Full wwPDB X-ray Structure Validation Report (i)

Feb 17, 2024 – 10:15 AM EST

PDB ID	:	3T3T
Title	:	1.38 A structure of human frataxin variant Q148G
Authors	:	Bridwell-Rabb, J.; Winn, A.M.; Barondeau, D.P.
Deposited on	:	2011-07-25
Resolution	:	1.38 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (i) 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 (1)) were used in the production of this report:

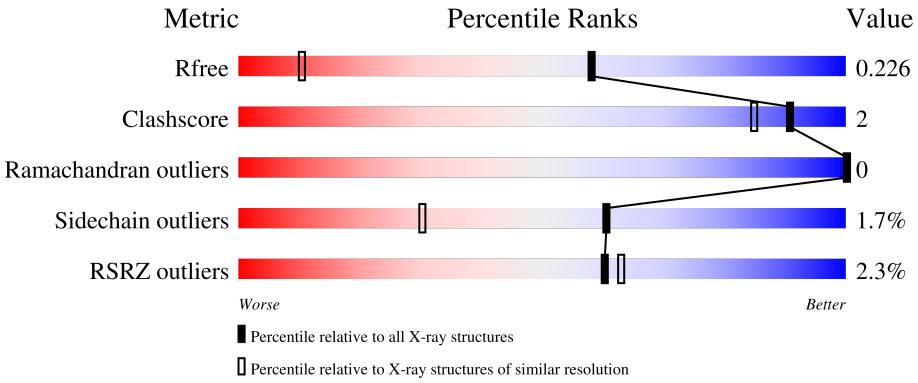
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.38 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	2907 (1.40-1.36)
Clashscore	141614	3037 (1.40-1.36)
Ramachandran outliers	138981	2970 (1.40-1.36)
Sidechain outliers	138945	2969 (1.40-1.36)
RSRZ outliers	127900	2846 (1.40-1.36)

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 <=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	129	2% 78% 13% 7%
1	B	129	2% 79% 13% 7%
1	C	129	2% 83% 10% 7%
1	D	129	2% 76% 16% 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4149 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.

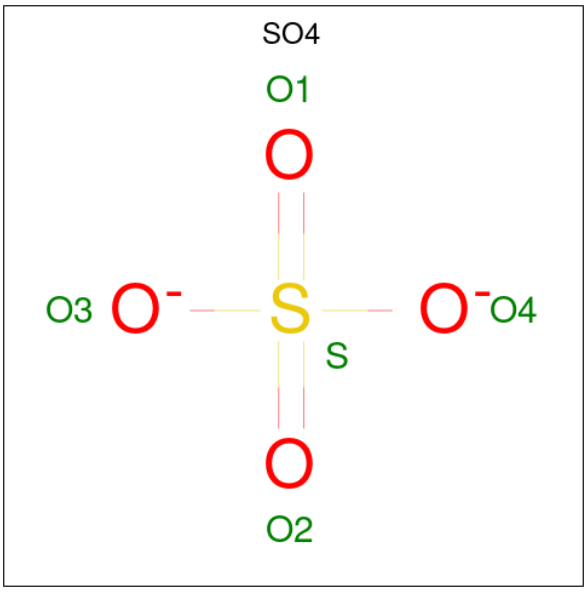
- Molecule 1 is a protein called Frataxin, mitochondrial.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	120	Total 952	C 608	N 150	O 194	0	3	0
1	B	120	Total 947	C 605	N 148	O 194	0	3	0
1	C	120	Total 948	C 606	N 150	O 192	0	1	0
1	D	120	Total 941	C 602	N 147	O 192	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	148	GLY	GLN	engineered mutation	UNP Q16595
B	148	GLY	GLN	engineered mutation	UNP Q16595
C	148	GLY	GLN	engineered mutation	UNP Q16595
D	148	GLY	GLN	engineered mutation	UNP Q16595

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

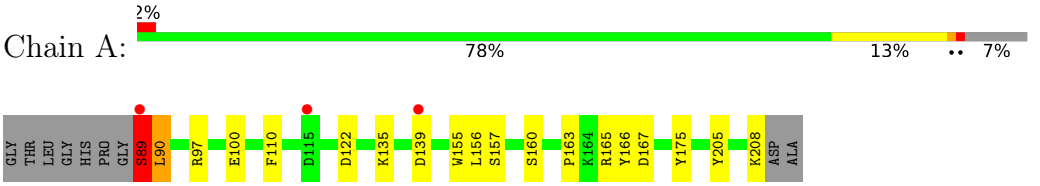
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	95	Total O 95 95	0	0
3	B	65	Total O 65 65	0	0
3	C	87	Total O 87 87	0	0
3	D	94	Total O 94 94	0	0

