wwPDB X-ray Structure Validation Summary Report (i)

Feb 4, 2024 – 08:46 PM EST

PDB ID	:	1SJB
Title	:	X-ray structure of o-succinylbenzoate synthase complexed with o-succinylbenzoic acid
Authors	:	Thoden, J.B.; Taylor-Ringia, E.A.; Garrett, J.B.; Gerlt, J.A.; Holden, H.M.; Rayment, I.
Deposited on	:	2004-03-03
Resolution	:	2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

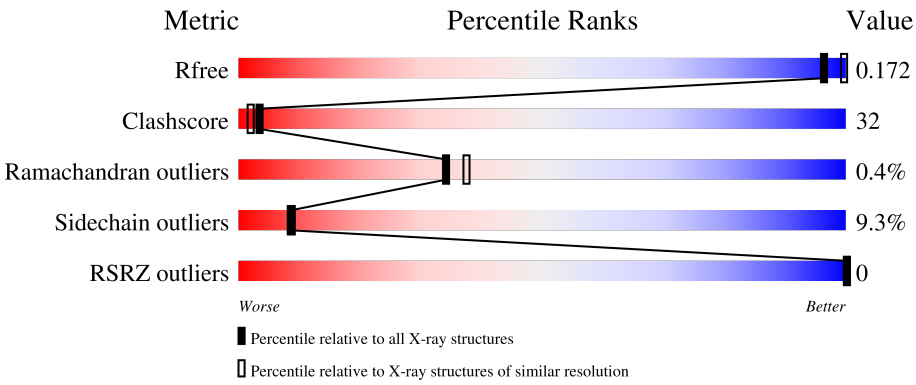
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	368	48% 40% 11% •
1	B	368	55% 33% 11% •
1	C	368	51% 38% 10% •
1	D	368	46% 42% 10% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11955 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.

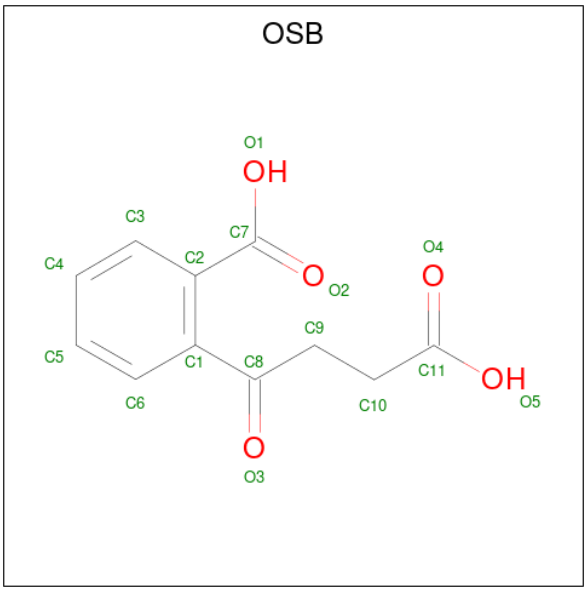
- Molecule 1 is a protein called N-acylamino acid racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	367	2772	1762	483	515	12	0	1	0
1	B	368	2781	1766	481	522	12	0	2	0
1	C	367	2782	1768	483	519	12	0	3	0
1	D	368	2778	1765	484	517	12	0	1	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0

- Molecule 3 is 2-SUCCINYLBENZOATE (three-letter code: OSB) (formula: $C_{11}H_{10}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 16 11 5	0	0
3	B	1	Total C O 16 11 5	0	0
3	C	1	Total C O 16 11 5	0	0
3	D	1	Total C O 16 11 5	0	0

- Molecule 4 is water.

