Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2024 – 09:12 PM EST

PDB ID	:	5QJ8
Title	:	PanDDA analysis group deposition of models with modelled events (e.g. bound ligands) – Crystal Structure of NUDT5 in complex with Z2856434829
Authors	:	Dubianok, Y.; Collins, P.; Krojer, T.; Wright, N.; Strain-Damerell, C.; Burgess-Brown, N.; Bountra, C.; Arrowsmith, C.H.; Edwards, A.; Huber, K.; von Delft, F.
Deposited on	:	2018-10-31
Resolution	:	1.76 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 ⓘ 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:

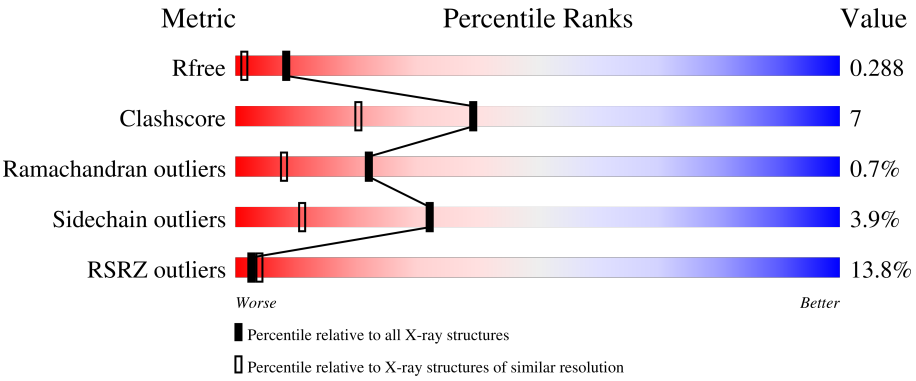
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.76 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	9% 83% 9% 7%
1	B	209	8% 79% 13% 7%
1	C	209	14% 75% 16% • 8%
1	D	209	21% 72% 19% 9%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5997 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
1	A	194	Total	C	N	O	S	0	0	0
			1462	925	244	285	8			
1	B	194	Total	C	N	O	S	0	0	0
			1464	924	244	288	8			
1	C	192	Total	C	N	O	S	0	0	0
			1402	884	234	277	7			
1	D	190	Total	C	N	O	S	0	1	0
			1404	887	235	274	8			

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

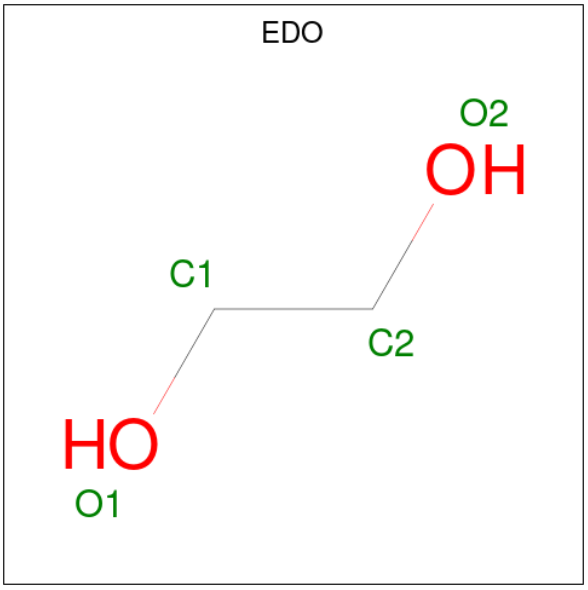
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

