Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:07 AM GMT

PDB ID	:	3KYD
Title	:	Human SUMO E1 SUMO1-AMP tetrahedral intermediate mimic
Authors	:	Lima, C.D.
Deposited on	:	2009-12-05
Resolution	:	2.61 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

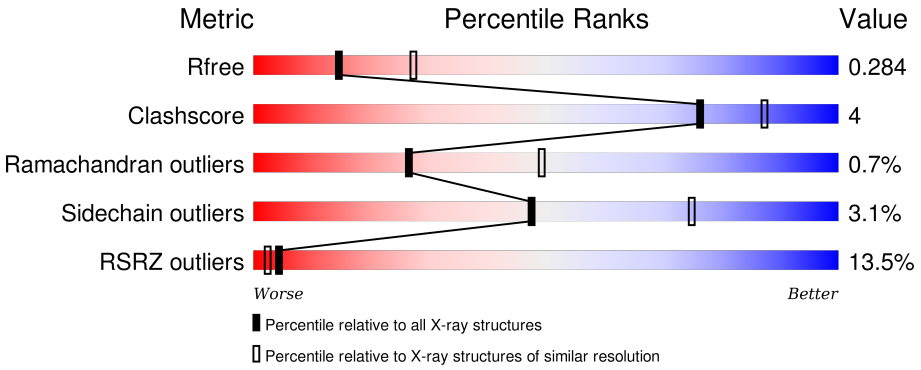
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.61 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}	91344	2700 (2.64-2.60)
Clashscore	102246	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (2.64-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	346	2% 79% 8% 13%
2	B	551	19% 76% 9% • 13%
3	D	115	5% 54% 13% 33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	A	347	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6978 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 SUMO-activating enzyme subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2353	1497	398	445	13			

- Molecule 2 is a protein called SUMO-activating enzyme subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	477	Total	C	N	O	S	0	0	0
			3740	2382	648	690	20			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	SER	-	EXPRESSION TAG	UNP Q9UBT2
B	0	LEU	-	EXPRESSION TAG	UNP Q9UBT2
B	229	CYS	SER	VARIANT	UNP Q9UBT2

- Molecule 3 is a protein called Small ubiquitin-related modifier 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	77	Total	C	N	O	S	0	0	0
			631	397	108	121	5			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-18	MET	-	EXPRESSION TAG	UNP P63165
D	-17	GLY	-	EXPRESSION TAG	UNP P63165
D	-16	SER	-	EXPRESSION TAG	UNP P63165
D	-15	SER	-	EXPRESSION TAG	UNP P63165
D	-14	HIS	-	EXPRESSION TAG	UNP P63165
D	-13	HIS	-	EXPRESSION TAG	UNP P63165
D	-12	HIS	-	EXPRESSION TAG	UNP P63165

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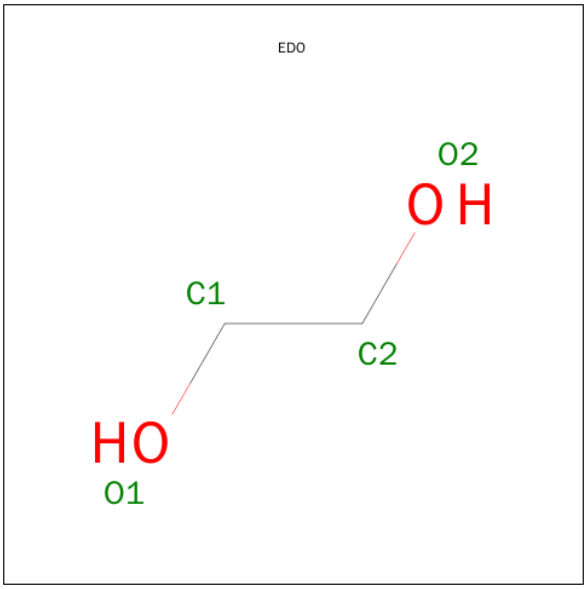
Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	HIS	-	EXPRESSION TAG	UNP P63165
D	-10	HIS	-	EXPRESSION TAG	UNP P63165
D	-9	HIS	-	EXPRESSION TAG	UNP P63165
D	-8	SER	-	EXPRESSION TAG	UNP P63165
D	-7	SER	-	EXPRESSION TAG	UNP P63165
D	-6	GLY	-	EXPRESSION TAG	UNP P63165
D	-5	LEU	-	EXPRESSION TAG	UNP P63165
D	-4	VAL	-	EXPRESSION TAG	UNP P63165
D	-3	PRO	-	EXPRESSION TAG	UNP P63165
D	-2	ARG	-	EXPRESSION TAG	UNP P63165
D	-1	SER	-	EXPRESSION TAG	UNP P63165
D	0	HIS	-	EXPRESSION TAG	UNP P63165
D	95	CYS	THR	ENGINEERED	UNP P63165