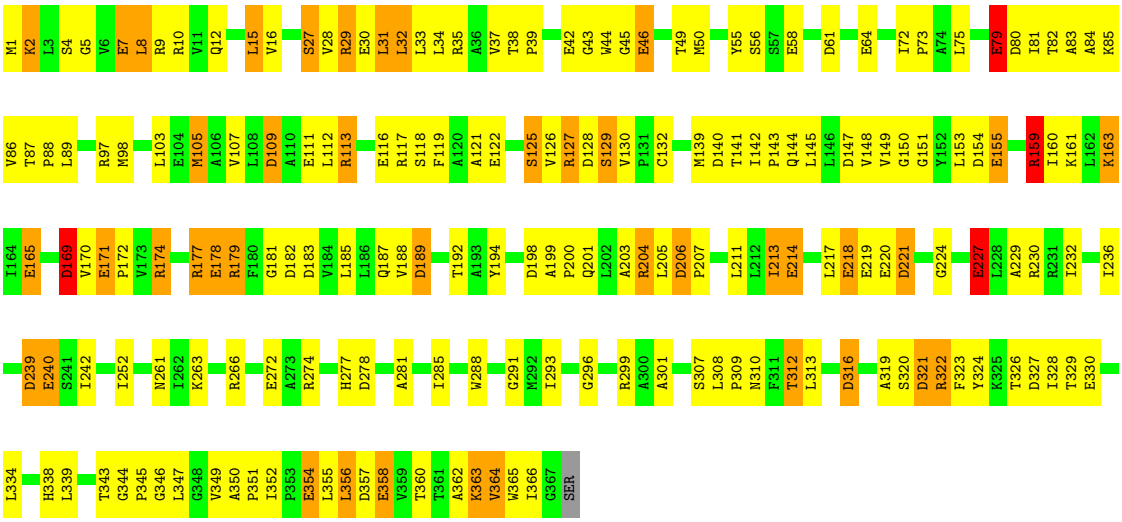
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	180	Total O 180 180	0	0
4	B	249	Total O 249 249	0	0
4	C	196	Total O 196 196	0	0
4	D	149	Total O 149 149	0	0

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.