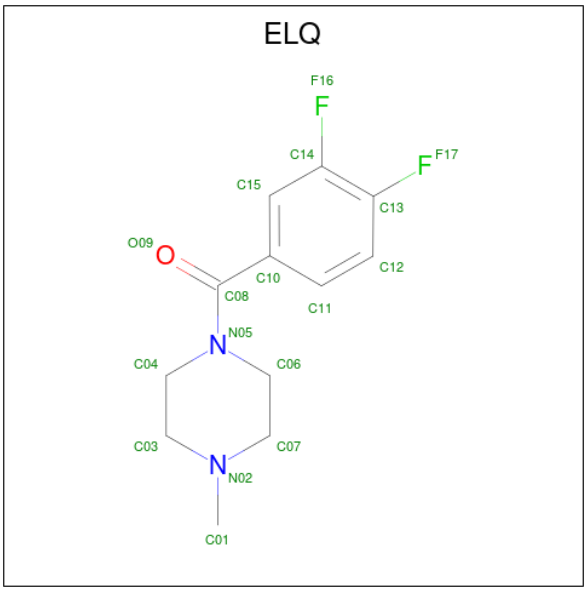
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cl 1 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is [3,4-bis(fluoranyl)phenyl]-(4-methylpiperazin-1-yl)methanone (three-letter code: ELQ) (formula: $C_{12}H_{14}F_2N_2O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	F	N	O	0	0
			17	12	2	2	1		

- Molecule 6 is water.

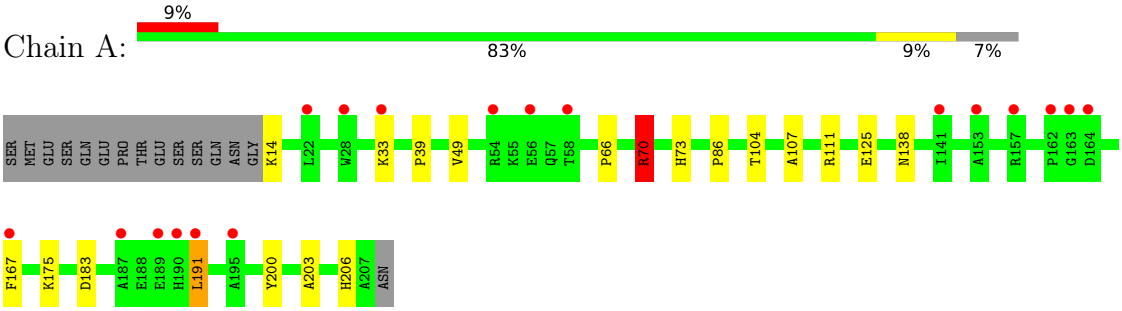
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	71	Total	O	0	0
			71	71		
6	B	71	Total	O	0	0
			71	71		
6	C	62	Total	O	0	0
			62	62		
6	D	27	Total	O	0	0
			27	27		

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.

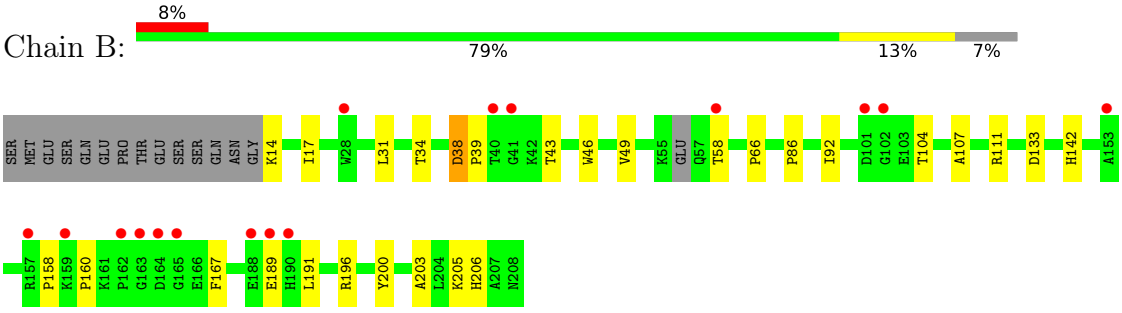
• Molecule 1: ADP-sugar pyrophosphatase

Chain A:



