Full wwPDB X-ray Structure Validation Report (i)

Feb 28, 2024 – 06:25 AM EST

PDB ID	:	5QTM
Title	:	PanDDA analysis group deposition – Crystal Structure of NUDT5 in complex with FS-2639
Authors	:	Dubianok, Y.; Krojer, T.; Kovacs, H.; Moriaud, F.; Wright, N.; Strain-Damerell, C.; Burgess-Brown, N.; Bountra, C.; Arrowsmith, C.H.; Edwards, A.; von Delft, F.
Deposited on	:	2019-08-14
Resolution	:	1.79 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 (i)) were used in the production of this report:

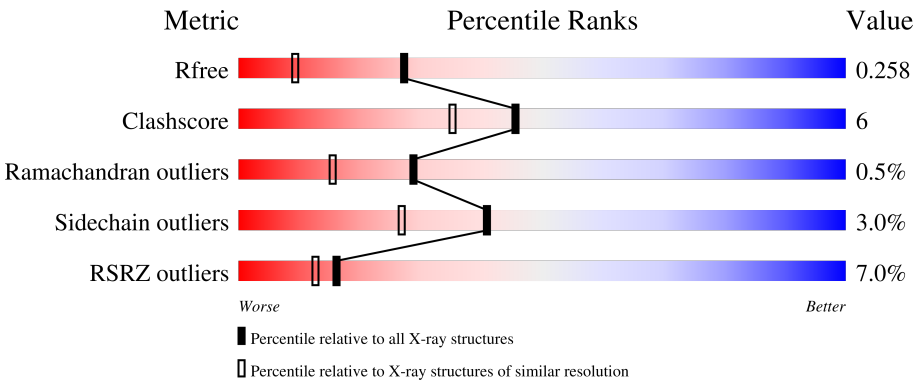
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.79 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	209	6%, 82%, 9%, •, 7%
1	B	209	6%, 79%, 13%, 7%
1	C	209	5%, 79%, 12%, •, 8%
1	D	209	9%, 77%, 15%, •, 7%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6182 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 ADP-sugar pyrophosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	194	1466	927	245	286	8	0	0	0
1	B	194	1468	926	245	289	8	0	0	0
1	C	192	1436	906	240	282	8	0	0	0
1	D	194	1448	915	242	283	8	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q9UKK9
B	0	SER	-	expression tag	UNP Q9UKK9
C	0	SER	-	expression tag	UNP Q9UKK9
D	0	SER	-	expression tag	UNP Q9UKK9

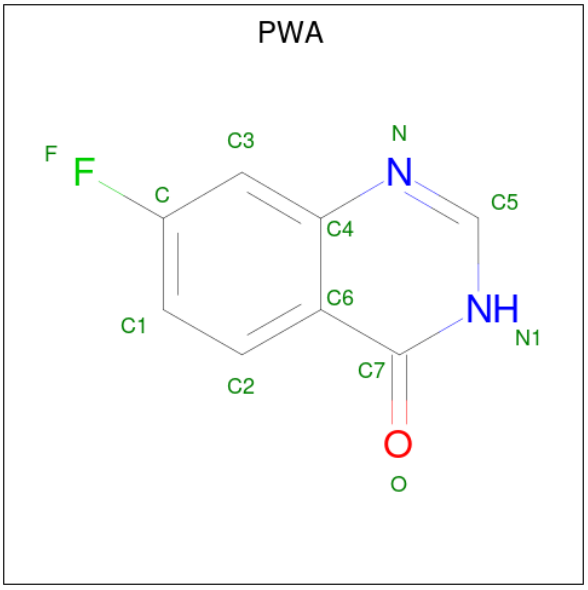
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	2	2	2	0	0
2	B	2	2	2	0	0
2	C	2	2	2	0	0
2	D	2	2	2	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

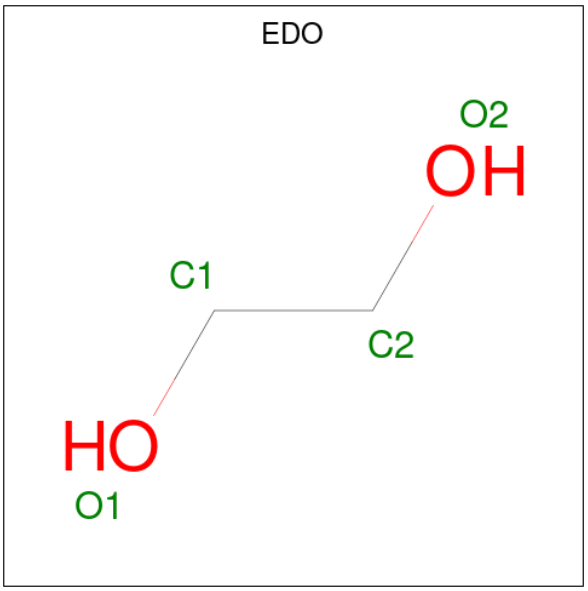
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
3	A	1	1	1	0	0