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

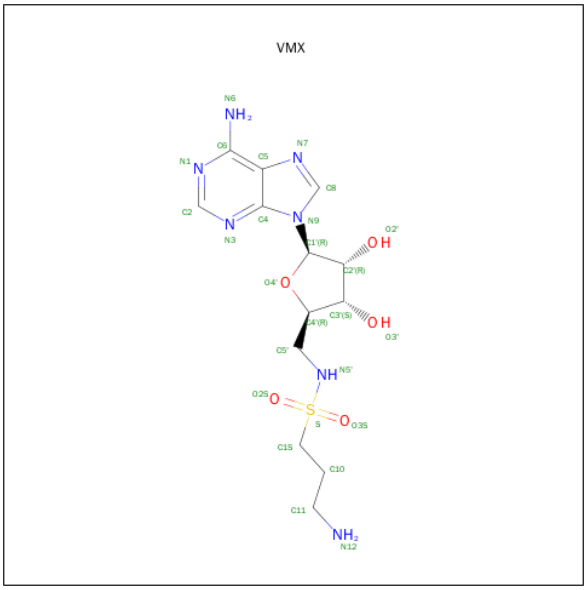


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Zn 1 1	0	0

- Molecule 6 is 5'-{[(3-AMINOPROPYL)SULFONYL]AMINO}-5'-DEOXYADENOSINE (three-letter code: VMX) (formula: $C_{13}H_{21}N_7O_5S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total C N O S 26 13 7 5 1	0	0

- Molecule 7 is water.

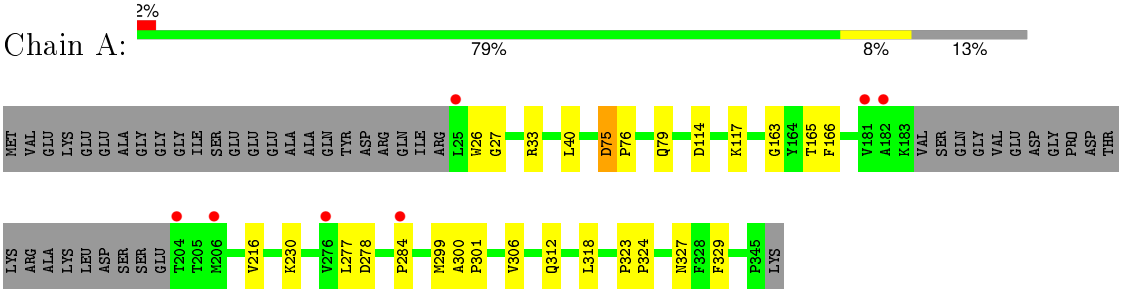
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	94	Total O 94 94	0	0
7	B	101	Total O 101 101	0	0
7	D	20	Total O 20 20	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