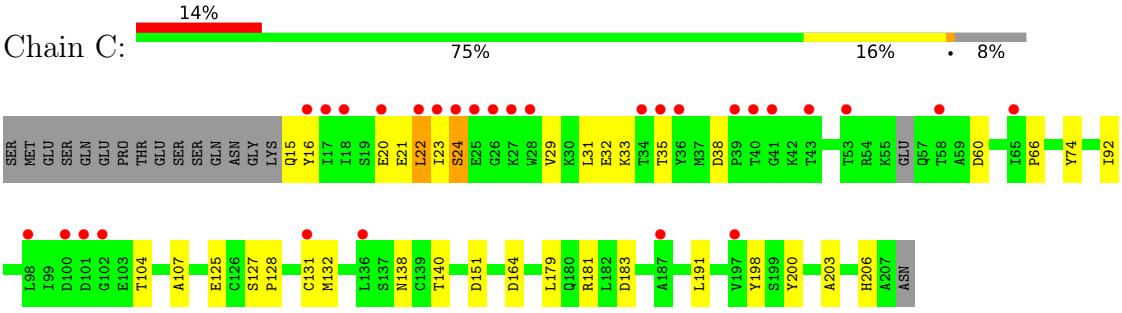
• Molecule 1: ADP-sugar pyrophosphatase

Chain B:



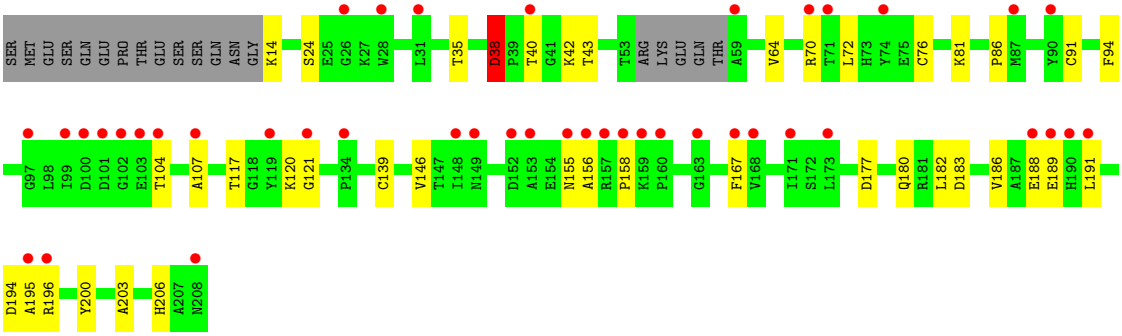
• Molecule 1: ADP-sugar pyrophosphatase

Chain C:



• Molecule 1: ADP-sugar pyrophosphatase

Chain D:


SER MET GLU SER GLN GLU PRO THR GLU SER SER GLN ASN GLY K14 S24 E25 G26 K27 W28 L31 T35 D38 P39 T40 G41 K42 T43 T53 ARG LYS GLU GLN THR A59 V64 R70 T71 L72 H73 Y74 E75 C76 K81 P86 M87 Y90 C91 F94
G97 L98 I99 D100 D101 G102 E103 T104 A107 T117 G118 Y119 K120 G121 P134 C139 V146 T147 I148 N149 D152 A153 E154 N155 A156 R157 P158 K159 P160 G163 F167 V168 I171 S172 L173 D177 Q180 R181 L182 D183 V186 A187 E188 E189 H190 L191
D194 A195 R196 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	49.53Å 59.99Å 79.65Å 79.56° 81.09° 75.49°	Depositor
Resolution (Å)	77.81 – 1.76 33.90 – 1.76	Depositor EDS
% Data completeness (in resolution range)	96.8 (77.81-1.76) 96.8 (33.90-1.76)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.234 , 0.278 0.250 , 0.288	Depositor DCC
R_{free} test set	4213 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	30.1	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 42.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5997	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.33% 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

