%)
2	TRQ	B	62	2	13,17,18	4.65	3 (23%)	14,24,26	3.53	6 (42%)

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	TRQ	I	62	2	-	0/4/19/21	0/2/2/2
2	TRQ	E	62	2	-	1/4/19/21	0/2/2/2
2	TRQ	G	62	2	-	1/4/19/21	0/2/2/2
2	TRQ	B	62	2	-	0/4/19/21	0/2/2/2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	62	TRQ	CH2-CZ2	-15.03	1.37	1.54
2	E	62	TRQ	CH2-CZ2	-14.90	1.37	1.54
2	I	62	TRQ	CH2-CZ2	-14.64	1.37	1.54
2	B	62	TRQ	CH2-CZ2	-14.51	1.37	1.54
2	G	62	TRQ	CE2-CZ2	-7.54	1.40	1.50

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	62	TRQ	O6-CH2-CZ2	-14.75	108.48	118.51
2	B	62	TRQ	O6-CH2-CZ2	-10.18	111.59	118.51
2	I	62	TRQ	O6-CH2-CZ2	-5.80	114.57	118.51
2	G	62	TRQ	CZ2-CE2-NE1	5.59	128.86	119.94
2	I	62	TRQ	CZ2-CE2-NE1	5.58	128.86	119.94

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	62	TRQ	O-C-CA-CB
2	G	62	TRQ	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	62	TRQ	5	0
2	E	62	TRQ	5	0
2	G	62	TRQ	5	0
2	B	62	TRQ	5	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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	A	360/390 (92%)	-0.81	0 100 100	7, 20, 36, 57	0
1	D	361/390 (92%)	-0.69	2 (0%) 89 88	7, 20, 37, 75	0
1	F	362/390 (92%)	-0.64	3 (0%) 86 84	8, 22, 41, 84	0
1	H	362/390 (92%)	-0.75	3 (0%) 86 84	9, 22, 39, 85	0
2	B	123/135 (91%)	-0.15	7 (5%) 23 18	16, 25, 74, 87	0
2	E	124/135 (91%)	-0.46	1 (0%) 86 84	9, 23, 67, 83	0
2	G	125/135 (92%)	-0.12	10 (8%) 12 9	13, 25, 78, 99	0
2	I	123/135 (91%)	-0.19	6 (4%) 29 23	13, 25, 72, 91	0
3	C	128/128 (100%)	1.14	29 (22%) 0 0	40, 66, 92, 96	0
All	All	2068/2228 (92%)	-0.49	61 (2%) 51 45	7, 22, 68, 99	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	9	GLY	6.8
2	G	10	ALA	6.6
3	C	22	VAL	6.5
2	I	12	HIS	5.5
2	B	13	ILE	5.1

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. 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
2	TRQ	I	62	16/17	0.96	0.11	20,26,28,28	0
2	TRQ	E	62	16/17	0.97	0.13	17,19,22,23	0
2	TRQ	G	62	16/17	0.97	0.13	15,21,26,30	0
2	TRQ	B	62	16/17	0.97	0.13	16,20,25,26	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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	CU	C	130	1/1	0.98	0.03	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.