



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 07:43 AM EDT

PDB ID : 1Y7I  
Title : Structural and biochemical studies identify tobacco SABP2 as a methylsalicylate esterase and further implicate it in plant innate immunity, Northeast Structural Genomics Target AR2241  
Authors : Forouhar, F.; Yang, Y.; Kumar, D.; Chen, Y.; Fridman, E.; Park, S.W.; Chiang, Y.; Acton, T.B.; Montelione, G.T.; Pichersky, E.; Klessig, D.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2004-12-08  
Resolution : 2.10 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](mailto: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>.

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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 : 2.35  
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)

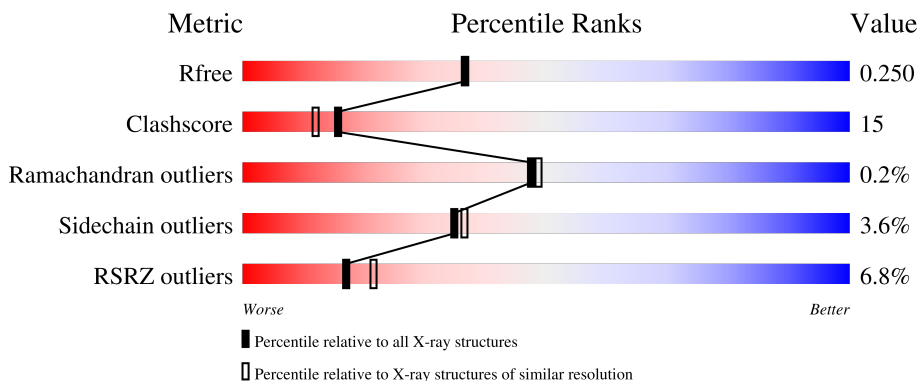
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	268	 7% 66% 29%
1	B	268	 6% 67% 29%

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 4612 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 salicylic acid-binding protein 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	258	2042	1317	331	380	5	9	0	0	0
1	B	262	2079	1340	339	386	5	9	0	0	0

There are 34 discrepancies between the modelled and reference sequences:

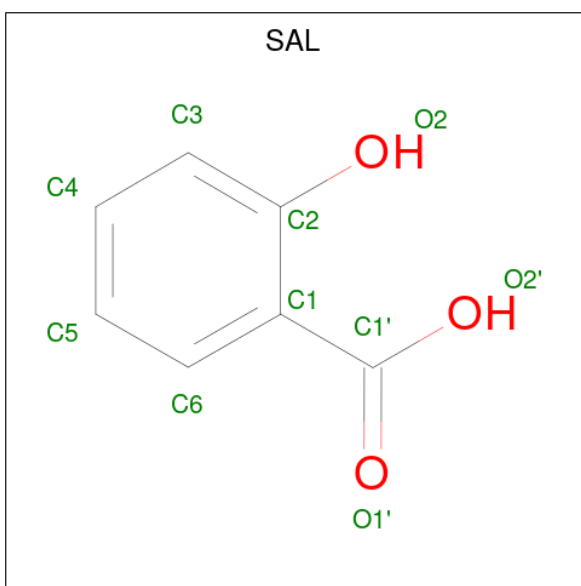
Chain	Residue	Modelled	Actual	Comment	Reference
A	63	MSE	MET	modified residue	UNP Q6RYA0
A	66	MSE	MET	modified residue	UNP Q6RYA0
A	85	MSE	MET	modified residue	UNP Q6RYA0
A	91	MSE	MET	modified residue	UNP Q6RYA0
A	108	MSE	MET	modified residue	UNP Q6RYA0
A	149	MSE	MET	modified residue	UNP Q6RYA0
A	183	MSE	MET	modified residue	UNP Q6RYA0
A	239	MSE	MET	modified residue	UNP Q6RYA0
A	241	MSE	MET	modified residue	UNP Q6RYA0
A	261	LEU	-	expression tag	UNP Q6RYA0
A	262	GLU	-	expression tag	UNP Q6RYA0
A	263	HIS	-	expression tag	UNP Q6RYA0
A	264	HIS	-	expression tag	UNP Q6RYA0
A	265	HIS	-	expression tag	UNP Q6RYA0
A	266	HIS	-	expression tag	UNP Q6RYA0
A	267	HIS	-	expression tag	UNP Q6RYA0
A	268	HIS	-	expression tag	UNP Q6RYA0
B	63	MSE	MET	modified residue	UNP Q6RYA0
B	66	MSE	MET	modified residue	UNP Q6RYA0
B	85	MSE	MET	modified residue	UNP Q6RYA0
B	91	MSE	MET	modified residue	UNP Q6RYA0
B	108	MSE	MET	modified residue	UNP Q6RYA0
B	149	MSE	MET	modified residue	UNP Q6RYA0
B	183	MSE	MET	modified residue	UNP Q6RYA0
B	239	MSE	MET	modified residue	UNP Q6RYA0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	241	MSE	MET	modified residue	UNP Q6RYA0
B	261	LEU	-	expression tag	UNP Q6RYA0
B	262	GLU	-	expression tag	UNP Q6RYA0
B	263	HIS	-	expression tag	UNP Q6RYA0
B	264	HIS	-	expression tag	UNP Q6RYA0
B	265	HIS	-	expression tag	UNP Q6RYA0
B	266	HIS	-	expression tag	UNP Q6RYA0
B	267	HIS	-	expression tag	UNP Q6RYA0
B	268	HIS	-	expression tag	UNP Q6RYA0

