



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 4, 2019 – 03:00 PM EDT

PDB ID : 6A2D
Title : Crystal structure of a synthase 2 from santalum album in complex with ligand1
Authors : Han, X.; Ko, T.P.; Liu, W.D.; Zheng, Y.Y.; Chen, C.C.; Guo, R.T.
Deposited on : 2018-06-10
Resolution : 1.96 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : rb-20031633
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

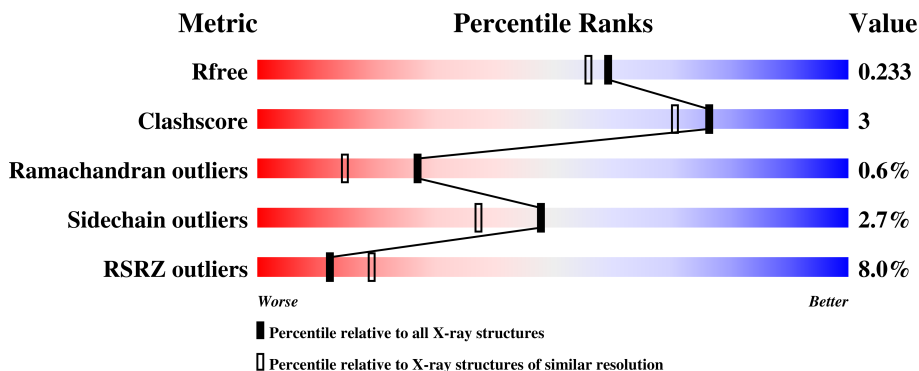
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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}	111664	2220 (1.96-1.96)
Clashscore	122126	2333 (1.96-1.96)
Ramachandran outliers	120053	2314 (1.96-1.96)
Sidechain outliers	120020	2314 (1.96-1.96)
RSRZ outliers	108989	2174 (1.96-1.96)

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 $\leq 5\%$. 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	566	 5% 83% 8% 9%
1	B	566	 10% 84% 7% 8%

2 Entry composition [i](#)

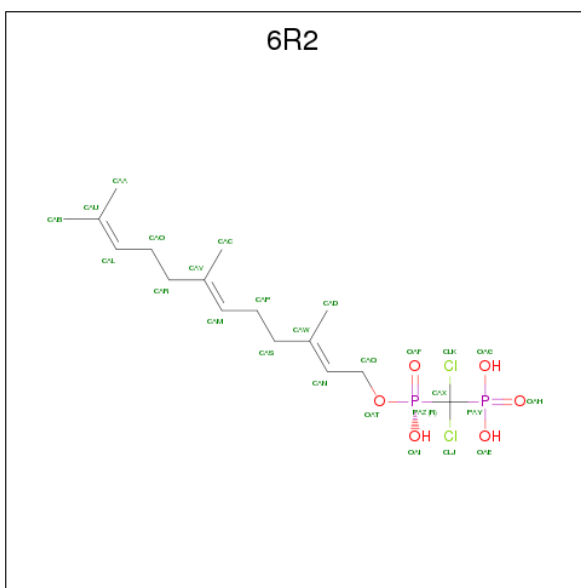
There are 4 unique types of molecules in this entry. The entry contains 9422 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Sesquisabinene B synthase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	515	Total	C	N	O	S	0	0	0
			4225	2728	700	778	19			
1	B	519	Total	C	N	O	S	0	0	0
			4260	2749	704	787	20			

- Molecule 2 is [bis(chloranyl)-[oxidanyl]-[(2 {E},6 {E})-3,7,11-trimethyldodeca-2,6,10-trienoxyl]phosphoryl]methyl]phosphonic acid (three-letter code: 6R2) (formula: C₁₆H₂₈Cl₂O₆P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	O	P		
2	A	1	Total	C	Cl	O	P	0	0
			26	16	2	6	2		
2	B	1	Total	C	Cl	O	P	0	0
			26	16	2	6	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