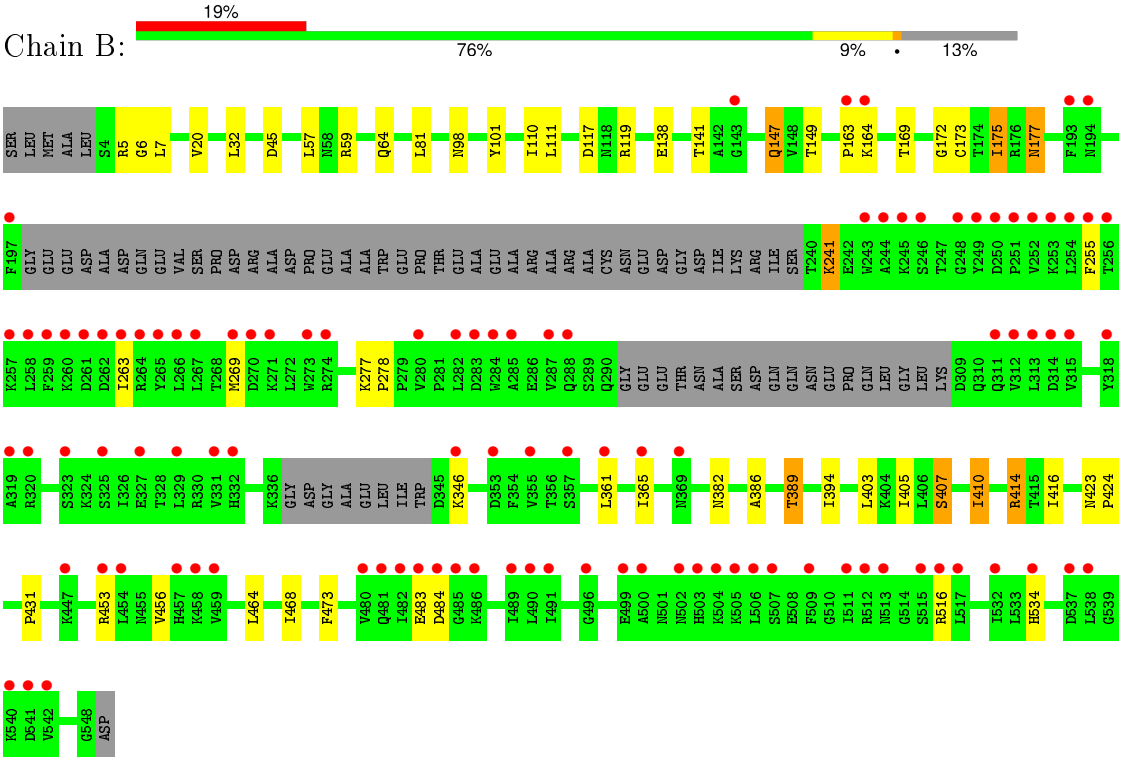
- Molecule 1: SUMO-activating enzyme subunit 1

Chain A:



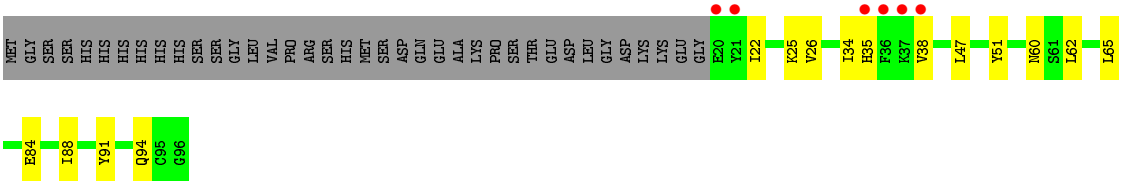
- Molecule 2: SUMO-activating enzyme subunit 2

Chain B:



- Molecule 3: Small ubiquitin-related modifier 1

Chain D:


MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG SER HIS MET SER ASP GLN GLU GLU ALA LYS PRO SER THR GLU ASP LEU GLY ASP LYS LYS GLU GLY
E20 Y21 I22 K25 V26 I34 H35 F36 K37 V38 L47 Y51 N60 S61 L62 L65
E84 I88 Y91 Q94 G95 G96

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	101.72Å 115.61Å 90.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.61 46.55 – 2.61	Depositor EDS
% Data completeness (in resolution range)	98.9 (25.00-2.61) 98.9 (46.55-2.61)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.79 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0093	Depositor
R, R_{free}	0.227 , 0.284 0.225 , 0.284	Depositor DCC
R_{free} test set	1671 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	53.7	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 79.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 33002 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6978	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, EDO, VMX

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	0.34	0/2395	0.47	0/3232
2	B	0.33	0/3809	0.48	0/5152
3	D	0.33	0/641	0.46	0/856
All	All	0.33	0/6845	0.47	0/9240

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2353	0	2360	11	0
2	B	3740	0	3796	35	0
3	D	631	0	627	10	0
4	A	8	0	12	0	0
4	D	4	0	6	0	0
5	B	1	0	0	0	0
6	D	26	0	19	1	0
7	A	94	0	0	0	0
7	B	101	0	0	2	0
7	D	20	0	0	0	0
All	All	6978	0	6820	51	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 4.

