Full wwPDB X-ray Structure Validation Report (i)

Feb 27, 2024 – 09:29 PM EST

PDB ID	:	5QJZ
Title	:	PanDDA analysis group deposition of models with modelled events (e.g. bound ligands) – Crystal Structure of NUDT5 in complex with Z1696822287
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	:	1.52 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:

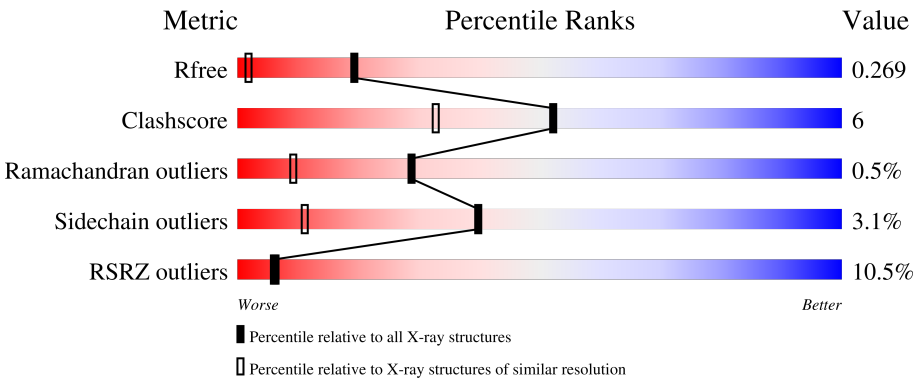
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.52 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	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)
RSRZ outliers	127900	3943 (1.54-1.50)

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% 80% 11% • 7%
1	B	209	11% 82% 11% 7%
1	C	209	13% 79% 11% • 8%
1	D	209	6% 80% 10% 9%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6010 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	1458	923	244	283	8	0	0	0
1	B	194	1464	924	244	288	8	0	0	0
1	C	192	1402	884	234	277	7	0	0	0
1	D	190	1404	887	235	274	8	0	1	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

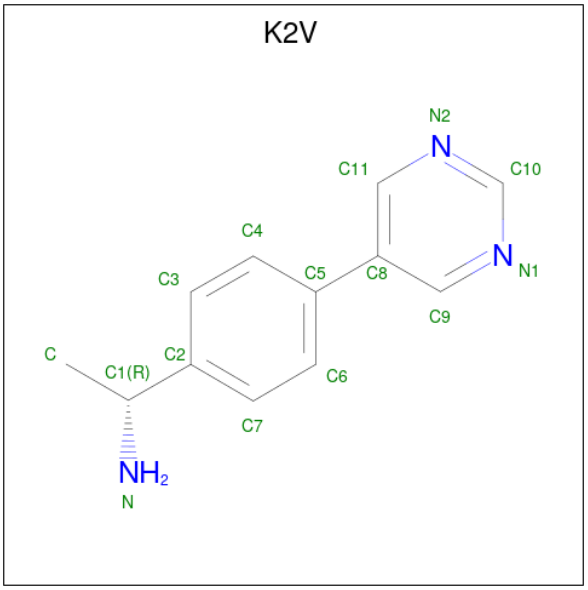
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

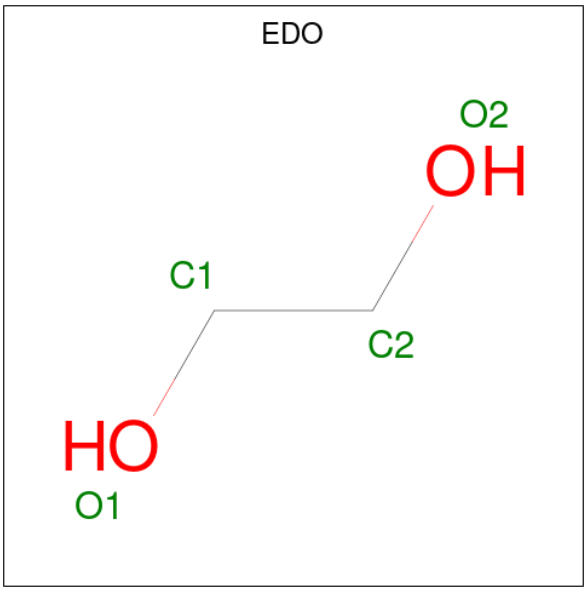
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
3	A	1	1	1	0	0