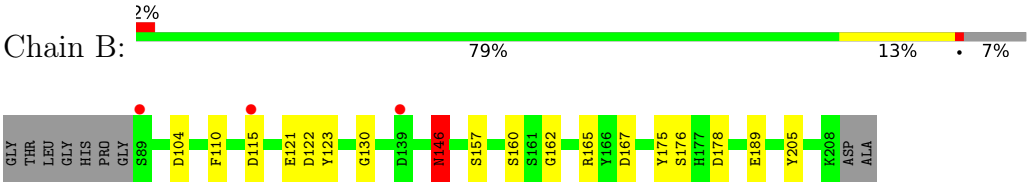
3 Residue-property plots (i)

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.

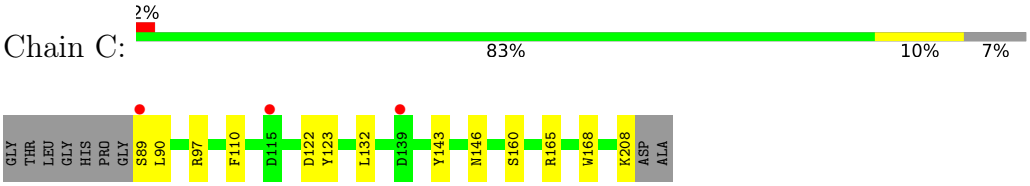
• Molecule 1: Frataxin, mitochondrial



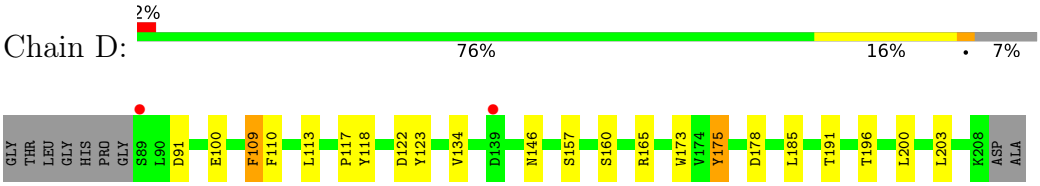
• Molecule 1: Frataxin, mitochondrial



• Molecule 1: Frataxin, mitochondrial



• Molecule 1: Frataxin, mitochondrial



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	46.41Å 68.56Å 89.97Å 90.00° 93.23° 90.00°	Depositor
Resolution (Å)	26.19 – 1.38 25.82 – 1.38	Depositor EDS
% Data completeness (in resolution range)	96.7 (26.19-1.38) 96.4 (25.82-1.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 1.38Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.198 , 0.227 0.197 , 0.226	Depositor DCC
R_{free} test set	5578 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	13.0	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.45 , 46.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4149	wwPDB-VP
Average B, all atoms (Å^2)	15.0	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 54.17 % 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 3.7928e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	A	1.60	8/986 (0.8%)	1.33	6/1337 (0.4%)
1	B	1.61	16/977 (1.6%)	1.44	9/1326 (0.7%)
1	C	1.45	4/974 (0.4%)	1.33	7/1321 (0.5%)
1	D	1.59	12/963 (1.2%)	1.55	13/1307 (1.0%)
All	All	1.56	40/3900 (1.0%)	1.41	35/5291 (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	0	1
1	B	0	2
All	All	0	3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	146[A]	ASN	CB-CG	9.45	1.72	1.51
1	B	146[B]	ASN	CB-CG	9.45	1.72	1.51
1	D	157	SER	CA-CB	8.99	1.66	1.52
1	C	160	SER	CB-OG	-8.87	1.30	1.42
1	A	157	SER	CA-CB	8.70	1.66	1.52
1	A	160	SER	CB-OG	-8.65	1.30	1.42
1	D	165[A]	ARG	CD-NE	-8.21	1.32	1.46
1	A	110	PHE	CE2-CZ	7.22	1.51	1.37
1	D	123	TYR	CE1-CZ	-7.21	1.29	1.38
1	B	146[A]	ASN	CG-OD1	7.12	1.39	1.24
1	B	146[B]	ASN	CG-OD1	7.12	1.39	1.24
1	D	165[A]	ARG	CZ-NH2	-6.93	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	165[A]	ARG	CZ-NH1	6.84	1.42	1.33
1	B	175	TYR	CD2-CE2	6.69	1.49	1.39
1	D	173	TRP	CG-CD1	6.31	1.45	1.36
1	D	109	PHE	CD2-CE2	6.22	1.51	1.39
1	B	205	TYR	CD1-CE1	6.08	1.48	1.39
1	D	134	VAL	CB-CG1	5.93	1.65	1.52
1	A	205	TYR	CE2-CZ	-5.69	1.31	1.38
1	C	168	TRP	CD2-CE2	5.69	1.48	1.41
1	B	110	PHE	CE2-CZ	5.57	1.48	1.37
1	A	175	TYR	CD1-CE1	5.55	1.47	1.39
1	D	175	TYR	CG-CD1	5.54	1.46	1.39
1	A	175	TYR	CE2-CZ	-5.53	1.31	1.38
1	D	100	GLU	CG-CD	5.50	1.60	1.51
1	A	100	GLU	CB-CG	5.50	1.62	1.52
1	B	121	GLU	CG-CD	5.50	1.60	1.51
1	B	123	TYR	CD1-CE1	5.47	1.47	1.39
1	B	157[A]	SER	CB-OG	-5.44	1.35	1.42
1	B	157[B]	SER	CB-OG	-5.44	1.35	1.42
1	B	176	SER	CB-OG	-5.42	1.35	1.42
1	C	143	TYR	CD1-CE1	5.29	1.47	1.39
1	B	146[A]	ASN	CA-CB	5.28	1.66	1.53
1	B	146[B]	ASN	CA-CB	5.28	1.66	1.53
1	D	160	SER	CB-OG	-5.27	1.35	1.42
1	B	160	SER	CA-CB	5.25	1.60	1.52
1	A	208	LYS	C-O	5.19	1.33	1.23
1	C	110	PHE	CE2-CZ	5.11	1.47	1.37
1	D	118	TYR	CD1-CE1	5.08	1.47	1.39
1	B	165[B]	ARG	CD-NE	-5.00	1.38	1.46