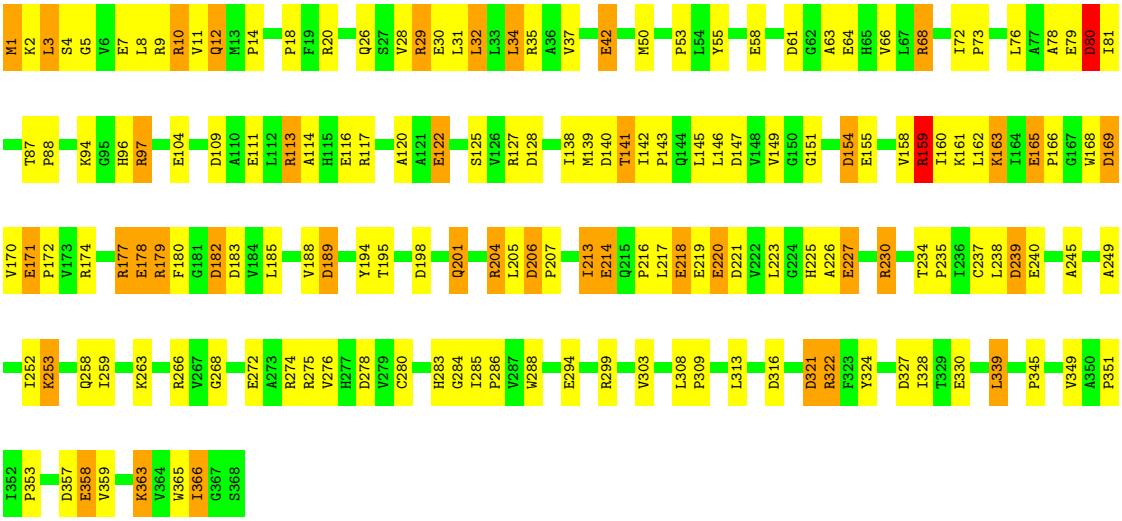
• Molecule 1: N-acylamino acid racemase

Chain A: 48% 40% 11% •



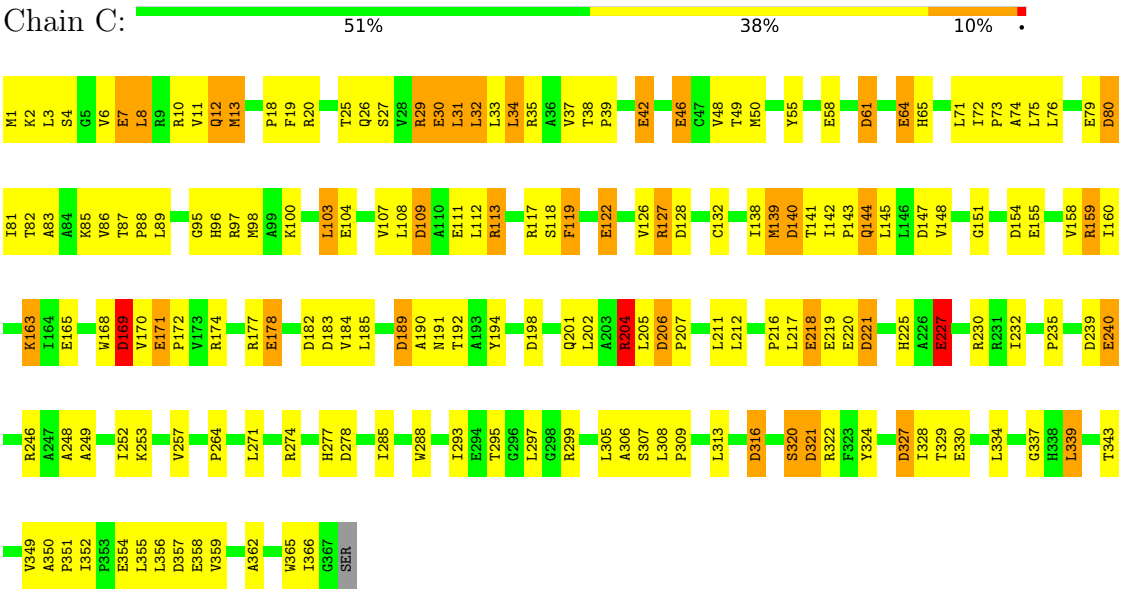
• Molecule 1: N-acylamino acid racemase

Chain B: 55% 33% 11% •



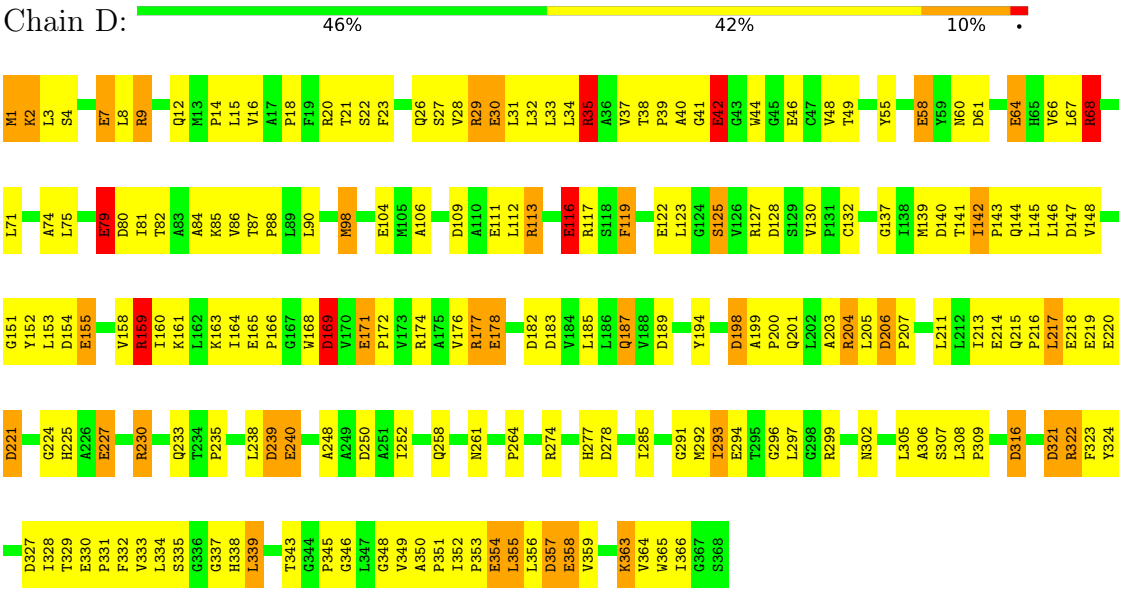
• Molecule 1: N-acylamino acid racemase

Chain C:



• Molecule 1: N-acylamino acid racemase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	216.00Å 216.00Å 261.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.20 29.95 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (30.00-2.20) 95.1 (29.95-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 2.20Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.204 , 0.272 0.174 , 0.172	Depositor DCC
R_{free} test set	11644 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å^2)	13.0	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 121.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.30$, $< L^2 > = 0.14$	Xtriage
Estimated twinning fraction	0.217 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.216 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.208 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	11955	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.30% 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, OSB

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	1.08	22/2832 (0.8%)	1.37	42/3856 (1.1%)
1	B	1.09	21/2845 (0.7%)	1.42	51/3873 (1.3%)
1	C	1.10	23/2850 (0.8%)	1.37	42/3880 (1.1%)
1	D	1.10	24/2838 (0.8%)	1.42	48/3864 (1.2%)
All	All	1.09	90/11365 (0.8%)	1.39	183/15473 (1.2%)

