



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:55 AM UTC

PDB ID : 2Y7K / pdb_00002y7k
Title : DntR Inducer Binding Domain in Complex with Salicylate. Monoclinic crystal form
Authors : Devesse, L.; Smirnova, I.; Lonneborg, R.; Kapp, U.; Brzezinski, P.; Leonard, G.A.; Dian, C.
Deposited on : 2011-01-31
Resolution : 1.95 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

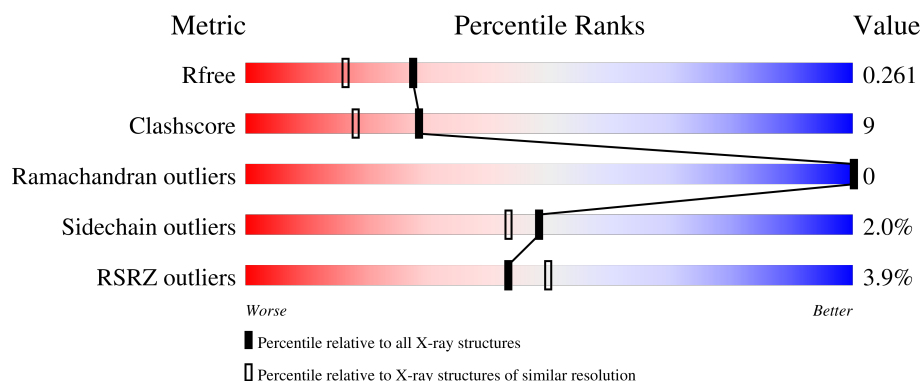
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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 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 $\leq 5\%$. 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	218	3% 81% 15% ..
1	B	218	5% 82% 14% ..
1	C	218	4% 78% 18% ..
1	D	218	4% 82% 13% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6992 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 LYSR-TYPE REGULATORY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	2	0
			1656	1068	293	283	12			
1	B	213	Total	C	N	O	S	0	1	0
			1671	1076	298	285	12			
1	C	212	Total	C	N	O	S	0	2	0
			1660	1072	289	285	14			
1	D	209	Total	C	N	O	S	0	1	0
			1650	1061	292	285	12			

There are 29 discrepancies between the modelled and reference sequences:

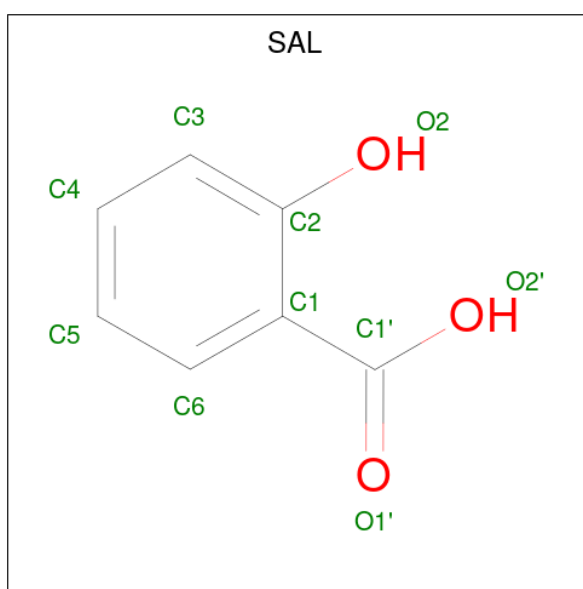
Chain	Residue	Modelled	Actual	Comment	Reference
A	90	MET	PHE	engineered mutation	UNP Q7WT50
A	302	HIS	-	expression tag	UNP Q7WT50
A	303	HIS	-	expression tag	UNP Q7WT50
A	304	HIS	-	expression tag	UNP Q7WT50
A	305	HIS	-	expression tag	UNP Q7WT50
A	306	HIS	-	expression tag	UNP Q7WT50
A	307	HIS	-	expression tag	UNP Q7WT50
B	90	MET	PHE	engineered mutation	UNP Q7WT50
B	302	HIS	-	expression tag	UNP Q7WT50
B	303	HIS	-	expression tag	UNP Q7WT50
B	304	HIS	-	expression tag	UNP Q7WT50
B	305	HIS	-	expression tag	UNP Q7WT50
B	306	HIS	-	expression tag	UNP Q7WT50
B	307	HIS	-	expression tag	UNP Q7WT50
C	90	MET	PHE	engineered mutation	UNP Q7WT50
C	90	MET	-	expression tag	UNP Q7WT50
C	302	HIS	-	expression tag	UNP Q7WT50
C	303	HIS	-	expression tag	UNP Q7WT50
C	304	HIS	-	expression tag	UNP Q7WT50
C	305	HIS	-	expression tag	UNP Q7WT50
C	306	HIS	-	expression tag	UNP Q7WT50