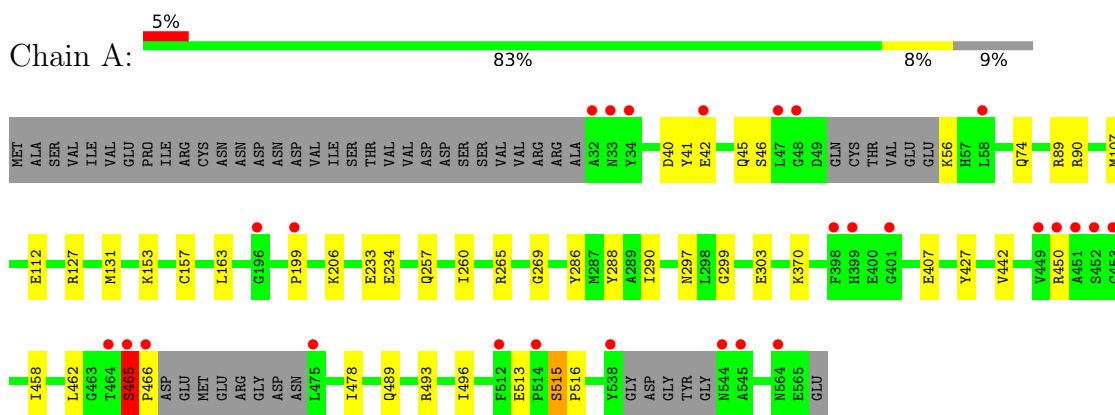
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	531	Total O 531 531	0	0
4	B	350	Total O 350 350	0	0

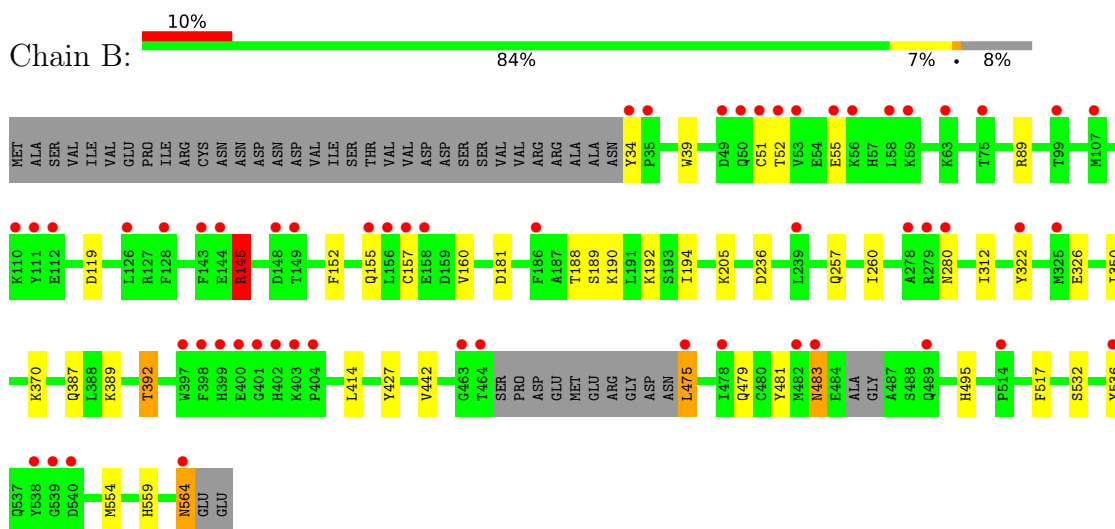
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Sesquisabinene B synthase 2



- Molecule 1: Sesquisabinene B synthase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	132.53Å 132.53Å 141.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.96 24.83 – 1.96	Depositor EDS
% Data completeness (in resolution range)	99.9 (25.00-1.96) 100.0 (24.83-1.96)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 1.96Å)	Xtrriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.178 , 0.225 0.190 , 0.233	Depositor DCC
R_{free} test set	4322 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtrriage
Anisotropy	0.017	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9422	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 6R2, MG

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	0.75	0/4330	0.79	0/5862
1	B	0.59	0/4366	0.72	0/5911
All	All	0.67	0/8696	0.76	0/11773

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	4225	0	4176	28	0
1	B	4260	0	4203	28	0
2	A	26	0	0	0	0
2	B	26	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	531	0	0	6	0
4	B	350	0	0	3	0
All	All	9422	0	8379	55	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 3.