- Molecule 2 is 2-HYDROXYBENZOIC ACID (three-letter code: SAL) (formula: C<sub>7</sub>H<sub>6</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 7 3	0	0
2	A	1	Total C O 10 7 3	0	0
2	B	1	Total C O 10 7 3	0	0

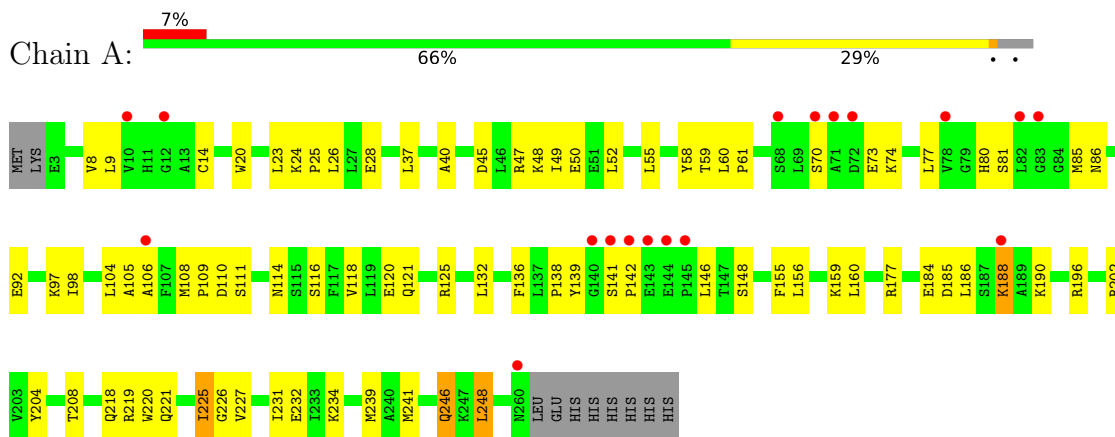
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	226	Total O 226 226	0	0
3	B	235	Total O 235 235	0	0

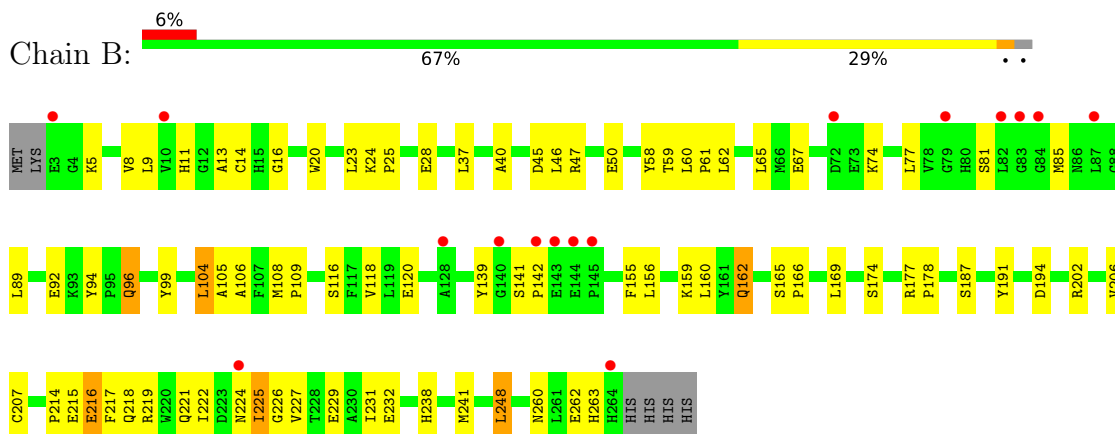
### 3 Residue-property plots [i](#)