All (51) 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:166:PHE:CE2	1:A:216:VAL:HG12	2.03	0.93
2:B:423:ASN:HB2	2:B:424:PRO:HD2	1.52	0.92
2:B:147:GLN:HE22	3:D:94:GLN:H	1.28	0.79
2:B:414:ARG:HG2	2:B:431:PRO:HB2	1.73	0.70
1:A:312:GLN:HB2	2:B:389:THR:HG21	1.73	0.69
2:B:147:GLN:NE2	3:D:94:GLN:H	1.91	0.67
2:B:263:ILE:HD13	2:B:365:ILE:HG21	1.78	0.65
2:B:241:LYS:H	2:B:241:LYS:HD3	1.63	0.61
2:B:263:ILE:HB	7:B:637:HOH:O	2.07	0.54
2:B:138:GLU:HB3	2:B:149:THR:HG22	1.91	0.52
2:B:141:THR:CG2	2:B:394:ILE:HG13	2.38	0.52
2:B:403:LEU:O	2:B:407:SER:HB2	2.09	0.52
1:A:277:LEU:HD13	1:A:284:PRO:HA	1.92	0.52
2:B:117:ASP:HB3	6:D:97:VMX:H1SA	1.95	0.49
2:B:141:THR:HG22	2:B:394:ILE:HG13	1.94	0.49
2:B:423:ASN:CB	2:B:424:PRO:HD2	2.34	0.48
1:A:33:ARG:HG2	1:A:318:LEU:O	2.14	0.48
1:A:26:TRP:CG	1:A:27:GLY:N	2.81	0.48
1:A:165:THR:OG1	1:A:329:PHE:HB3	2.13	0.48
3:D:38:VAL:HG21	3:D:47:LEU:HD12	1.96	0.48
2:B:473:PHE:N	7:B:636:HOH:O	2.39	0.47
2:B:255:PHE:CE1	2:B:361:LEU:HD21	2.49	0.47
3:D:25:LYS:HG2	3:D:35:HIS:CD2	2.50	0.47
2:B:163:PRO:HD2	3:D:60:ASN:HB2	1.97	0.47
2:B:20:VAL:HG12	2:B:111:LEU:HB3	1.96	0.46
3:D:22:ILE:HG23	3:D:84:GLU:HA	1.97	0.46
3:D:65:LEU:HD12	3:D:91:TYR:CE1	2.51	0.45
2:B:172:GLY:O	2:B:386:ALA:HB2	2.18	0.45
2:B:464:LEU:HA	2:B:468:ILE:HD12	1.99	0.45
2:B:169:THR:HA	2:B:382:ASN:HB3	1.97	0.44
2:B:277:LYS:HA	2:B:278:PRO:HD3	1.84	0.44
2:B:423:ASN:HB2	2:B:424:PRO:CD	2.36	0.44
1:A:300:ALA:HB3	1:A:301:PRO:HD3	1.98	0.44
2:B:98:ASN:HB3	2:B:101:TYR:CE1	2.53	0.43
2:B:59:ARG:HH12	2:B:64:GLN:HA	1.83	0.43
3:D:34:ILE:HD12	3:D:51:TYR:CE1	2.53	0.43
2:B:147:GLN:HE22	3:D:94:GLN:N	2.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:26:VAL:HG22	3:D:88:ILE:HB	2.00	0.42
2:B:483:GLU:HB2	2:B:516:ARG:HB2	2.01	0.42
1:A:75:ASP:H	1:A:76:PRO:CD	2.31	0.42
1:A:114:ASP:HB3	1:A:117:LYS:HG2	2.02	0.42
2:B:110:ILE:HG13	2:B:110:ILE:H	1.68	0.42
2:B:414:ARG:HG2	2:B:431:PRO:CB	2.47	0.41
2:B:177:ASN:HD22	2:B:177:ASN:HA	1.58	0.41
2:B:175:ILE:H	2:B:175:ILE:HG13	1.63	0.41
1:A:323:PRO:HA	1:A:324:PRO:HD3	1.92	0.41
2:B:164:LYS:HA	2:B:164:LYS:HD3	1.97	0.41
1:A:163:GLY:HA3	1:A:306:VAL:HG21	2.03	0.40
2:B:147:GLN:HA	2:B:416:ILE:O	2.21	0.40
2:B:456:VAL:HG12	2:B:534:HIS:CE1	2.56	0.40
2:B:405:ILE:HG12	2:B:410:ILE:HG23	2.03	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	297/346 (86%)	278 (94%)	17 (6%)	2 (1%)	26 49
2	B	469/551 (85%)	443 (94%)	22 (5%)	4 (1%)	21 41
3	D	75/115 (65%)	73 (97%)	2 (3%)	0	100 100
All	All	841/1012 (83%)	794 (94%)	41 (5%)	6 (1%)	26 49