- Molecule 4 is (1R)-1-[4-(pyrimidin-5-yl)phenyl]ethan-1-amine (three-letter code: K2V) (formula: $C_{12}H_{13}N_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
4	A	1	15	12	3	0	0
4	B	1	15	12	3	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
			Total	C	O		
5	B	1	4	2	2	0	0
			Total	C	O		
5	C	1	4	2	2	0	0

- Molecule 6 is water.

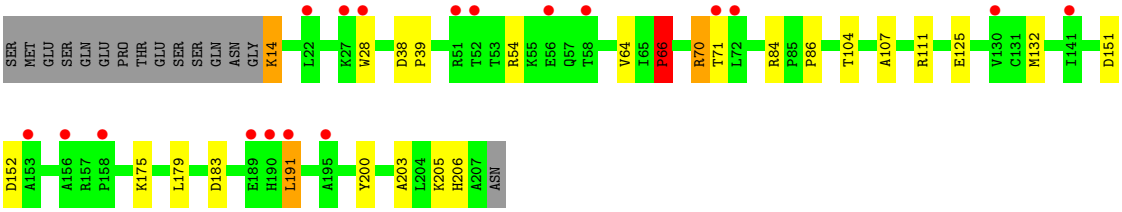
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	71	71	71	0	0
			Total	O		
6	B	70	70	70	0	0
			Total	O		
6	C	67	67	67	0	0
			Total	O		
6	D	23	23	23	0	0

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.

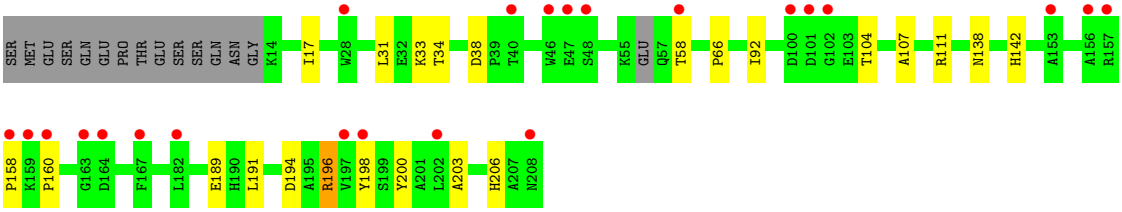
• Molecule 1: ADP-sugar pyrophosphatase

Chain A:



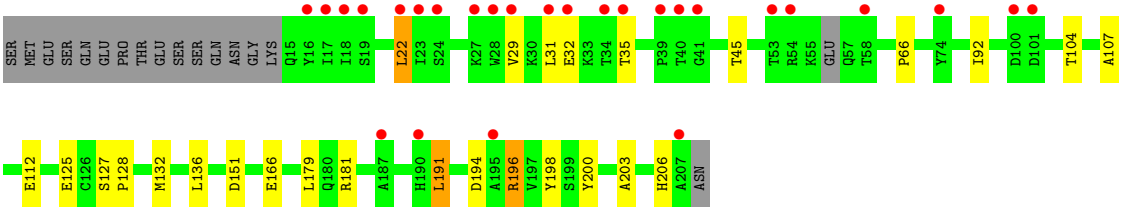
• Molecule 1: ADP-sugar pyrophosphatase

Chain B:



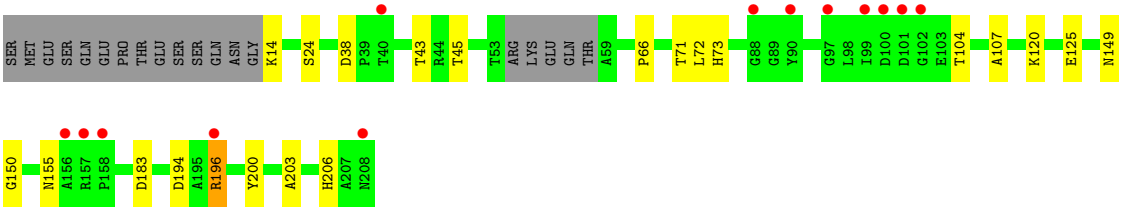
• Molecule 1: ADP-sugar pyrophosphatase

Chain C:



• Molecule 1: ADP-sugar pyrophosphatase

Chain D:


SER MET GLU SER GLN GLU PRO THR GLU SER SER GLN ASN GLY K14 S24 D38 P39 T40 T43 R44 T45 T53 ARG LYS GLU GLN THR A59 P66 T71 L72 H73 G88 G89 Y90 G97 L98 I99 D100 D101 G102 E103 T104 A107 K120 E125 N149
G150 N155 A156 R157 P158 D183 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	49.43Å 59.82Å 79.90Å 79.61° 81.70° 75.99°	Depositor
Resolution (Å)	78.15 – 1.52 41.48 – 1.52	Depositor EDS
% Data completeness (in resolution range)	94.0 (78.15-1.52) 94.1 (41.48-1.52)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 1.52Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.226 , 0.263 0.238 , 0.269	Depositor DCC
R_{free} test set	6347 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	29.5	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.5	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	0.96	EDS
Total number of atoms	6010	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 6.67% 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: MG, EDO, CL, K2V

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	1.03	0/1486	1.07	8/2027 (0.4%)
1	B	0.93	1/1492 (0.1%)	1.01	3/2035 (0.1%)
1	C	1.01	0/1429	1.02	3/1958 (0.2%)
1	D	1.01	0/1430	1.02	6/1954 (0.3%)
All	All	0.99	1/5837 (0.0%)	1.03	20/7974 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	198	TYR	CE1-CZ	-5.90	1.30	1.38