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: salicylic acid-binding protein 2



- Molecule 1: salicylic acid-binding protein 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.22Å 48.02Å 92.59Å 90.00° 110.63° 90.00°	Depositor
Resolution (Å)	29.53 – 2.10 29.53 – 2.09	Depositor EDS
% Data completeness (in resolution range)	91.9 (29.53-2.10) 96.3 (29.53-2.09)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.90 (at 2.10Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.197 , 0.248 0.201 , 0.250	Depositor DCC
$R_{free}$ test set	3423 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.6	Xtrriage
Anisotropy	0.462	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 50.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4612	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SAL

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	0/2085	0.55	0/2808
1	B	0.34	0/2124	0.55	0/2861
All	All	0.34	0/4209	0.55	0/5669

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 [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	2042	0	2015	59	0
1	B	2079	0	2046	63	0
2	A	20	0	8	0	0
2	B	10	0	4	0	0
3	A	226	0	0	4	0
3	B	235	0	0	3	0
All	All	4612	0	4073	121	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 15.

All (121) 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:B:108:MSE:HE3	1:B:225:ILE:HG12	1.42	0.99
1:A:208:THR:HG21	1:A:234:LYS:HD2	1.54	0.89
1:A:121:GLN:HB3	1:A:125:ARG:HH12	1.36	0.89
1:A:85:MSE:SE	1:A:109:PRO:HG3	2.23	0.89
1:A:70:SER:HB3	1:A:73:GLU:HB2	1.57	0.86
1:B:85:MSE:SE	1:B:109:PRO:HG3	2.27	0.84
1:B:81:SER:HA	1:B:106:ALA:HA	1.60	0.83
1:A:108:MSE:HE3	1:A:225:ILE:HG12	1.59	0.82
1:B:207:CYS:H	1:B:218:GLN:HE22	1.23	0.82
1:A:108:MSE:H	1:A:221:GLN:HE22	1.28	0.79
1:A:81:SER:HA	1:A:106:ALA:HA	1.67	0.77
1:B:108:MSE:H	1:B:221:GLN:HE22	1.34	0.76
1:B:5:LYS:NZ	1:B:260:ASN:HD21	1.83	0.75
1:A:185:ASP:HA	1:A:188:LYS:HE3	1.71	0.73
1:A:108:MSE:H	1:A:221:GLN:NE2	1.84	0.73
1:B:5:LYS:HZ1	1:B:260:ASN:HD21	1.36	0.73
1:B:108:MSE:H	1:B:221:GLN:NE2	1.90	0.68
1:A:121:GLN:HB3	1:A:125:ARG:NH1	2.09	0.68
1:B:202:ARG:O	1:B:227:VAL:HG22	1.95	0.67
1:A:48:LYS:HG2	1:B:46:LEU:HD13	1.77	0.66
1:A:118:VAL:HG11	1:A:221:GLN:NE2	2.10	0.65