- Molecule 4 is 7-fluoroquinazolin-4(3H)-one (three-letter code: PWA) (formula: $C_8H_5FN_2O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
4	A	1	12	8	1	2	1	0	0
			Total	C	F	N	O		
4	B	1	12	8	1	2	1	0	0
			Total	C	F	N	O		
4	D	1	12	8	1	2	1	0	0
			Total	C	F	N	O		
4	D	1	12	8	1	2	1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 6 is water.

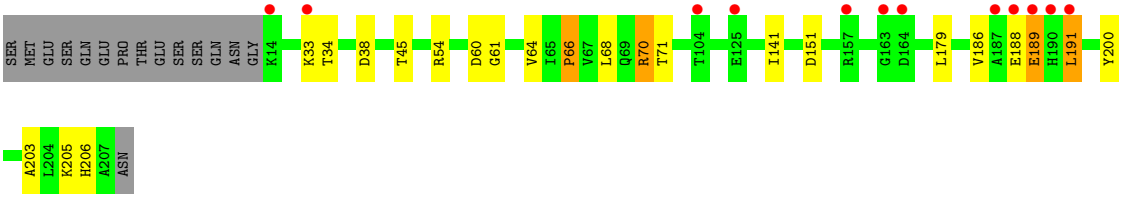
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	77	77	77	0	0
6	B	79	79	79	0	0
6	C	74	74	74	0	0
6	D	45	45	45	0	0

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.

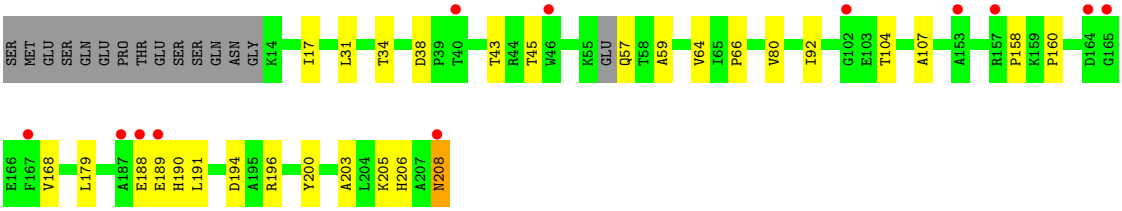
• Molecule 1: ADP-sugar pyrophosphatase

Chain A:



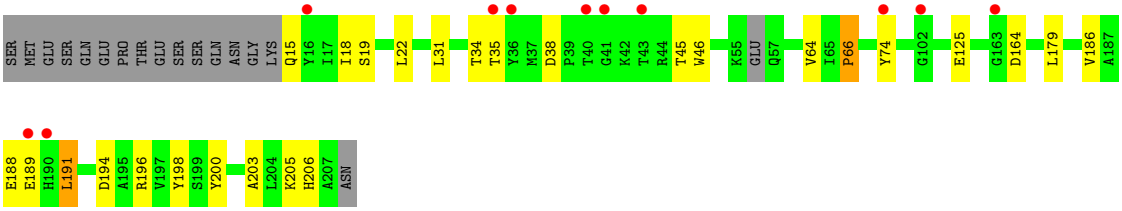
• Molecule 1: ADP-sugar pyrophosphatase

Chain B:



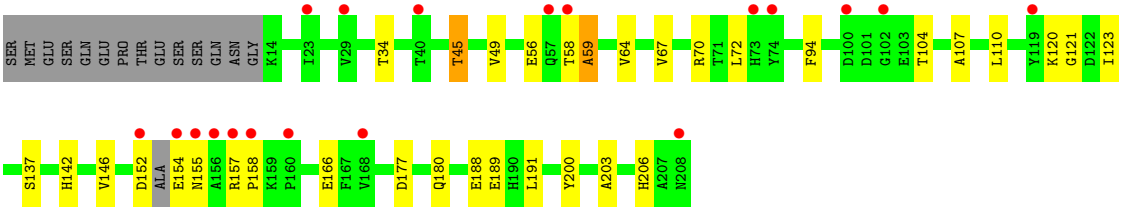
• Molecule 1: ADP-sugar pyrophosphatase

Chain C:



• Molecule 1: ADP-sugar pyrophosphatase

Chain D:


SER
MET
GLU
SER
GLN
GLU
PRO
THR
GLU
SER
SER
GLN
ASN
GLY
K14
I23
V29
T34
T40
T45
V49
E56
Q57
T58
A59
V64
V67
R70
T71
L72
H73
Y74
F94
D100
D101
G102
E103
T104
A107
L110
Y119
K120
G121
D122
I123
S137
H142
V146
D152
ALA
E154
N155
A156
R157
P158
K159
P160
E166
F167
V168
D177
Q180
E188
E189
H190
L191
Y200
A203
H206
A207
N208

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	49.27Å 59.81Å 80.07Å 79.33° 81.48° 75.66°	Depositor
Resolution (Å)	47.50 – 1.79 47.46 – 1.79	Depositor EDS
% Data completeness (in resolution range)	96.2 (47.50-1.79) 96.3 (47.46-1.79)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.214 , 0.247 0.229 , 0.258	Depositor DCC
R_{free} test set	3972 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	26.8	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 40.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6182	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, PWA, MG, CL

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	0.72	0/1494	0.82	1/2037 (0.0%)
1	B	0.69	0/1496	0.82	0/2040
1	C	0.69	0/1463	0.82	0/1998
1	D	0.71	0/1476	0.83	0/2017
All	All	0.70	0/5929	0.82	1/8092 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	70	ARG	NE-CZ-NH2	-5.17	117.72	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1466	0	1437	17	0
1	B	1468	0	1420	22	0
1	C	1436	0	1374	20	0
1	D	1448	0	1386	25	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	1	0	0	0	0
4	A	12	0	0	0	0
4	B	12	0	0	0	0
4	D	24	0	0	0	0
5	A	4	0	6	0	0
5	B	8	0	12	1	0
5	C	16	0	24	0	0
5	D	4	0	6	1	0
6	A	77	0	0	0	0
6	B	79	0	0	1	0
6	C	74	0	0	4	0
6	D	45	0	0	0	0
All	All	6182	0	5665	74	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 6.