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	307	HIS	-	expression tag	UNP Q7WT50
D	90	MET	PHE	engineered mutation	UNP Q7WT50
D	302	HIS	-	expression tag	UNP Q7WT50
D	303	HIS	-	expression tag	UNP Q7WT50
D	304	HIS	-	expression tag	UNP Q7WT50
D	305	HIS	-	expression tag	UNP Q7WT50
D	306	HIS	-	expression tag	UNP Q7WT50
D	307	HIS	-	expression tag	UNP Q7WT50

- Molecule 2 is 2-HYDROXYBENZOIC ACID (CCD ID: SAL) (formula: $C_7H_6O_3$).



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
2	B	1	Total C O 10 7 3	0	0
2	C	1	Total C O 10 7 3	0	0
2	D	1	Total C O 10 7 3	0	0

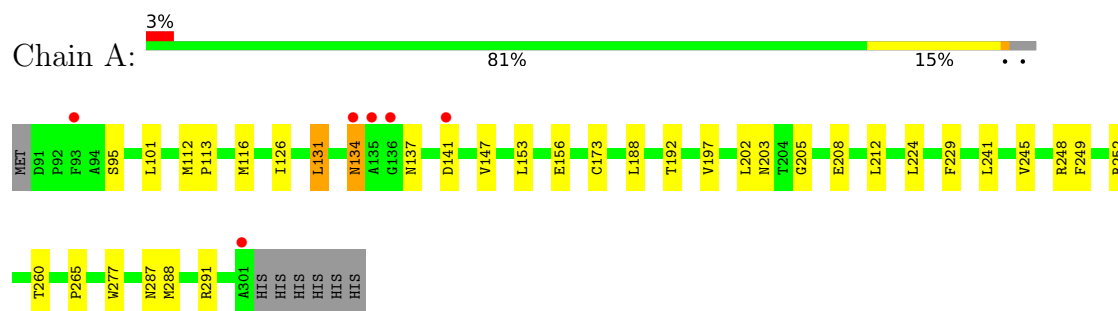
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	72	Total 72	O 72	0	0
3	B	73	Total 73	O 73	0	0
3	C	85	Total 85	O 85	0	0
3	D	65	Total 65	O 65	0	0

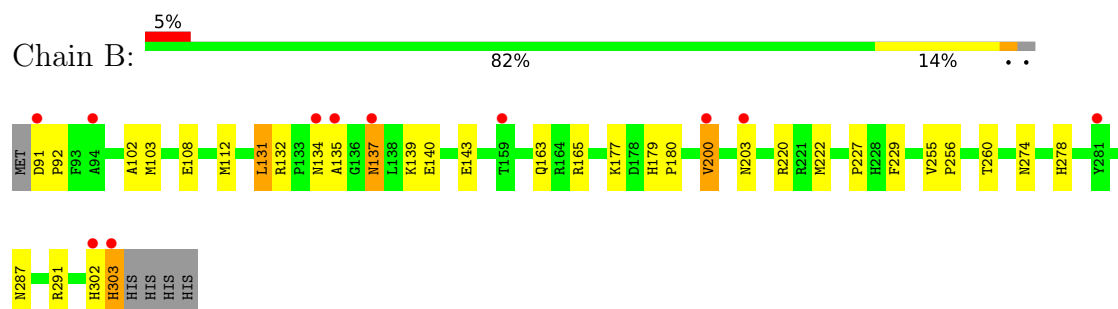
3 Residue-property plots [i](#)

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.