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	70	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	B	196	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	C	196	ARG	NE-CZ-NH1	7.69	124.15	120.30
1	C	151	ASP	CB-CG-OD2	-7.39	111.64	118.30
1	A	183	ASP	CB-CG-OD1	7.14	124.73	118.30
1	B	111	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	A	54	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	D	38	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	54	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	B	194	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	A	152	ASP	CB-CG-OD1	5.40	123.16	118.30
1	C	181	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	D	196[A]	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	D	196[B]	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	D	183	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	A	152	ASP	CB-CG-OD2	-5.13	113.68	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	84	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	A	111	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	D	196[A]	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	D	196[B]	ARG	NE-CZ-NH2	-5.03	117.78	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	1458	0	1427	19	0
1	B	1464	0	1414	15	0
1	C	1402	0	1298	24	0
1	D	1404	0	1338	19	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	A	1	0	0	0	0
4	A	15	0	0	0	0
4	B	15	0	0	0	0
5	A	4	0	6	0	0
5	B	4	0	6	1	0
5	C	4	0	6	0	0
6	A	71	0	0	1	0
6	B	70	0	0	2	0
6	C	67	0	0	4	0
6	D	23	0	0	1	0
All	All	6010	0	5495	62	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 (62) 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:C:22:LEU:HD13	1:C:22:LEU:O	1.51	1.11
1:C:22:LEU:HD13	1:C:22:LEU:C	1.73	1.08
1:D:196[B]:ARG:HH21	1:D:196[B]:ARG:HG3	0.96	1.07
1:D:196[B]:ARG:HG3	1:D:196[B]:ARG:NH2	1.68	0.94
1:B:92:ILE:HD11	1:B:191:LEU:HD13	1.53	0.90
1:D:196[B]:ARG:HH21	1:D:196[B]:ARG:CG	1.85	0.88
1:C:125:GLU:OE1	6:C:401:HOH:O	1.93	0.85
1:D:120:LYS:H	1:D:155:ASN:HD21	1.27	0.83
1:C:22:LEU:O	1:C:22:LEU:CD1	2.26	0.83
1:A:191:LEU:C	1:A:191:LEU:HD23	2.00	0.81
1:A:104:THR:HG23	1:A:107:ALA:H	1.46	0.81
1:C:31:LEU:HD23	1:C:32:GLU:H	1.53	0.74
1:A:203:ALA:HB3	1:B:203:ALA:HB3	1.70	0.73
1:C:22:LEU:C	1:C:22:LEU:CD1	2.49	0.71
1:D:196[B]:ARG:NH2	1:D:196[B]:ARG:CG	2.49	0.71
1:C:104:THR:HG23	1:C:107:ALA:H	1.56	0.70
1:C:112:GLU:OE2	6:C:402:HOH:O	2.10	0.69
1:A:206:HIS:HD2	1:B:200:TYR:OH	1.77	0.67
1:A:191:LEU:HD23	1:A:191:LEU:O	1.95	0.66
1:C:166:GLU:OE2	6:C:402:HOH:O	2.14	0.65
1:C:200:TYR:OH	1:D:206:HIS:HD2	1.80	0.64
1:C:179:LEU:HD11	1:C:198:TYR:CZ	2.33	0.64
1:A:191:LEU:C	1:A:191:LEU:CD2	2.69	0.61
1:C:206:HIS:HD2	1:D:200:TYR:OH	1.82	0.61
1:B:92:ILE:CD1	1:B:191:LEU:HD13	2.28	0.60
1:C:203:ALA:HB3	1:D:203:ALA:HB3	1.84	0.60
1:B:104:THR:HG23	1:B:107:ALA:H	1.68	0.59
1:D:104:THR:HG23	1:D:107:ALA:H	1.68	0.58
1:C:31:LEU:HD23	1:C:32:GLU:N	2.19	0.57
1:C:194:ASP:OD2	1:C:196:ARG:NH2	2.37	0.57
1:C:132:MET:O	1:D:196[B]:ARG:NH1	2.38	0.56
1:C:206:HIS:HE1	1:D:125:GLU:OE1	1.87	0.56
1:A:28:TRP:CZ3	6:B:457:HOH:O	2.53	0.56
1:A:71:THR:HG23	1:A:151:ASP:OD2	2.07	0.55
1:C:203:ALA:HB2	1:D:200:TYR:CD1	2.43	0.54
6:C:401:HOH:O	1:D:206:HIS:HE1	1.91	0.53
1:A:200:TYR:CD1	1:B:203:ALA:HB2	2.44	0.53
1:C:200:TYR:CD1	1:D:203:ALA:HB2	2.44	0.52
1:D:194:ASP:OD1	1:D:196[A]:ARG:HD3	2.10	0.52
1:A:179:LEU:HD23	1:A:205:LYS:HD2	1.94	0.48
1:B:189:GLU:OE2	1:B:191:LEU:HD11	2.14	0.48
1:A:191:LEU:O	1:A:191:LEU:CD2	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:GLU:OE1	1:B:206:HIS:HE1	1.96	0.47
1:C:191:LEU:HD12	1:C:191:LEU:C	2.35	0.47
1:D:71:THR:O	1:D:73:HIS:ND1	2.41	0.47
1:B:58:THR:CB	1:B:142:HIS:NE2	2.79	0.46
1:A:70:ARG:HD3	6:A:439:HOH:O	2.16	0.46
1:A:132:MET:O	1:B:196:ARG:NH2	2.49	0.45
1:A:86:PRO:O	1:B:138:ASN:HB3	2.15	0.45
1:A:175:LYS:NZ	1:B:206:HIS:O	2.48	0.45
1:B:17:ILE:HD12	1:B:34:THR:CG2	2.46	0.45
1:C:136:LEU:HD13	1:C:136:LEU:O	2.18	0.44
1:B:158:PRO:O	1:B:160:PRO:HD3	2.18	0.43
1:A:14:LYS:HE2	1:A:39:PRO:O	2.19	0.43
1:A:64:VAL:O	1:A:66:PRO:HD3	2.19	0.43
1:D:150:GLY:O	6:D:401:HOH:O	2.21	0.43
1:C:92:ILE:HG13	1:C:191:LEU:HD13	2.01	0.42
1:D:194:ASP:OD2	1:D:196[B]:ARG:NH1	2.52	0.42
1:C:200:TYR:OH	1:D:206:HIS:CD2	2.68	0.41
1:A:200:TYR:OH	1:B:206:HIS:HD2	2.02	0.41
1:C:127:SER:HB2	1:C:128:PRO:HD2	2.03	0.40
5:B:301:EDO:C2	6:B:402:HOH:O	2.69	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%)	189 (98%)	2 (1%)	1 (0%)	29 9
1	B	190/209 (91%)	183 (96%)	6 (3%)	1 (0%)	29 9
1	C	188/209 (90%)	183 (97%)	4 (2%)	1 (0%)	29 9
1	D	187/209 (90%)	181 (97%)	5 (3%)	1 (0%)	29 9
All	All	757/836 (91%)	736 (97%)	17 (2%)	4 (0%)	29 9