All (74) 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:A:191:LEU:O	1:A:191:LEU:HD23	1.43	1.18
1:B:92:ILE:HD11	1:B:191:LEU:HD13	1.53	0.90
1:A:191:LEU:HD23	1:A:191:LEU:C	1.98	0.84
1:C:206:HIS:HD2	1:D:200:TYR:OH	1.65	0.77
1:A:71:THR:HG23	1:A:151:ASP:OD2	1.86	0.76
1:B:104:THR:HG23	1:B:107:ALA:H	1.50	0.75
1:A:203:ALA:HB3	1:B:203:ALA:HB3	1.72	0.72
5:B:301:EDO:H21	6:B:454:HOH:O	1.89	0.71
1:C:15:GLN:N	6:C:402:HOH:O	2.23	0.70
1:C:203:ALA:HB3	1:D:203:ALA:HB3	1.71	0.70
1:B:188:GLU:HG2	1:B:189:GLU:HG3	1.73	0.70
1:C:125:GLU:OE1	6:C:401:HOH:O	2.13	0.67
1:D:188:GLU:HG3	1:D:189:GLU:HG3	1.77	0.67
1:D:120:LYS:H	1:D:155:ASN:HD21	1.42	0.66
1:A:188:GLU:C	1:A:189:GLU:HG3	2.19	0.64
1:D:58:THR:HG23	1:D:142:HIS:NE2	2.13	0.64
1:D:104:THR:HG23	1:D:107:ALA:H	1.62	0.64
1:A:206:HIS:HD2	1:B:200:TYR:OH	1.81	0.63
1:D:58:THR:HG23	1:D:58:THR:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:HIS:CD2	1:D:200:TYR:OH	2.52	0.59
1:B:179:LEU:HD23	1:B:205:LYS:HE2	1.85	0.59
1:B:208:ASN:HD22	1:B:208:ASN:H	1.53	0.55
1:B:158:PRO:O	1:B:160:PRO:HD3	2.07	0.54
1:C:200:TYR:OH	1:D:206:HIS:HD2	1.89	0.54
1:B:194:ASP:OD2	1:B:196:ARG:NH2	2.34	0.54
1:A:179:LEU:HD23	1:A:205:LYS:HD2	1.90	0.53
1:C:179:LEU:HD11	1:C:198:TYR:CZ	2.43	0.53
1:B:179:LEU:CD2	1:B:205:LYS:HE2	2.39	0.53
6:C:401:HOH:O	1:D:206:HIS:HE1	1.91	0.52
1:C:74:TYR:HB3	6:C:441:HOH:O	2.10	0.52
1:A:68:LEU:HG	1:A:70:ARG:HD2	1.92	0.51
1:C:191:LEU:HD12	1:C:191:LEU:O	2.11	0.50
1:D:121:GLY:HA3	1:D:146:VAL:CG1	2.41	0.50
1:A:191:LEU:C	1:A:191:LEU:CD2	2.73	0.50
1:A:54:ARG:HD3	1:A:60:ASP:OD1	2.12	0.49
1:C:22:LEU:C	1:C:22:LEU:HD13	2.33	0.49
1:C:19:SER:OG	1:C:35:THR:HG22	2.13	0.48
1:C:194:ASP:OD2	1:C:196:ARG:NH2	2.46	0.48
1:D:64:VAL:O	1:D:94:PHE:HB3	2.14	0.47
1:D:49:VAL:O	1:D:137:SER:HA	2.14	0.47
1:A:200:TYR:OH	1:B:206:HIS:HD2	1.96	0.47
1:C:188:GLU:C	1:C:189:GLU:HG3	2.34	0.47
1:B:104:THR:HG22	1:B:107:ALA:CB	2.44	0.47
1:D:152:ASP:O	1:D:155:ASN:N	2.48	0.47
1:A:186:VAL:HA	1:A:191:LEU:CD2	2.44	0.47
1:D:58:THR:O	1:D:58:THR:CG2	2.63	0.46
1:C:203:ALA:HB2	1:D:200:TYR:CD1	2.51	0.46
1:C:179:LEU:HD23	1:C:205:LYS:HD2	1.97	0.46
1:D:191:LEU:C	1:D:191:LEU:HD12	2.37	0.45
1:D:67:VAL:HG21	5:D:502:EDO:H22	1.99	0.45
1:C:186:VAL:HA	1:C:191:LEU:HD11	1.99	0.44
1:A:64:VAL:O	1:A:66:PRO:HD3	2.18	0.43
1:B:34:THR:O	1:B:45:THR:HA	2.18	0.43
1:C:200:TYR:CD1	1:D:203:ALA:HB2	2.54	0.43
1:B:64:VAL:O	1:B:66:PRO:HD3	2.19	0.43
1:D:34:THR:O	1:D:45:THR:HA	2.19	0.42
1:A:200:TYR:CD1	1:B:203:ALA:HB2	2.55	0.42
1:B:104:THR:HG22	1:B:107:ALA:HB3	2.02	0.42
1:B:208:ASN:HD22	1:B:208:ASN:N	2.16	0.42
1:D:58:THR:O	1:D:59:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:ILE:HD12	1:B:34:THR:CG2	2.51	0.41
1:C:34:THR:OG1	1:C:46:TRP:HB3	2.20	0.41
1:C:64:VAL:O	1:C:66:PRO:HD3	2.20	0.41
1:A:61:GLY:O	1:A:141:ILE:HA	2.20	0.41
1:D:58:THR:O	1:D:142:HIS:NE2	2.54	0.41
1:D:157:ARG:N	1:D:158:PRO:CD	2.84	0.41
1:A:206:HIS:CD2	1:B:200:TYR:OH	2.69	0.41
1:B:80:VAL:HB	1:B:168:VAL:CG1	2.50	0.41
1:B:190:HIS:O	1:B:190:HIS:CG	2.73	0.41
1:D:110:LEU:HG	1:D:123:ILE:HD11	2.01	0.41
1:D:177:ASP:OD1	1:D:180:GLN:CB	2.69	0.41
1:B:57:GLN:HB3	1:B:59:ALA:O	2.20	0.40
1:C:18:ILE:HB	1:C:35:THR:HG23	2.04	0.40
1:A:34:THR:O	1:A:45:THR:HA	2.21	0.40

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	192/209 (92%)	186 (97%)	5 (3%)	1 (0%)	29 15
1	B	190/209 (91%)	184 (97%)	6 (3%)	0	100 100
1	C	188/209 (90%)	185 (98%)	2 (1%)	1 (0%)	29 15
1	D	190/209 (91%)	181 (95%)	7 (4%)	2 (1%)	14 4
All	All	760/836 (91%)	736 (97%)	20 (3%)	4 (0%)	29 15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	59	ALA