5.1 Standard geometry

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

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	0.95	0/1490	0.99	4/2032 (0.2%)
1	B	0.86	0/1492	0.97	3/2035 (0.1%)
1	C	0.91	0/1429	1.00	4/1958 (0.2%)
1	D	0.88	0/1430	0.97	3/1954 (0.2%)
All	All	0.90	0/5841	0.98	14/7979 (0.2%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	70	ARG	NE-CZ-NH1	8.17	124.39	120.30
1	B	196	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	A	111	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	183	ASP	CB-CG-OD1	6.66	124.29	118.30
1	A	70	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	C	151	ASP	CB-CG-OD1	5.65	123.39	118.30
1	D	38	ASP	CB-CG-OD1	5.58	123.32	118.30
1	D	183	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	B	111	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	C	151	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	C	183	ASP	CB-CG-OD1	5.30	123.07	118.30
1	B	133	ASP	CB-CG-OD1	5.29	123.06	118.30
1	D	183	ASP	CB-CG-OD1	5.22	123.00	118.30
1	C	181	ARG	NE-CZ-NH1	5.22	122.91	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	1462	0	1431	21	0
1	B	1464	0	1414	21	0
1	C	1402	0	1298	25	0
1	D	1404	0	1338	36	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	B	1	0	0	0	0
4	B	4	0	6	1	0
4	C	4	0	6	0	0
5	B	17	0	0	0	0
6	A	71	0	0	1	0
6	B	71	0	0	1	0
6	C	62	0	0	4	0
6	D	27	0	0	0	0
All	All	5997	0	5493	83	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 7.