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	PRO
1	B	66	PRO
1	C	66	PRO
1	D	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	153/179 (86%)	149 (97%)	4 (3%)	46	16
1	B	154/179 (86%)	151 (98%)	3 (2%)	57	26
1	C	139/179 (78%)	134 (96%)	5 (4%)	35	8
1	D	143/179 (80%)	137 (96%)	6 (4%)	30	5
All	All	589/716 (82%)	571 (97%)	18 (3%)	40	11

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

Mol	Chain	Res	Type
1	A	14	LYS
1	A	38	ASP
1	A	66	PRO
1	A	191	LEU
1	B	31	LEU
1	B	33	LYS
1	B	38	ASP
1	C	22	LEU
1	C	29	VAL
1	C	35	THR
1	C	45	THR
1	C	191	LEU
1	D	14	LYS
1	D	24	SER
1	D	43	THR
1	D	45	THR

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Mol	Chain	Res	Type
1	D	72	LEU
1	D	149	ASN

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	206	HIS
1	B	73	HIS
1	B	190	HIS
1	B	206	HIS
1	C	206	HIS
1	D	69	GLN
1	D	149	ASN
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 14 ligands modelled in this entry, 9 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
5	EDO	B	301	-	3,3,3	0.66	0	2,2,2	0.28	0
4	K2V	A	304	-	15,16,16	1.46	2 (13%)	19,21,21	0.74	0
5	EDO	C	301	-	3,3,3	0.72	0	2,2,2	0.45	0
4	K2V	B	304	-	15,16,16	1.37	2 (13%)	19,21,21	0.73	0
5	EDO	A	305	-	3,3,3	0.41	0	2,2,2	0.78	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
5	EDO	B	301	-	-	0/1/1/1	-
4	K2V	A	304	-	-	2/8/8/8	0/2/2/2
5	EDO	C	301	-	-	0/1/1/1	-
4	K2V	B	304	-	-	0/8/8/8	0/2/2/2
5	EDO	A	305	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	304	K2V	C10-N2	2.51	1.38	1.33
4	B	304	K2V	C3-C2	2.40	1.42	1.39
4	A	304	K2V	C7-C2	2.26	1.42	1.39
4	A	304	K2V	C11-C8	2.13	1.43	1.39