All (55) 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:465:SER:HB2	1:A:466:PRO:CD	1.46	1.45
1:A:465:SER:CB	1:A:466:PRO:HD3	1.72	1.19
1:A:515:SER:HB2	1:A:516:PRO:HD3	1.31	1.11
1:A:515:SER:CB	1:A:516:PRO:HD3	1.84	1.06
1:A:465:SER:CB	1:A:466:PRO:CD	2.29	1.05
1:A:515:SER:HB2	1:A:516:PRO:CD	1.87	1.04
1:A:297:ASN:HB2	4:A:1449:HOH:O	1.83	0.79
1:A:465:SER:HB2	1:A:466:PRO:HD3	0.76	0.75
1:A:515:SER:HB3	1:A:516:PRO:HD3	1.72	0.72
1:A:515:SER:CB	1:A:516:PRO:CD	2.49	0.70
1:A:489:GLN:HE22	1:A:493:ARG:HE	1.44	0.64
1:A:41:TYR:O	1:A:45:GLN:HG3	1.99	0.61
1:B:160:VAL:HG22	1:B:194:ILE:CD1	2.33	0.59
1:A:206:LYS:HE2	1:A:234:GLU:OE2	2.05	0.56
1:B:152:PHE:N	4:B:1007:HOH:O	2.37	0.56
1:A:286:TYR:CE2	1:A:290:ILE:HD11	2.41	0.55
1:B:312:ILE:HG23	1:B:387:GLN:HE22	1.72	0.54
1:B:427:TYR:CD2	1:B:442:VAL:HG21	2.42	0.54
1:A:450:ARG:NE	4:A:1005:HOH:O	2.36	0.54
1:A:112:GLU:HG3	4:A:1209:HOH:O	2.07	0.53
1:A:153:LYS:HE2	4:A:1435:HOH:O	2.09	0.53
1:A:427:TYR:CD2	1:A:442:VAL:HG21	2.43	0.53
1:A:206:LYS:CE	1:A:234:GLU:OE2	2.57	0.52
1:A:458:ILE:HG23	1:A:496:ILE:CG2	2.41	0.51
1:B:157:CYS:CB	1:B:190:LYS:HD2	2.41	0.51
1:B:483:ASN:O	1:B:483:ASN:ND2	2.42	0.50
1:A:299:GLY:O	1:A:303:GLU:HG3	2.11	0.50
1:B:475:LEU:N	1:B:475:LEU:HD12	2.27	0.50
1:A:157:CYS:HA	1:A:163:LEU:HD11	1.96	0.48
1:A:462:LEU:HD23	1:A:478:ILE:HD11	1.97	0.46
1:B:322:TYR:CD2	1:B:350:ILE:HD11	2.50	0.46
1:B:427:TYR:CE2	1:B:442:VAL:HG21	2.51	0.46
1:B:205:LYS:NZ	4:B:1024:HOH:O	2.47	0.46
1:B:481:TYR:CE1	1:B:495:HIS:CE1	3.05	0.45
1:A:233:GLU:HG2	4:A:1451:HOH:O	2.17	0.45
1:A:127:ARG:O	1:A:131:MET:HG2	2.17	0.45
1:A:257:GLN:O	1:A:260:ILE:HG22	2.17	0.45
1:B:188:THR:O	1:B:192:LYS:HG3	2.17	0.44
1:B:257:GLN:O	1:B:260:ILE:HG22	2.18	0.44
1:B:564:ASN:HD22	1:B:564:ASN:C	2.20	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:ASP:OD1	1:B:145:ARG:HG3	2.18	0.43
1:B:389:LYS:O	1:B:392:THR:HG22	2.18	0.43
1:B:257:GLN:HA	1:B:260:ILE:HG22	2.00	0.43
1:A:269:GLY:O	1:B:370:LYS:HE2	2.19	0.43
1:B:554:MET:CE	1:B:559:HIS:CE1	3.02	0.43
1:B:532:SER:O	1:B:536:TYR:HB3	2.19	0.42
1:B:322:TYR:HD2	1:B:350:ILE:HD11	1.85	0.42
1:B:34:TYR:HA	4:B:1142:HOH:O	2.20	0.42
1:B:414:LEU:HD12	1:B:414:LEU:C	2.40	0.42
1:B:236:ASP:OD1	1:B:236:ASP:N	2.41	0.41
1:B:39:TRP:HB3	1:B:280:ASN:OD1	2.20	0.41
1:B:442:VAL:HG22	1:B:517:PHE:HE1	1.85	0.41
1:B:160:VAL:HG13	1:B:194:ILE:HD11	2.03	0.41
1:B:554:MET:HE2	1:B:559:HIS:CE1	2.56	0.41
1:A:265:ARG:CD	4:A:1461: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	507/566 (90%)	494 (97%)	10 (2%)	3 (1%)	27	15
1	B	513/566 (91%)	497 (97%)	13 (2%)	3 (1%)	27	15
All	All	1020/1132 (90%)	991 (97%)	23 (2%)	6 (1%)	27	15