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	ASN
2	B	175	ILE
2	B	484	ASP

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Mol	Chain	Res	Type
2	B	346	LYS
2	B	6	GLY
1	A	75	ASP

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	259/296 (88%)	254 (98%)	5 (2%)	65 85
2	B	414/475 (87%)	397 (96%)	17 (4%)	37 65
3	D	71/104 (68%)	70 (99%)	1 (1%)	74 90
All	All	744/875 (85%)	721 (97%)	23 (3%)	47 75

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

Mol	Chain	Res	Type
1	A	40	LEU
1	A	79	GLN
1	A	230	LYS
1	A	278	ASP
1	A	299	MET
2	B	5	ARG
2	B	7	LEU
2	B	32	LEU
2	B	45	ASP
2	B	57	LEU
2	B	81	LEU
2	B	119	ARG
2	B	147	GLN
2	B	173	CYS
2	B	177	ASN
2	B	241	LYS
2	B	269	MET
2	B	389	THR
2	B	407	SER

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Mol	Chain	Res	Type
2	B	410	ILE
2	B	414	ARG
2	B	453	ARG
3	D	62	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	ASN
2	B	74	GLN
2	B	82	GLN
2	B	93	HIS
2	B	147	GLN
2	B	177	ASN
2	B	382	ASN
2	B	412	GLN
2	B	419	ASN
2	B	455	ASN
3	D	35	HIS
3	D	94	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	A	347	-	3,3,3	0.43	0	2,2,2	0.52	0
4	EDO	A	348	-	3,3,3	0.47	0	2,2,2	0.38	0
6	VMX	D	97	3,2	23,28,28	1.43	2 (8%)	22,41,41	3.25	6 (27%)
4	EDO	D	98	-	3,3,3	0.47	0	2,2,2	0.43	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	A	347	-	-	0/1/1/1	0/0/0/0
4	EDO	A	348	-	-	0/1/1/1	0/0/0/0
6	VMX	D	97	3,2	-	0/11/31/31	0/3/3/3
4	EDO	D	98	-	-	0/1/1/1	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	97	VMX	C1S-S	-4.77	1.66	1.78
6	D	97	VMX	O4'-C1'	3.99	1.46	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	97	VMX	N3-C2-N1	-8.49	122.39	128.89
6	D	97	VMX	O3S-S-O2S	-5.51	109.82	119.34
6	D	97	VMX	C1'-N9-C4	-2.94	122.50	126.94
6	D	97	VMX	C2'-C1'-N9	-2.23	110.88	114.29
6	D	97	VMX	C4'-O4'-C1'	2.09	112.01	109.72
6	D	97	VMX	O4'-C1'-N9	9.67	128.34	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	97	VMX	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	301/346 (86%)	0.06	7 (2%) 64 57	14, 21, 28, 30	0
2	B	477/551 (86%)	1.01	102 (21%) 1 0	16, 23, 31, 55	0
3	D	77/115 (66%)	0.39	6 (7%) 16 11	20, 23, 27, 28	0
All	All	855/1012 (84%)	0.62	115 (13%) 4 2	14, 22, 29, 55	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	490	LEU	7.0
2	B	263	ILE	6.8
2	B	511	ILE	6.7
2	B	243	TRP	6.2