All (83) 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:196[B]:ARG:HH21	1:D:196[B]:ARG:CG	1.50	1.21
1:C:22:LEU:HD13	1:C:22:LEU:O	1.47	1.10
1:C:22:LEU:O	1:C:22:LEU:CD1	2.00	1.10
1:D:196[B]:ARG:HG3	1:D:196[B]:ARG:NH2	1.48	1.00
1:C:22:LEU:HD13	1:C:22:LEU:C	1.87	0.95
1:C:125:GLU:OE1	6:C:401:HOH:O	1.87	0.91
1:D:188:GLU:HG3	1:D:189:GLU:N	1.94	0.83
1:B:92:ILE:HD11	1:B:191:LEU:HD13	1.62	0.80
1:D:188:GLU:HG3	1:D:189:GLU:HG3	1.67	0.76
1:C:104:THR:HG23	1:C:107:ALA:H	1.52	0.75
1:D:155:ASN:O	1:D:158:PRO:HD3	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LEU:CD2	1:A:191:LEU:C	2.55	0.74
1:C:22:LEU:O	1:C:22:LEU:HD12	1.88	0.73
1:A:175:LYS:NZ	1:B:206:HIS:O	2.20	0.71
1:A:191:LEU:HD22	1:A:191:LEU:O	1.91	0.71
1:D:196[B]:ARG:NH2	1:D:196[B]:ARG:N	2.38	0.71
1:D:196[B]:ARG:HH21	1:D:196[B]:ARG:HG3	0.64	0.70
1:D:120:LYS:H	1:D:155:ASN:HD21	1.40	0.69
1:D:188:GLU:HG3	1:D:189:GLU:CG	2.23	0.69
1:D:188:GLU:CG	1:D:189:GLU:HG3	2.24	0.67
1:C:200:TYR:CD1	1:D:203:ALA:HB2	2.30	0.67
1:D:196[B]:ARG:CG	1:D:196[B]:ARG:NH2	2.23	0.64
1:B:104:THR:HG23	1:B:107:ALA:H	1.64	0.63
1:A:104:THR:HG23	1:A:107:ALA:H	1.64	0.62
1:A:206:HIS:HD2	1:B:200:TYR:OH	1.80	0.62
1:A:203:ALA:HB3	1:B:203:ALA:HB3	1.83	0.60
1:A:70:ARG:NH1	6:A:401:HOH:O	2.36	0.59
1:A:191:LEU:C	1:A:191:LEU:HD23	2.23	0.58
1:C:23:ILE:O	1:C:24:SER:CB	2.51	0.58
1:D:196[B]:ARG:NH2	1:D:196[B]:ARG:H	2.02	0.57
1:D:35:THR:HG23	1:D:43:THR:HG23	1.86	0.57
1:C:38:ASP:HB2	1:D:167:PHE:CE2	2.41	0.56
1:C:179:LEU:HD11	1:C:198:TYR:CZ	2.41	0.56
1:C:191:LEU:HD12	1:C:191:LEU:C	2.26	0.55
1:D:188:GLU:CG	1:D:189:GLU:N	2.69	0.54
1:B:17:ILE:HD12	1:B:34:THR:CG2	2.38	0.54
1:D:81:LYS:HA	1:D:91:CYS:O	2.07	0.53
1:D:196[B]:ARG:H	1:D:196[B]:ARG:CZ	2.22	0.53
1:A:191:LEU:C	1:A:191:LEU:HD22	2.25	0.53
1:C:203:ALA:HB3	1:D:203:ALA:HB3	1.91	0.53
1:D:191:LEU:C	1:D:191:LEU:HD12	2.29	0.52
1:A:200:TYR:CD1	1:B:203:ALA:HB2	2.44	0.52
1:D:155:ASN:O	1:D:156:ALA:C	2.48	0.52
1:A:104:THR:CG2	1:A:107:ALA:H	2.22	0.52
1:D:195:ALA:HB3	1:D:196[B]:ARG:HH12	1.75	0.51
1:C:20:GLU:HA	1:C:33:LYS:O	2.10	0.51
1:D:177:ASP:OD1	1:D:180:GLN:CB	2.58	0.51
6:C:401:HOH:O	1:D:206:HIS:HE1	1.92	0.51
1:C:200:TYR:OH	1:D:206:HIS:HD2	1.94	0.50
1:D:38:ASP:OD1	1:D:40:THR:N	2.39	0.49
1:B:189:GLU:HB3	1:B:191:LEU:HD12	1.95	0.48
1:C:206:HIS:HD2	1:D:200:TYR:OH	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:ASP:OD2	1:C:140:THR:N	2.30	0.48
1:C:203:ALA:HB2	1:D:200:TYR:CD1	2.48	0.48
1:C:15:GLN:N	6:C:405:HOH:O	2.46	0.47
1:A:49:VAL:HG21	1:B:49:VAL:HG11	1.97	0.47
1:A:203:ALA:HB2	1:B:200:TYR:CD1	2.50	0.46
1:C:92:ILE:HG13	1:C:191:LEU:HD13	1.98	0.46
1:B:92:ILE:CD1	1:B:191:LEU:HD13	2.39	0.46
1:B:158:PRO:O	1:B:160:PRO:HD3	2.16	0.46
1:C:138:ASN:HB3	1:D:86:PRO:O	2.16	0.45
1:D:121:GLY:HA3	1:D:146:VAL:CG1	2.47	0.45
1:A:104:THR:HG22	1:A:107:ALA:CB	2.47	0.45
1:C:131:CYS:SG	1:D:194:ASP:HA	2.57	0.45
1:C:74:TYR:HB3	6:C:426:HOH:O	2.18	0.44
1:D:182:LEU:O	1:D:186:VAL:HG23	2.17	0.44
1:A:125:GLU:OE1	1:B:206:HIS:HE1	1.99	0.44
1:B:17:ILE:HD12	1:B:34:THR:HG21	1.97	0.44
1:D:104:THR:HG23	1:D:107:ALA:H	1.82	0.44
1:A:200:TYR:OH	1:B:206:HIS:HD2	2.00	0.43
1:A:86:PRO:HD3	1:B:46:TRP:CD1	2.54	0.43
1:A:138:ASN:HB3	1:B:86:PRO:O	2.18	0.42
1:C:127:SER:HB2	1:C:128:PRO:HD2	2.01	0.42
1:A:39:PRO:HG2	1:B:167:PHE:CD2	2.54	0.42
4:B:302:EDO:C2	6:B:411:HOH:O	2.68	0.42
1:A:167:PHE:CZ	1:B:39:PRO:HD2	2.55	0.42
1:B:58:THR:CB	1:B:142:HIS:NE2	2.83	0.42
1:D:64:VAL:O	1:D:94:PHE:HB3	2.19	0.42
1:D:196[B]:ARG:NH2	1:D:196[B]:ARG:CA	2.83	0.41
1:C:21:GLU:O	1:C:32:GLU:HA	2.20	0.41
1:A:70:ARG:HB3	1:A:73:HIS:HB2	2.02	0.41
1:C:132:MET:O	1:D:196[B]:ARG:NH1	2.53	0.41
1:B:38:ASP:C	1:B:38:ASP:OD1	2.60	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%)	187 (97%)	4 (2%)	1 (0%)	29 12
1	B	190/209 (91%)	183 (96%)	6 (3%)	1 (0%)	29 12
1	C	188/209 (90%)	176 (94%)	9 (5%)	3 (2%)	9 1
1	D	187/209 (90%)	174 (93%)	13 (7%)	0	100 100
All	All	757/836 (91%)	720 (95%)	32 (4%)	5 (1%)	22 8