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	465	SER
1	A	515	SER
1	B	51	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	145	ARG
1	B	55	GLU
1	A	199	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	462/507 (91%)	449 (97%)	13 (3%)	47	35
1	B	466/507 (92%)	454 (97%)	12 (3%)	49	39
All	All	928/1014 (92%)	903 (97%)	25 (3%)	48	37

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	A	42	GLU
1	A	46	SER
1	A	56	LYS
1	A	74	GLN
1	A	89	ARG
1	A	90	ARG
1	A	107	MET
1	A	288	TYR
1	A	370	LYS
1	A	407	GLU
1	A	465	SER
1	A	513	GLU
1	B	52	THR
1	B	89	ARG
1	B	145	ARG
1	B	155	GLN
1	B	181	ASP
1	B	189	SER
1	B	326	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	392	THR
1	B	475	LEU
1	B	479	GLN
1	B	483	ASN
1	B	564	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	479	GLN
1	A	489	GLN
1	B	559	HIS
1	B	564	ASN

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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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
2	6R2	A	900	3	25,25,25	3.62	10 (40%)	23,36,36	1.94	8 (34%)
2	6R2	B	900	3	25,25,25	3.74	10 (40%)	23,36,36	2.18	11 (47%)

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
2	6R2	A	900	3	-	0/34/37/37	0/0/0/0
2	6R2	B	900	3	-	0/34/37/37	0/0/0/0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	6R2	CAX-CLJ	-4.70	1.76	1.79
2	A	900	6R2	PAY-CAX	-2.94	1.83	1.86
2	A	900	6R2	CAX-CLK	-2.38	1.77	1.79
2	B	900	6R2	PAZ-CAX	-2.22	1.84	1.86
2	A	900	6R2	PAZ-OAI	2.31	1.61	1.56
2	B	900	6R2	PAY-CAX	2.64	1.89	1.86
2	B	900	6R2	PAY-OAG	2.77	1.59	1.54
2	A	900	6R2	PAZ-OAF	3.24	1.56	1.51
2	B	900	6R2	PAZ-OAI	3.85	1.64	1.56
2	A	900	6R2	PAZ-OAT	4.23	1.63	1.57
2	B	900	6R2	PAZ-OAT	5.14	1.65	1.57
2	B	900	6R2	PAY-OAH	6.13	1.60	1.50
2	B	900	6R2	CAL-CAU	6.79	1.52	1.32
2	A	900	6R2	CAL-CAU	7.25	1.53	1.32
2	B	900	6R2	CAX-CLK	7.27	1.85	1.79
2	A	900	6R2	CAM-CAV	7.44	1.51	1.33
2	A	900	6R2	PAY-OAH	8.05	1.63	1.50
2	B	900	6R2	CAM-CAV	8.05	1.52	1.33
2	A	900	6R2	CAN-CAW	8.27	1.53	1.33
2	B	900	6R2	CAN-CAW	8.55	1.53	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	6R2	OAG-PAY-OAH	-3.39	105.44	113.06
2	B	900	6R2	OAT-PAZ-OAF	-3.38	109.47	115.45
2	B	900	6R2	CAO-CAL-CAU	-2.85	117.84	127.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	6R2	CAP-CAM-CAV	-2.60	121.29	127.67
2	A	900	6R2	CAS-CAP-CAM	-2.52	103.55	111.88
2	B	900	6R2	CAR-CAV-CAM	-2.31	116.36	121.11
2	A	900	6R2	CAO-CAL-CAU	-2.25	119.94	127.77
2	B	900	6R2	CAS-CAW-CAN	-2.07	116.85	121.11
2	A	900	6R2	CAP-CAM-CAV	-2.02	122.71	127.67
2	B	900	6R2	OAE-PAY-OAG	2.03	113.72	107.99