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Mol	Chain	Res	Type
1	D	56	GLU
1	A	66	PRO
1	C	66	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	
1	A	155/179 (87%)	151 (97%)	4 (3%)	46	32
1	B	155/179 (87%)	151 (97%)	4 (3%)	46	32
1	C	149/179 (83%)	144 (97%)	5 (3%)	37	22
1	D	150/179 (84%)	145 (97%)	5 (3%)	38	23
All	All	609/716 (85%)	591 (97%)	18 (3%)	41	27

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LYS
1	A	38	ASP
1	A	189	GLU
1	A	191	LEU
1	B	31	LEU
1	B	38	ASP
1	B	43	THR
1	B	208	ASN
1	C	31	LEU
1	C	38	ASP
1	C	45	THR
1	C	164	ASP
1	C	191	LEU
1	D	45	THR
1	D	70	ARG
1	D	72	LEU
1	D	154	GLU
1	D	166	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	HIS
1	A	180	GLN
1	A	206	HIS
1	B	15	GLN
1	B	73	HIS
1	B	206	HIS
1	B	208	ASN
1	C	206	HIS
1	D	155	ASN
1	D	206	HIS

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)

Of 21 ligands modelled in this entry, 9 are monoatomic - leaving 12 for Mogul analysis.

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	PWA	B	304	-	13,13,13	1.68	3 (23%)	15,18,18	1.00	0
5	EDO	B	305	-	3,3,3	0.10	0	2,2,2	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	EDO	B	301	-	3,3,3	0.26	0	2,2,2	0.33	0
5	EDO	C	305	-	3,3,3	0.11	0	2,2,2	0.16	0
4	PWA	D	505	-	13,13,13	1.56	2 (15%)	15,18,18	0.93	1 (6%)
5	EDO	C	301	-	3,3,3	0.12	0	2,2,2	0.08	0
4	PWA	A	304	-	13,13,13	1.85	4 (30%)	15,18,18	1.03	2 (13%)
5	EDO	A	305	-	3,3,3	0.30	0	2,2,2	0.09	0
5	EDO	C	306	-	3,3,3	0.13	0	2,2,2	0.20	0
4	PWA	D	501	-	13,13,13	1.48	2 (15%)	15,18,18	1.34	3 (20%)
5	EDO	D	502	-	3,3,3	0.19	0	2,2,2	0.05	0
5	EDO	C	304	-	3,3,3	0.09	0	2,2,2	0.13	0

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	PWA	B	304	-	-	-	0/2/2/2
5	EDO	B	305	-	-	0/1/1/1	-
5	EDO	B	301	-	-	1/1/1/1	-
5	EDO	C	305	-	-	0/1/1/1	-
5	EDO	C	301	-	-	1/1/1/1	-
4	PWA	D	505	-	-	-	0/2/2/2
4	PWA	A	304	-	-	-	0/2/2/2
5	EDO	A	305	-	-	0/1/1/1	-
5	EDO	C	306	-	-	1/1/1/1	-
4	PWA	D	501	-	-	-	0/2/2/2
5	EDO	D	502	-	-	1/1/1/1	-
5	EDO	C	304	-	-	0/1/1/1	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	304	PWA	C1-C	4.07	1.45	1.37
4	D	505	PWA	C1-C	3.65	1.44	1.37
4	D	501	PWA	C1-C	3.62	1.44	1.37
4	B	304	PWA	C1-C	3.39	1.43	1.37
4	A	304	PWA	C5-N	3.08	1.35	1.29
4	A	304	PWA	C5-N1	2.93	1.40	1.35
4	B	304	PWA	C6-C7	-2.85	1.42	1.47
4	D	501	PWA	C5-N1	2.49	1.40	1.35
4	A	304	PWA	C7-N1	2.37	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	505	PWA	C7-N1	2.31	1.42	1.38
4	B	304	PWA	C5-N1	2.25	1.39	1.35

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	501	PWA	O-C7-N1	-2.79	116.93	120.32
4	D	501	PWA	O-C7-C6	2.51	127.64	123.30
4	D	501	PWA	C1-C-C3	-2.21	120.42	123.29
4	A	304	PWA	F-C-C1	2.10	122.11	118.54
4	D	505	PWA	C6-C7-N1	2.06	116.05	114.31
4	A	304	PWA	C1-C-C3	-2.04	120.64	123.29