The worst 5 of 90 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	122	GLU	CD-OE2	8.16	1.34	1.25
1	A	171	GLU	CD-OE2	8.10	1.34	1.25
1	C	155	GLU	CD-OE2	7.55	1.33	1.25
1	B	358	GLU	CD-OE2	7.50	1.33	1.25
1	D	354	GLU	CD-OE2	7.49	1.33	1.25

The worst 5 of 183 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	159	ARG	NE-CZ-NH1	9.53	125.07	120.30
1	B	221	ASP	CB-CG-OD2	-9.47	109.78	118.30
1	D	68[A]	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	D	68[B]	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	A	322	ARG	NE-CZ-NH1	8.96	124.78	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	2772	0	2814	199	1
1	B	2781	0	2812	135	0
1	C	2782	0	2818	178	0
1	D	2778	0	2819	214	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	16	0	8	4	0
3	B	16	0	8	2	0
3	C	16	0	8	0	0
3	D	16	0	8	3	0
4	A	180	0	0	2	0
4	B	249	0	0	6	0
4	C	196	0	0	13	0
4	D	149	0	0	7	0
All	All	11955	0	11295	724	1

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 32.

The worst 5 of 724 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:38:THR:HB	1:D:39:PRO:HD2	1.20	1.17
1:A:149:VAL:HG13	1:A:160:ILE:HD13	1.25	1.11
1:D:352:ILE:O	1:D:355:LEU:HB2	1.51	1.10
1:D:49:THR:HG22	1:D:98:MET:HE3	1.27	1.07
1:A:58:GLU:HB2	1:A:98:MET:CE	1.84	1.06

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:GLU:OE2	1:D:117:ARG:NH2[17_555]	1.82	0.38

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	366/368 (100%)	338 (92%)	27 (7%)	1 (0%)	41	46
1	B	368/368 (100%)	352 (96%)	15 (4%)	1 (0%)	41	46
1	C	368/368 (100%)	346 (94%)	22 (6%)	0	100	100
1	D	367/368 (100%)	337 (92%)	26 (7%)	4 (1%)	14	12
All	All	1469/1472 (100%)	1373 (94%)	90 (6%)	6 (0%)	34	37