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	24	SER
1	C	22	LEU
1	A	66	PRO
1	B	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	154/179 (86%)	150 (97%)	4 (3%)	46 23
1	B	154/179 (86%)	149 (97%)	5 (3%)	39 16
1	C	139/179 (78%)	134 (96%)	5 (4%)	35 13
1	D	143/179 (80%)	134 (94%)	9 (6%)	18 3
All	All	590/716 (82%)	567 (96%)	23 (4%)	32 11

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	33	LYS
1	A	70	ARG

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Mol	Chain	Res	Type
1	A	191	LEU
1	B	14	LYS
1	B	31	LEU
1	B	38	ASP
1	B	43	THR
1	B	205	LYS
1	C	16	TYR
1	C	29	VAL
1	C	31	LEU
1	C	35	THR
1	C	164	ASP
1	D	14	LYS
1	D	24	SER
1	D	38	ASP
1	D	42	LYS
1	D	70	ARG
1	D	72	LEU
1	D	76	CYS
1	D	117	THR
1	D	139	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	HIS
1	A	206	HIS
1	B	206	HIS
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 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 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	EDO	C	301	-	3,3,3	0.65	0	2,2,2	0.12	0
5	ELQ	B	305	-	18,18,18	2.03	4 (22%)	25,25,25	1.50	4 (16%)
4	EDO	B	302	-	3,3,3	0.50	0	2,2,2	0.03	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	EDO	C	301	-	-	0/1/1/1	-
5	ELQ	B	305	-	-	0/8/18/18	1/2/2/2
4	EDO	B	302	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	305	ELQ	C08-N05	4.80	1.45	1.34
5	B	305	ELQ	C07-N02	3.09	1.53	1.46
5	B	305	ELQ	C04-N05	2.91	1.52	1.47
5	B	305	ELQ	C03-N02	2.56	1.51	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	305	ELQ	C10-C08-N05	4.58	124.54	118.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	305	ELQ	C07-N02-C03	2.72	113.33	109.52
5	B	305	ELQ	O09-C08-C10	-2.36	115.63	120.23
5	B	305	ELQ	C15-C10-C08	-2.22	115.18	120.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	302	EDO	O1-C1-C2-O2

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	305	ELQ	C03-C04-C06-C07-N02-N05

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	302	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