2	A	900	6R2	OAE-PAY-OAG	2.69	115.58	107.99
2	B	900	6R2	CAD-CAW-CAS	2.85	120.19	115.29
2	B	900	6R2	CAA-CAU-CAB	2.96	121.24	114.59
2	A	900	6R2	CAD-CAW-CAS	2.97	120.40	115.29
2	A	900	6R2	PAZ-OAT-CAQ	3.17	127.13	121.30
2	A	900	6R2	CAC-CAV-CAR	3.29	120.95	115.29
2	A	900	6R2	OAI-PAZ-OAF	3.54	119.88	111.34
2	B	900	6R2	CAC-CAV-CAR	3.57	121.44	115.29
2	B	900	6R2	PAZ-OAT-CAQ	4.24	129.09	121.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	515/566 (90%)	0.07	27 (5%) 27 37	13, 26, 58, 91	0
1	B	519/566 (91%)	0.53	56 (10%) 6 10	17, 38, 78, 140	0
All	All	1034/1132 (91%)	0.31	83 (8%) 12 19	13, 33, 72, 140	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	51	CYS	23.8
1	A	544	ASN	9.2
1	B	399	HIS	7.7
1	B	52	THR	6.7
1	B	464	THR	6.1
1	B	50	GLN	6.1
1	B	401	GLY	5.9
1	B	279	ARG	5.7
1	B	56	LYS	5.5
1	A	538	TYR	5.3
1	A	32	ALA	5.1
1	B	53	VAL	5.1
1	B	55	GLU	4.9
1	B	278	ALA	4.5
1	B	149	THR	4.2
1	A	451	ALA	4.1
1	B	538	TYR	3.6
1	A	475	LEU	3.5
1	B	398	PHE	3.5
1	A	196	GLY	3.4
1	B	514	PRO	3.4
1	A	47	LEU	3.4
1	A	453	CYS	3.4
1	B	239	LEU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	157	CYS	3.3
1	A	399	HIS	3.3
1	A	465	SER	3.2
1	B	34	TYR	3.2
1	B	158	GLU	3.2
1	B	186	PHE	3.1
1	B	110	LYS	3.1
1	B	280	ASN	3.1
1	B	75	THR	3.1
1	B	112	GLU	3.0
1	B	463	GLY	2.9
1	B	478	ILE	2.9
1	A	398	PHE	2.9
1	B	155	GLN	2.9
1	B	148	ASP	2.9
1	B	35	PRO	2.9
1	A	401	GLY	2.8
1	B	483	ASN	2.8
1	B	111	TYR	2.7
1	A	450	ARG	2.7
1	A	42	GLU	2.6
1	A	564	ASN	2.6
1	B	403	LYS	2.6
1	B	49	ASP	2.5
1	B	107	MET	2.5
1	A	545	ALA	2.5
1	A	512	PHE	2.4
1	B	128	PHE	2.4
1	B	540	ASP	2.4
1	B	325	MET	2.4
1	B	99	THR	2.4
1	B	404	PRO	2.4
1	B	59	LYS	2.4
1	A	449	VAL	2.3
1	B	156	LEU	2.3
1	A	48	GLY	2.3
1	B	539	GLY	2.3
1	A	464	THR	2.2
1	B	144	GLU	2.2
1	A	58	LEU	2.2
1	B	143	PHE	2.2
1	B	482	MET	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	402	HIS	2.2
1	B	63	LYS	2.2
1	A	466	PRO	2.2
1	B	397	TRP	2.2
1	A	452	SER	2.2
1	B	58	LEU	2.2
1	B	126	LEU	2.2
1	B	400	GLU	2.2
1	B	475	LEU	2.1
1	B	564	ASN	2.1
1	B	536	TYR	2.1
1	B	489	GLN	2.1
1	A	199	PRO	2.1
1	A	514	PRO	2.1
1	A	34	TYR	2.0
1	B	322	TYR	2.0
1	A	33	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 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. 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	MG	B	901	1/1	0.68	0.10	44,44,44,44	0
3	MG	A	902	1/1	0.90	0.07	25,25,25,25	0
2	6R2	B	900	26/26	0.91	0.17	34,48,62,66	0
3	MG	B	902	1/1	0.93	0.08	37,37,37,37	0
2	6R2	A	900	26/26	0.96	0.11	22,31,46,51	0
3	MG	A	901	1/1	0.97	0.03	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.