1:A:246:GLN:HG2	3:A:505:HOH:O	1.97	0.64
1:A:49:ILE:HD12	1:A:52:LEU:HD12	1.78	0.64
1:B:74:LYS:HE2	1:B:96:GLN:O	1.97	0.64
1:A:92:GLU:O	1:A:196:ARG:HD3	1.98	0.63
1:A:108:MSE:HE3	1:A:225:ILE:CG1	2.29	0.61
1:A:185:ASP:O	1:A:188:LYS:HG2	2.01	0.60
1:B:156:LEU:HD23	1:B:160:LEU:HD12	1.84	0.60
1:A:74:LYS:HD3	3:A:690:HOH:O	2.02	0.59
1:B:24:LYS:HB3	1:B:25:PRO:HD3	1.83	0.59
1:B:108:MSE:O	1:B:118:VAL:HG21	2.03	0.58
1:B:118:VAL:HG23	3:B:510:HOH:O	2.02	0.58
1:B:141:SER:HB2	1:B:142:PRO:HD2	1.84	0.58
1:A:37:LEU:HD23	1:A:37:LEU:H	1.68	0.58
1:A:55:LEU:HD22	1:A:186:LEU:HD21	1.86	0.57
1:B:224:ASN:ND2	1:B:225:ILE:HG22	2.19	0.57
1:A:59:THR:HG23	1:A:86:ASN:HB3	1.87	0.57
1:B:241:MSE:SE	1:B:241:MSE:H	2.38	0.56
1:A:24:LYS:HB3	1:A:25:PRO:HD3	1.88	0.56
1:A:8:VAL:HB	1:A:77:LEU:HD13	1.88	0.55
1:A:23:LEU:HD22	1:A:248:LEU:HD13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:GLU:H	1:B:216:GLU:CD	2.08	0.55
1:A:116:SER:O	1:A:120:GLU:HG3	2.07	0.54
1:A:246:GLN:H	1:A:246:GLN:CD	2.11	0.54
1:B:23:LEU:HD22	1:B:248:LEU:HD13	1.89	0.54
1:A:60:LEU:HB3	1:A:61:PRO:HD3	1.90	0.53
1:A:156:LEU:HD23	1:A:160:LEU:HD12	1.91	0.53
1:A:108:MSE:N	1:A:221:GLN:HE22	2.03	0.52
1:B:24:LYS:O	1:B:28:GLU:HG3	2.09	0.52
1:A:241:MSE:H	1:A:241:MSE:SE	2.44	0.51
1:A:141:SER:HB2	1:A:142:PRO:HD2	1.91	0.51
1:A:155:PHE:O	1:A:159:LYS:HB2	2.11	0.51
1:A:24:LYS:O	1:A:28:GLU:HG3	2.11	0.51
1:A:74:LYS:HD2	1:A:97:LYS:HA	1.93	0.50
1:B:8:VAL:HB	1:B:77:LEU:HD23	1.93	0.50
1:B:160:LEU:HD22	1:B:238:HIS:CD2	2.46	0.50
1:A:132:LEU:HD12	1:A:155:PHE:HA	1.93	0.50
1:B:104:LEU:O	1:B:105:ALA:C	2.50	0.49
1:A:225:ILE:HG13	1:A:226:GLY:N	2.26	0.48
1:B:40:ALA:HB3	1:B:58:TYR:HA	1.95	0.48
1:B:202:ARG:NE	1:B:225:ILE:HD11	2.29	0.48
1:B:224:ASN:HD22	1:B:225:ILE:HG22	1.77	0.48
1:A:136:PHE:HA	1:A:148:SER:O	2.14	0.48
1:B:231:ILE:HG22	1:B:232:GLU:N	2.29	0.48
1:B:45:ASP:OD2	1:B:47:ARG:HB2	2.13	0.47
1:A:104:LEU:O	1:A:105:ALA:C	2.51	0.47
1:B:109:PRO:O	1:B:225:ILE:HD13	2.14	0.47
1:B:162:GLN:H	1:B:162:GLN:HG3	1.32	0.47
1:B:11:HIS:CD2	1:B:16:GLY:HA2	2.50	0.47
1:B:206:VAL:HA	1:B:218:GLN:NE2	2.30	0.46
1:A:202:ARG:O	1:A:227:VAL:HG22	2.15	0.46
1:B:165:SER:HB2	1:B:166:PRO:HD2	1.98	0.46
1:A:231:ILE:HG22	1:A:232:GLU:N	2.30	0.45
1:B:219:ARG:HH11	1:B:219:ARG:HG3	1.81	0.45