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	165[A]	ARG	NE-CZ-NH2	-19.34	110.63	120.30
1	D	165[A]	ARG	NE-CZ-NH1	15.78	128.19	120.30
1	B	146[A]	ASN	N-CA-CB	9.63	127.94	110.60
1	B	146[B]	ASN	N-CA-CB	9.63	127.94	110.60
1	B	175	TYR	CB-CG-CD2	-8.62	115.83	121.00
1	B	178	ASP	CB-CG-OD1	8.26	125.73	118.30
1	A	167	ASP	CB-CG-OD1	-7.90	111.19	118.30
1	C	97	ARG	NE-CZ-NH1	-7.80	116.40	120.30
1	C	165[A]	ARG	NE-CZ-NH1	-7.80	116.40	120.30
1	C	165[B]	ARG	NE-CZ-NH1	-7.80	116.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	178	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	A	122	ASP	CB-CG-OD1	6.85	124.47	118.30
1	D	185	LEU	CB-CG-CD2	6.36	121.81	111.00
1	B	115	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	C	123	TYR	CB-CG-CD1	-6.04	117.38	121.00
1	B	189	GLU	OE1-CD-OE2	5.98	130.48	123.30
1	A	135	LYS	CD-CE-NZ	-5.96	97.98	111.70
1	D	113	LEU	CB-CG-CD1	-5.93	100.91	111.00
1	D	122	ASP	CB-CG-OD1	5.86	123.57	118.30
1	D	118	TYR	CB-CG-CD2	-5.74	117.55	121.00
1	D	110	PHE	CB-CG-CD1	5.70	124.79	120.80
1	D	91	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	A	90	LEU	CB-CG-CD2	-5.48	101.68	111.00
1	B	104	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	122	ASP	CB-CG-OD1	5.36	123.13	118.30
1	B	167	ASP	CB-CG-OD1	-5.33	113.50	118.30
1	A	166	TYR	CG-CD1-CE1	-5.33	117.04	121.30
1	D	165[A]	ARG	CG-CD-NE	5.32	122.98	111.80
1	D	178	ASP	CB-CG-OD1	5.28	123.05	118.30
1	C	132	LEU	CB-CG-CD2	-5.27	102.04	111.00
1	D	165[A]	ARG	CB-CG-CD	-5.26	97.91	111.60
1	A	97	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	C	208	LYS	CB-CA-C	-5.12	100.17	110.40
1	C	122	ASP	CB-CG-OD1	5.10	122.89	118.30
1	D	117	PRO	N-CD-CG	-5.05	95.63	103.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	89	SER	Peptide
1	B	146[A]	ASN	Sidechain
1	B	146[B]	ASN	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	952	0	920	4	0
1	B	947	0	910	2	0
1	C	948	0	918	0	0
1	D	941	0	907	8	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	95	0	0	1	3
3	B	65	0	0	0	1
3	C	87	0	0	0	1
3	D	94	0	0	1	5
All	All	4149	0	3655	13	6

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 2.