2	B	249	TYR	6.1
2	B	541	ASP	6.0
2	B	245	LYS	5.8
2	B	313	LEU	5.8
2	B	284	TRP	5.7
2	B	454	LEU	5.3
2	B	459	VAL	5.3
2	B	319	ALA	5.3
2	B	486	LYS	5.0
2	B	320	ARG	4.9
2	B	507	SER	4.9
2	B	453	ARG	4.6
2	B	258	LEU	4.6
2	B	457	HIS	4.6
2	B	532	ILE	4.5
2	B	482	ILE	4.5
2	B	246	SER	4.4
2	B	480	VAL	4.3
2	B	315	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
2	B	491	ILE	4.2
2	B	254	LEU	4.1
2	B	265	TYR	4.1
2	B	244	ALA	4.0
2	B	193	PHE	4.0
2	B	512	ARG	3.9
2	B	269	MET	3.7
2	B	516	ARG	3.7
2	B	357	SER	3.6
2	B	542	VAL	3.6
2	B	273	TRP	3.6
2	B	271	LYS	3.6
2	B	264	ARG	3.5
2	B	500	ALA	3.5
2	B	483	GLU	3.4
2	B	503	HIS	3.4
2	B	513	ASN	3.4
2	B	312	VAL	3.4
2	B	250	ASP	3.3
2	B	318	TYR	3.3
3	D	36	PHE	3.2
2	B	502	ASN	3.2
2	B	504	LYS	3.2
2	B	285	ALA	3.2
2	B	499	GLU	3.2
2	B	361	LEU	3.1
2	B	283	ASP	3.1
1	A	182	ALA	3.1
2	B	262	ASP	3.1
2	B	274	ARG	3.1
2	B	447	LYS	3.1
2	B	538	LEU	3.1
2	B	331	VAL	3.0
2	B	506	LEU	3.0
2	B	253	LYS	3.0
3	D	21	TYR	3.0
2	B	256	THR	2.9
2	B	252	VAL	2.9
2	B	267	LEU	2.9
2	B	458	LYS	2.9
1	A	276	VAL	2.8
2	B	259	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	329	LEU	2.8
2	B	369	ASN	2.8
2	B	194	ASN	2.8
2	B	257	LYS	2.7
2	B	280	VAL	2.7
2	B	537	ASP	2.7
2	B	517	LEU	2.7
2	B	505	LYS	2.7
3	D	37	LYS	2.7
1	A	204	THR	2.6
2	B	485	GLY	2.6
2	B	515	SER	2.6
2	B	534	HIS	2.6
1	A	181	VAL	2.6
3	D	38	VAL	2.5
2	B	496	GLY	2.5
1	A	284	PRO	2.5
2	B	282	LEU	2.5
2	B	327	GLU	2.4
1	A	25	LEU	2.4
2	B	163	PRO	2.4
2	B	355	VAL	2.4
2	B	484	ASP	2.4
2	B	255	PHE	2.4
2	B	260	LYS	2.4
2	B	540	LYS	2.3
2	B	365	ILE	2.3
2	B	270	ASP	2.3
2	B	251	PRO	2.3
2	B	311	GLN	2.3
2	B	481	GLN	2.3
2	B	287	VAL	2.3
2	B	509	PHE	2.3
2	B	261	ASP	2.3
2	B	332	HIS	2.3
3	D	20	GLU	2.2
2	B	197	PHE	2.2
2	B	314	ASP	2.2
2	B	346	LYS	2.2
2	B	489	ILE	2.2
2	B	353	ASP	2.2
2	B	323	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	248	GLY	2.2
1	A	206	MET	2.1
2	B	266	LEU	2.1
2	B	325	SER	2.1
2	B	164	LYS	2.1
2	B	288	GLN	2.1
3	D	35	HIS	2.0
2	B	143	GLY	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
4	EDO	A	347	4/4	0.94	0.29	2.91	58,58,59,59	0
6	VMX	D	97	26/26	0.95	0.21	-0.16	17,18,23,24	0
5	ZN	B	550	1/1	0.98	0.15	-0.27	50,50,50,50	0
4	EDO	A	348	4/4	0.94	0.16	-	74,74,74,74	0
4	EDO	D	98	4/4	0.55	0.32	-	99,99,99,99	0

6.5 Other polymers (i)

There are no such residues in this entry.