1:A:81:SER:CA	1:A:106:ALA:HA	2.42	0.45
1:A:204:TYR:OH	1:A:218:GLN:HG2	2.17	0.45
1:A:37:LEU:H	1:A:37:LEU:CD2	2.29	0.45
1:B:5:LYS:HZ1	1:B:260:ASN:ND2	2.10	0.45
1:B:14:CYS:HA	1:B:177:ARG:O	2.17	0.45
1:A:108:MSE:SE	1:A:225:ILE:HD11	2.67	0.44
1:A:80:HIS:CG	1:A:241:MSE:HE1	2.52	0.44
1:B:214:PRO:HB2	1:B:216:GLU:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:LEU:HB3	1:A:20:TRP:CE2	2.53	0.43
1:B:60:LEU:HB3	1:B:61:PRO:HD3	2.00	0.43
1:B:155:PHE:O	1:B:159:LYS:HB2	2.18	0.43
1:B:202:ARG:HE	1:B:225:ILE:HD11	1.82	0.43
1:B:162:GLN:HE21	1:B:162:GLN:HB2	1.62	0.43
1:A:45:ASP:OD2	1:A:47:ARG:HB2	2.17	0.43
1:B:50:GLU:HA	1:B:139:TYR:CD2	2.54	0.43
1:B:67:GLU:HB2	1:B:94:TYR:OH	2.19	0.43
1:A:138:PRO:HA	1:A:146:LEU:O	2.19	0.43
1:B:108:MSE:HA	1:B:109:PRO:HD3	1.87	0.43
1:B:217:PHE:O	1:B:221:GLN:HG3	2.19	0.43
1:A:111:SER:O	1:A:190:LYS:HE2	2.18	0.42
1:B:96:GLN:H	1:B:96:GLN:CD	2.21	0.42
3:A:559:HOH:O	1:B:174:SER:HB2	2.18	0.42
1:B:225:ILE:HG13	1:B:226:GLY:O	2.19	0.42
1:A:40:ALA:HB3	1:A:58:TYR:HA	2.02	0.42
1:B:109:PRO:HA	1:B:118:VAL:HG21	2.02	0.42
1:A:219:ARG:NH1	1:A:232:GLU:OE1	2.52	0.42
1:B:116:SER:OG	1:B:187:SER:HA	2.20	0.42
1:A:77:LEU:HD23	1:A:98:ILE:HG23	2.01	0.42
1:B:9:LEU:HB3	1:B:20:TRP:CE2	2.55	0.42
1:B:13:ALA:O	1:B:14:CYS:HB2	2.19	0.42
1:B:215:GLU:O	1:B:219:ARG:HG2	2.20	0.42
1:A:50:GLU:HA	1:A:139:TYR:CD2	2.55	0.42
1:B:65:LEU:C	1:B:65:LEU:HD23	2.40	0.41
1:B:177:ARG:HB3	1:B:178:PRO:HD2	2.03	0.41
1:B:59:THR:HG22	1:B:59:THR:O	2.21	0.41
1:B:92:GLU:HG2	1:B:191:TYR:O	2.20	0.41
1:B:229:GLU:HB2	3:B:531:HOH:O	2.21	0.41
1:A:160:LEU:O	1:A:239:MSE:HG2	2.21	0.41
1:B:262:GLU:HG3	1:B:263:HIS:ND1	2.36	0.41
1:A:110:ASP:OD2	1:A:110:ASP:C	2.59	0.40
1:A:121:GLN:HG3	1:A:220:TRP:CH2	2.56	0.40
1:A:14:CYS:HA	1:A:177:ARG:O	2.21	0.40
1:B:74:LYS:HD2	1:B:99:TYR:CE2	2.57	0.40
1:B:222:ILE:O	1:B:226:GLY:HA2	2.21	0.40
1:A:118:VAL:HG11	1:A:221:GLN:HE21	1.84	0.40
1:A:184:GLU:HB2	3:A:553:HOH:O	2.21	0.40
1:B:169:LEU:HD11	3:B:616:HOH:O	2.20	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	256/268 (96%)	243 (95%)	12 (5%)	1 (0%)	34	32
1	B	260/268 (97%)	247 (95%)	13 (5%)	0	100	100
All	All	516/536 (96%)	490 (95%)	25 (5%)	1 (0%)	47	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	LYS