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	40	ALA
1	D	306	ALA
1	D	321	ASP
1	B	53	PRO
1	A	79	GLU

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	291/291 (100%)	265 (91%)	26 (9%)	9	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	293/291 (101%)	269 (92%)	24 (8%)	11	11
1	C	293/291 (101%)	265 (90%)	28 (10%)	8	8
1	D	292/291 (100%)	261 (89%)	31 (11%)	6	6
All	All	1169/1164 (100%)	1060 (91%)	109 (9%)	9	8

5 of 109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	32	LEU
1	C	227	GLU
1	D	177	ARG
1	C	80	ASP
1	C	144	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	69	HIS
1	D	26	GLN
1	B	69	HIS
1	C	338	HIS
1	B	65	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 8 ligands modelled in this entry, 4 are 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	$\#\|Z\| > 2$
3	OSB	A	1000	2	16,16,16	1.49	3 (18%)	20,21,21	3.52	7 (35%)
3	OSB	C	1200	2	16,16,16	1.32	1 (6%)	20,21,21	2.73	5 (25%)
3	OSB	D	1300	2	16,16,16	1.26	1 (6%)	20,21,21	2.28	4 (20%)
3	OSB	B	1100	2	16,16,16	1.32	2 (12%)	20,21,21	2.57	4 (20%)

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
3	OSB	A	1000	2	-	9/13/13/13	0/1/1/1
3	OSB	C	1200	2	-	2/13/13/13	0/1/1/1
3	OSB	D	1300	2	-	5/13/13/13	0/1/1/1
3	OSB	B	1100	2	-	4/13/13/13	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1000	OSB	C9-C8	3.40	1.56	1.51
3	C	1200	OSB	C9-C8	2.56	1.54	1.51
3	D	1300	OSB	C9-C8	2.28	1.54	1.51
3	A	1000	OSB	C2-C7	-2.25	1.44	1.49
3	B	1100	OSB	C2-C7	-2.18	1.45	1.49

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1000	OSB	C10-C9-C8	12.11	127.41	112.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1200	OSB	C10-C9-C8	10.54	125.51	112.76
3	B	1100	OSB	C10-C9-C8	10.10	124.98	112.76
3	D	1300	OSB	C10-C9-C8	8.05	122.51	112.76
3	A	1000	OSB	C9-C10-C11	5.74	125.97	113.60

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1000	OSB	O3-C8-C9-C10
3	A	1000	OSB	C1-C8-C9-C10
3	B	1100	OSB	C6-C1-C8-O3
3	D	1300	OSB	C6-C1-C8-O3
3	A	1000	OSB	C6-C1-C8-O3

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1000	OSB	4	0
3	D	1300	OSB	3	0
3	B	1100	OSB	2	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	367/368 (99%)	-1.30	0	100	100	22, 51, 85, 99	0
1	B	368/368 (100%)	-1.46	0	100	100	22, 37, 66, 94	0
1	C	367/368 (99%)	-1.35	0	100	100	25, 47, 80, 100	0
1	D	368/368 (100%)	-1.22	0	100	100	24, 53, 88, 100	0
All	All	1470/1472 (99%)	-1.33	0	100	100	22, 47, 82, 100	0

There are no RSRZ outliers to report.

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
3	OSB	D	1300	16/16	0.94	0.12	50,72,100,100	0
3	OSB	A	1000	16/16	0.97	0.08	41,61,100,100	0
3	OSB	B	1100	16/16	0.98	0.06	20,49,66,71	0
3	OSB	C	1200	16/16	0.98	0.10	16,48,81,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	C	1201	1/1	0.98	0.06	67,67,67,67	0
2	MG	A	1001	1/1	0.99	0.03	49,49,49,49	0
2	MG	D	1301	1/1	0.99	0.16	69,69,69,69	0
2	MG	B	1101	1/1	1.00	0.03	45,45,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.