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	305	EDO	O1-C1-C2-O2
4	A	304	K2V	C-C1-C2-C7
4	A	304	K2V	C-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	301	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%)	0.38	18 (9%)	8	9	23, 35, 54, 65	12 (6%)
1	B	194/209 (92%)	0.36	23 (11%)	4	4	24, 38, 62, 71	6 (3%)
1	C	192/209 (91%)	0.58	27 (14%)	2	2	23, 39, 67, 80	9 (4%)
1	D	190/209 (90%)	0.45	13 (6%)	17	18	27, 41, 65, 75	5 (2%)
All	All	770/836 (92%)	0.44	81 (10%)	6	6	23, 39, 65, 80	32 (4%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	28	TRP	12.3
1	D	196[A]	ARG	11.7
1	C	23	ILE	9.2
1	A	191	LEU	8.8
1	D	208	ASN	8.2
1	C	31	LEU	8.1
1	C	29	VAL	8.0
1	A	28	TRP	6.8
1	B	46	TRP	6.5
1	C	18	ILE	6.4
1	B	208	ASN	6.1
1	C	22	LEU	5.6
1	C	16	TYR	5.4
1	A	58	THR	5.2
1	B	28	TRP	4.6
1	D	90	TYR	4.2
1	B	48	SER	4.0
1	A	141	ILE	3.9
1	A	56	GLU	3.9
1	C	187	ALA	3.8
1	C	24	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	102	GLY	3.7
1	A	190	HIS	3.5
1	C	58	THR	3.5
1	C	190	HIS	3.4
1	B	40	THR	3.4
1	C	53	THR	3.4
1	D	100	ASP	3.4
1	D	157	ARG	3.4
1	B	159	LYS	3.2
1	C	40	THR	3.2
1	D	99	ILE	3.2
1	C	35	THR	3.2
1	C	19	SER	3.2
1	B	157	ARG	3.1
1	C	32	GLU	3.1
1	D	40	THR	3.1
1	A	22	LEU	3.1
1	B	58	THR	3.1
1	B	197	VAL	3.0
1	D	156	ALA	3.0
1	A	156	ALA	2.9
1	B	160	PRO	2.9
1	C	74	TYR	2.8
1	C	17	ILE	2.8
1	A	195	ALA	2.8
1	C	27	LYS	2.8
1	B	182	LEU	2.7
1	B	202	LEU	2.7
1	A	158	PRO	2.7
1	B	153	ALA	2.7
1	B	167	PHE	2.7
1	D	158	PRO	2.7
1	D	101	ASP	2.7
1	B	158	PRO	2.7
1	B	163	GLY	2.7
1	A	52	THR	2.6
1	A	71	THR	2.6
1	A	189	GLU	2.6
1	C	54	ARG	2.6
1	A	72	LEU	2.6
1	C	41	GLY	2.5
1	B	100	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	101	ASP	2.4
1	C	101	ASP	2.3
1	C	39	PRO	2.3
1	C	100	ASP	2.3
1	D	88	GLY	2.3
1	D	97	GLY	2.3
1	B	198	TYR	2.2
1	B	47	GLU	2.2
1	C	207	ALA	2.1
1	C	34	THR	2.1
1	A	153	ALA	2.1
1	B	102	GLY	2.1
1	A	27	LYS	2.1
1	C	195	ALA	2.1
1	A	51	ARG	2.0
1	B	164	ASP	2.0
1	A	130	VAL	2.0
1	B	156	ALA	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	A	305	4/4	0.55	0.35	37,37,37,42	4
4	K2V	B	304	15/15	0.70	0.24	32,43,49,50	15
4	K2V	A	304	15/15	0.80	0.17	42,58,63,64	15
3	CL	A	303	1/1	0.89	0.05	72,72,72,72	0
5	EDO	B	301	4/4	0.90	0.14	53,58,65,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	D	301	1/1	0.93	0.03	37,37,37,37	0
5	EDO	C	301	4/4	0.93	0.07	40,54,55,56	0
2	MG	C	303	1/1	0.95	0.04	37,37,37,37	0
2	MG	D	302	1/1	0.96	0.07	43,43,43,43	0
2	MG	C	302	1/1	0.97	0.05	50,50,50,50	0
2	MG	B	303	1/1	0.97	0.08	46,46,46,46	0
2	MG	B	302	1/1	0.98	0.01	34,34,34,34	0
2	MG	A	302	1/1	0.98	0.05	35,35,35,35	0
2	MG	A	301	1/1	0.99	0.09	33,33,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.