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	194/209 (92%)	0.38	18 (9%) 8 11	22, 32, 51, 64	13 (6%)
1	B	194/209 (92%)	0.31	16 (8%) 11 15	23, 36, 61, 76	3 (1%)
1	C	192/209 (91%)	0.68	29 (15%) 2 3	21, 38, 68, 79	7 (3%)
1	D	190/209 (90%)	1.21	43 (22%) 0 0	27, 47, 68, 81	17 (8%)
All	All	770/836 (92%)	0.64	106 (13%) 2 4	21, 38, 65, 81	40 (5%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	196[A]	ARG	16.9
1	A	191	LEU	9.2
1	D	191	LEU	8.4
1	D	153	ALA	8.1
1	C	28	TRP	8.1
1	C	40	THR	6.7
1	D	160	PRO	6.0
1	C	23	ILE	5.8
1	C	39	PRO	5.7
1	D	208	ASN	5.3
1	C	26	GLY	5.2
1	D	90	TYR	5.2
1	D	26	GLY	5.2
1	D	28	TRP	5.1
1	C	53	THR	4.9
1	C	35	THR	4.8
1	A	187	ALA	4.4
1	A	190	HIS	4.4
1	C	18	ILE	4.4
1	D	99	ILE	4.3
1	A	164	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	28	TRP	4.2
1	D	100	ASP	4.1
1	B	190	HIS	3.9
1	B	58	THR	3.9
1	A	163	GLY	3.6
1	D	101	ASP	3.6
1	A	56	GLU	3.6
1	B	189	GLU	3.6
1	B	157	ARG	3.5
1	C	41	GLY	3.5
1	D	74	TYR	3.5
1	D	158	PRO	3.5
1	D	159	LYS	3.4
1	D	156	ALA	3.4
1	B	163	GLY	3.4
1	D	40	THR	3.4
1	C	16	TYR	3.3
1	A	157	ARG	3.3
1	B	165	GLY	3.2
1	B	28	TRP	3.2
1	A	153	ALA	3.2
1	C	102	GLY	3.2
1	D	121	GLY	3.1
1	C	25	GLU	3.1
1	C	36	TYR	3.1
1	D	195	ALA	3.1
1	C	22	LEU	3.0
1	D	97	GLY	3.0
1	A	162	PRO	3.0
1	C	43	THR	2.9
1	D	167	PHE	2.9
1	C	24	SER	2.9
1	C	17	ILE	2.9
1	C	101	ASP	2.9
1	C	187	ALA	2.8
1	B	40	THR	2.8
1	B	164	ASP	2.7
1	D	119	TYR	2.7
1	D	190	HIS	2.7
1	D	148	ILE	2.7
1	D	168	VAL	2.6
1	A	33	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	159	LYS	2.6
1	D	188	GLU	2.6
1	C	197	VAL	2.6
1	B	102	GLY	2.6
1	D	157	ARG	2.5
1	D	152	ASP	2.5
1	D	189	GLU	2.5
1	D	59	ALA	2.5
1	D	149	ASN	2.5
1	C	20	GLU	2.5
1	A	54	ARG	2.4
1	C	34	THR	2.4
1	D	70	ARG	2.4
1	B	188	GLU	2.4
1	D	71	THR	2.4
1	D	163	GLY	2.4
1	C	65	ILE	2.4
1	C	27	LYS	2.4
1	C	58	THR	2.4
1	A	189	GLU	2.3
1	D	102	GLY	2.3
1	B	101	ASP	2.3
1	D	173	LEU	2.3
1	D	104	THR	2.3
1	D	107	ALA	2.3
1	D	87	MET	2.3
1	A	195	ALA	2.3
1	A	167	PHE	2.3
1	B	162	PRO	2.2
1	C	100	ASP	2.2
1	A	22	LEU	2.2
1	C	136	LEU	2.2
1	D	155	ASN	2.2
1	C	131	CYS	2.1
1	A	141	ILE	2.1
1	A	58	THR	2.0
1	B	153	ALA	2.0
1	D	103	GLU	2.0
1	D	171	ILE	2.0
1	B	41	GLY	2.0
1	D	134	PRO	2.0
1	C	98	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	31	LEU	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, 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
5	ELQ	B	305	17/17	0.69	0.31	56,62,68,68	17
3	CL	B	301	1/1	0.82	0.10	69,69,69,69	0
2	MG	B	304	1/1	0.86	0.11	71,71,71,71	0
4	EDO	C	301	4/4	0.89	0.12	36,47,49,57	0
2	MG	D	301	1/1	0.93	0.05	40,40,40,40	0
2	MG	A	302	1/1	0.93	0.04	65,65,65,65	0
2	MG	C	302	1/1	0.94	0.13	70,70,70,70	0
4	EDO	B	302	4/4	0.94	0.09	46,46,47,50	0
2	MG	D	302	1/1	0.96	0.07	46,46,46,46	0
2	MG	B	303	1/1	0.97	0.05	34,34,34,34	0
2	MG	C	303	1/1	0.98	0.06	35,35,35,35	0
2	MG	A	301	1/1	0.99	0.06	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.