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	301	EDO	O1-C1-C2-O2
5	D	502	EDO	O1-C1-C2-O2
5	C	306	EDO	O1-C1-C2-O2
5	B	301	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	301	EDO	1	0
5	D	502	EDO	1	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	194/209 (92%)	0.22	12 (6%)	20	16	18, 27, 51, 61	16 (8%)
1	B	194/209 (92%)	0.25	12 (6%)	20	16	20, 31, 57, 69	11 (5%)
1	C	192/209 (91%)	0.19	11 (5%)	23	19	19, 33, 57, 66	25 (13%)
1	D	194/209 (92%)	0.47	19 (9%)	7	5	20, 36, 64, 77	20 (10%)
All	All	774/836 (92%)	0.28	54 (6%)	16	13	18, 32, 58, 77	72 (9%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	191	LEU	9.8
1	B	187	ALA	8.0
1	B	188	GLU	7.5
1	A	187	ALA	7.1
1	B	167	PHE	7.0
1	B	189	GLU	5.9
1	C	190	HIS	5.3
1	C	189	GLU	5.2
1	A	189	GLU	5.0
1	A	14	LYS	4.9
1	A	188	GLU	4.7
1	D	40	THR	4.6
1	C	40	THR	4.3
1	A	163	GLY	4.0
1	D	73	HIS	4.0
1	A	190	HIS	3.7
1	D	58	THR	3.7
1	A	125	GLU	3.5
1	D	155	ASN	3.4
1	D	158	PRO	3.3
1	D	156	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	33	LYS	3.3
1	D	74	TYR	3.2
1	A	164	ASP	3.1
1	B	46	TRP	3.1
1	D	152	ASP	3.1
1	A	104	THR	3.0
1	D	154	GLU	3.0
1	B	102	GLY	3.0
1	C	16	TYR	2.9
1	B	208	ASN	2.7
1	B	164	ASP	2.6
1	D	100	ASP	2.6
1	C	35	THR	2.6
1	B	153	ALA	2.6
1	D	157	ARG	2.5
1	D	160	PRO	2.4
1	B	165	GLY	2.4
1	D	102	GLY	2.4
1	C	74	TYR	2.4
1	C	41	GLY	2.3
1	C	43	THR	2.3
1	B	157	ARG	2.3
1	D	168	VAL	2.2
1	A	157	ARG	2.1
1	D	29	VAL	2.1
1	C	163	GLY	2.1
1	D	23	ILE	2.1
1	D	119	TYR	2.1
1	C	102	GLY	2.1
1	C	36	TYR	2.1
1	D	57	GLN	2.1
1	B	40	THR	2.0
1	D	208	ASN	2.0

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 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(Å^2)	Q<0.9
5	EDO	B	301	4/4	0.81	0.14	24,25,25,25	4
5	EDO	C	306	4/4	0.84	0.12	43,43,44,45	4
5	EDO	C	304	4/4	0.86	0.13	33,35,35,36	4
5	EDO	C	301	4/4	0.87	0.14	38,52,53,58	0
4	PWA	D	505	12/12	0.87	0.13	34,40,46,51	12
3	CL	A	303	1/1	0.87	0.08	69,69,69,69	0
4	PWA	D	501	12/12	0.88	0.11	37,38,42,42	12
5	EDO	D	502	4/4	0.90	0.20	50,53,55,56	0
5	EDO	A	305	4/4	0.91	0.10	27,28,28,30	0
4	PWA	B	304	12/12	0.91	0.12	23,26,30,33	12
2	MG	A	302	1/1	0.92	0.08	49,49,49,49	0
4	PWA	A	304	12/12	0.93	0.10	26,30,38,38	12
2	MG	C	302	1/1	0.93	0.16	64,64,64,64	0
5	EDO	C	305	4/4	0.94	0.10	26,28,29,31	4
2	MG	C	303	1/1	0.95	0.03	35,35,35,35	0
2	MG	B	302	1/1	0.97	0.04	29,29,29,29	0
2	MG	D	503	1/1	0.97	0.04	32,32,32,32	0
2	MG	D	504	1/1	0.98	0.16	42,42,42,42	0
2	MG	B	303	1/1	0.98	0.15	72,72,72,72	0
5	EDO	B	305	4/4	0.98	0.07	28,31,32,32	0
2	MG	A	301	1/1	0.98	0.07	26,26,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.