All (13) 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:D:200:LEU:HD12	1:D:203:LEU:CD1	2.16	0.75
1:D:200:LEU:HD12	1:D:203:LEU:HD11	1.71	0.71
1:D:109:PHE:CE2	1:D:200:LEU:HD11	2.39	0.57
1:D:109:PHE:CZ	1:D:200:LEU:HD11	2.40	0.55
1:A:165[A]:ARG:NH2	3:A:438:HOH:O	2.42	0.52
1:B:130:GLY:O	1:B:146[A]:ASN:HB2	2.11	0.50
1:D:200:LEU:HD12	1:D:203:LEU:HD12	1.93	0.50
1:D:175:TYR:HE1	3:D:531:HOH:O	1.95	0.49
1:D:191:THR:HA	1:D:196:THR:O	2.21	0.40
1:A:89:SER:CB	1:A:90:LEU:C	2.90	0.40
1:D:196:THR:O	1:D:196:THR:HG23	2.21	0.40
1:A:155:TRP:CH2	1:B:162:GLY:HA2	2.56	0.40
1:A:156:LEU:O	1:A:163:PRO:HA	2.21	0.40

All (6) 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:C:303:HOH:O	3:D:337:HOH:O[2_656]	1.19	1.01
3:A:444:HOH:O	3:D:493:HOH:O[2_646]	1.30	0.90
3:D:499:HOH:O	3:D:531:HOH:O[2_656]	1.88	0.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:435:HOH:O	3:B:469:HOH:O[2_645]	1.95	0.25
3:D:497:HOH:O	3:D:532:HOH:O[2_656]	2.10	0.10
3:A:444:HOH:O	3:D:492:HOH:O[2_646]	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	
1	A	121/129 (94%)	119 (98%)	2 (2%)	0	100	100
1	B	120/129 (93%)	116 (97%)	4 (3%)	0	100	100
1	C	119/129 (92%)	118 (99%)	1 (1%)	0	100	100
1	D	118/129 (92%)	115 (98%)	3 (2%)	0	100	100
All	All	478/516 (93%)	468 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	106/108 (98%)	104 (98%)	2 (2%)	57	24
1	B	105/108 (97%)	103 (98%)	2 (2%)	57	24
1	C	104/108 (96%)	101 (97%)	3 (3%)	42	11
1	D	103/108 (95%)	102 (99%)	1 (1%)	76	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	418/432 (97%)	410 (98%)	8 (2%)	60 24

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	SER
1	A	139	ASP
1	B	146[A]	ASN
1	B	146[B]	ASN
1	C	89	SER
1	C	90	LEU
1	C	146	ASN
1	D	146	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	146	ASN
1	D	146	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 monosaccharides 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	$\#\|Z\| > 2$
2	SO4	B	563	-	4,4,4	0.46	0	6,6,6	0.71	0
2	SO4	D	566	-	4,4,4	0.45	0	6,6,6	1.40	1 (16%)
2	SO4	A	564	-	4,4,4	0.80	0	6,6,6	0.78	0
2	SO4	C	565	-	4,4,4	0.93	0	6,6,6	1.40	1 (16%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	566	SO4	O4-S-O3	-2.95	96.49	109.06
2	C	565	SO4	O4-S-O1	-2.40	96.77	109.31

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, 95^{th} 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	120/129 (93%)	0.18	3 (2%)	57	60	9, 14, 25, 41	0
1	B	120/129 (93%)	0.04	3 (2%)	57	60	8, 13, 23, 40	0
1	C	120/129 (93%)	0.11	3 (2%)	57	60	8, 13, 27, 42	0
1	D	120/129 (93%)	0.02	2 (1%)	70	72	8, 12, 22, 37	0
All	All	480/516 (93%)	0.09	11 (2%)	60	63	8, 13, 25, 42	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	89	SER	6.5
1	B	89	SER	6.4
1	D	89	SER	6.1
1	C	139	ASP	4.9
1	A	139	ASP	4.3
1	C	89	SER	3.5
1	C	115	ASP	3.2
1	D	139	ASP	3.2
1	B	139	ASP	3.1
1	A	115	ASP	2.3
1	B	115	ASP	2.3

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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, 95^{th} 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(Å^2)	Q<0.9
2	SO4	A	564	5/5	0.80	0.31	27,28,34,36	0
2	SO4	C	565	5/5	0.82	0.25	26,29,37,40	0
2	SO4	B	563	5/5	0.91	0.19	21,26,29,32	0
2	SO4	D	566	5/5	0.91	0.20	21,23,27,33	0

6.5 Other polymers

There are no such residues in this entry.