### 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	220/221 (100%)	215 (98%)	5 (2%)	50	55
1	B	224/221 (101%)	213 (95%)	11 (5%)	25	23
All	All	444/442 (100%)	428 (96%)	16 (4%)	35	36

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	114	ASN
1	A	225	ILE
1	A	246	GLN
1	A	248	LEU

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Mol	Chain	Res	Type
1	B	37	LEU
1	B	62	LEU
1	B	89	LEU
1	B	96	GLN
1	B	104	LEU
1	B	120	GLU
1	B	162	GLN
1	B	194	ASP
1	B	216	GLU
1	B	225	ILE
1	B	248	LEU

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	6	HIS
1	A	114	ASN
1	A	158	HIS
1	A	221	GLN
1	B	123	ASN
1	B	162	GLN
1	B	218	GLN
1	B	221	GLN
1	B	224	ASN
1	B	260	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 monosaccharides in this entry.

## 5.6 Ligand geometry

3 ligands are modelled in this entry.

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	SAL	A	502	-	10,10,10	1.85	4 (40%)	13,13,13	1.28	2 (15%)
2	SAL	A	501	-	10,10,10	1.76	4 (40%)	13,13,13	1.13	1 (7%)
2	SAL	B	503	-	10,10,10	1.69	4 (40%)	13,13,13	1.15	2 (15%)

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	SAL	A	502	-	-	0/4/4/4	0/1/1/1
2	SAL	A	501	-	-	0/4/4/4	0/1/1/1
2	SAL	B	503	-	-	0/4/4/4	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	SAL	O1'-C1'	3.20	1.32	1.22
2	A	502	SAL	O1'-C1'	3.18	1.32	1.22
2	B	503	SAL	O1'-C1'	3.00	1.31	1.22
2	A	502	SAL	C1-C2	2.93	1.45	1.40
2	A	501	SAL	C6-C1	2.67	1.44	1.39
2	A	502	SAL	C6-C1	2.37	1.43	1.39
2	B	503	SAL	C6-C1	2.35	1.43	1.39
2	B	503	SAL	O2'-C1'	-2.21	1.23	1.30
2	B	503	SAL	C1-C2	2.14	1.44	1.40
2	A	502	SAL	O2'-C1'	-2.12	1.24	1.30
2	A	501	SAL	O2'-C1'	-2.12	1.24	1.30
2	A	501	SAL	C1-C2	2.01	1.44	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	502	SAL	O2'-C1'-C1	2.85	123.52	115.31
2	B	503	SAL	O2'-C1'-C1	2.63	122.88	115.31
2	A	501	SAL	O2'-C1'-C1	2.48	122.46	115.31
2	A	502	SAL	O1'-C1'-C1	-2.43	116.05	121.94
2	B	503	SAL	O1'-C1'-C1	-2.10	116.85	121.94

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	249/268 (92%)	0.23	18 (7%) 15 19	13, 24, 54, 66	0
1	B	253/268 (94%)	0.24	16 (6%) 20 24	9, 25, 50, 66	0
All	All	502/536 (93%)	0.24	34 (6%) 17 21	9, 25, 51, 66	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	142	PRO	5.0
1	A	142	PRO	4.8
1	A	140	GLY	4.1
1	A	143	GLU	4.0
1	B	264	HIS	4.0
1	A	141	SER	3.9
1	B	144	GLU	3.7
1	B	140	GLY	3.6
1	A	144	GLU	3.5
1	A	145	PRO	3.2
1	A	260	ASN	3.1
1	B	143	GLU	3.1
1	A	188	LYS	2.9
1	A	71	ALA	2.9
1	B	87	LEU	2.9
1	B	224	ASN	2.7
1	A	82	LEU	2.7
1	A	10	VAL	2.6
1	A	68	SER	2.6
1	B	3	GLU	2.5
1	A	78	VAL	2.5
1	A	72	ASP	2.4
1	B	72	ASP	2.4
1	B	145	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	128	ALA	2.3
1	B	83	GLY	2.2
1	A	70	SER	2.2
1	B	10	VAL	2.2
1	A	12	GLY	2.2
1	B	82	LEU	2.1
1	B	84	GLY	2.1
1	A	83	GLY	2.0
1	A	106	ALA	2.0
1	B	79	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 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	SAL	A	502	10/10	0.84	0.17	30,33,39,40	0
2	SAL	B	503	10/10	0.90	0.22	25,27,29,30	0
2	SAL	A	501	10/10	0.92	0.18	15,19,22,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.