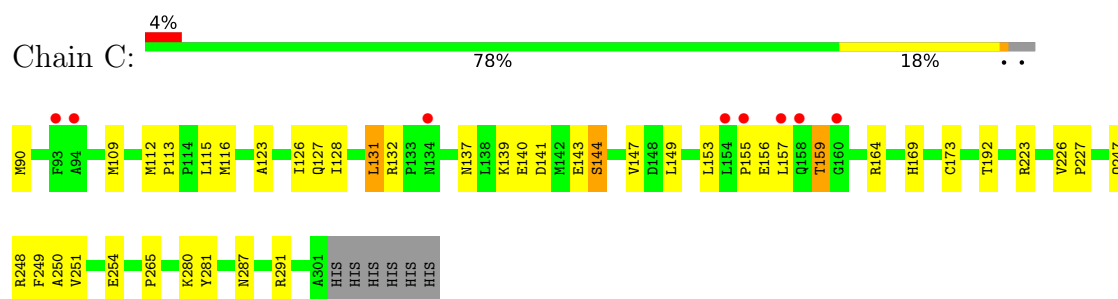
• Molecule 1: LYSR-TYPE REGULATORY PROTEIN



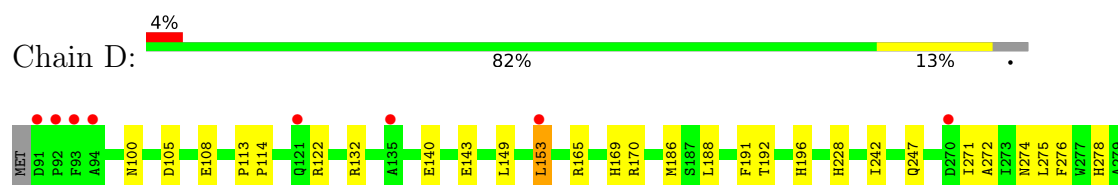
• Molecule 1: LYSR-TYPE REGULATORY PROTEIN



• Molecule 1: LYSR-TYPE REGULATORY PROTEIN



• Molecule 1: LYSR-TYPE REGULATORY PROTEIN



K280		R283		S299	GLU	ALA	HIS	HIS	HIS	HIS	HIS	HIS
------	--	------	--	------	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.91Å 82.11Å 86.27Å 90.00° 111.33° 90.00°	Depositor
Resolution (Å)	40.00 – 1.95 40.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.3 (40.00-1.95) 99.2 (40.00-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.200 , 0.250 (Not available) , 0.261	Depositor DCC
R_{free} test set	3147 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 35.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6992	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% 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: 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	0.91	0/1707	1.03	4/2320 (0.2%)
1	B	0.91	1/1719 (0.1%)	1.03	3/2334 (0.1%)
1	C	0.87	1/1711 (0.1%)	1.02	5/2324 (0.2%)
1	D	0.83	0/1698	0.96	3/2306 (0.1%)
All	All	0.88	2/6835 (0.0%)	1.01	15/9284 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	303	HIS	CB-CG	-6.18	1.41	1.50
1	C	113	PRO	CA-C	5.52	1.57	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	112	MET	CA-C-N	-7.52	112.63	120.38
1	C	112	MET	C-N-CA	-7.52	112.63	120.38
1	A	202	LEU	N-CA-C	7.21	120.69	110.23
1	B	200	VAL	CB-CA-C	-6.71	102.61	111.81
1	C	153	LEU	CA-C-N	-6.62	114.28	122.42
1	C	153	LEU	C-N-CA	-6.62	114.28	122.42
1	D	153	LEU	CA-C-N	-6.49	114.69	123.46
1	D	153	LEU	C-N-CA	-6.49	114.69	123.46
1	D	153	LEU	CB-CA-C	-6.32	100.55	111.30
1	A	113	PRO	CA-C-N	-6.17	112.65	119.19
1	A	113	PRO	C-N-CA	-6.17	112.65	119.19
1	A	229	PHE	N-CA-C	5.84	117.73	111.36
1	C	132	ARG	CB-CA-C	5.61	117.51	109.26
1	B	135	ALA	N-CA-C	5.17	118.37	111.75
1	B	229	PHE	N-CA-C	5.00	119.24	112.04

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	1656	0	1647	26	0
1	B	1671	0	1653	28	0
1	C	1660	0	1642	38	0
1	D	1650	0	1642	26	0
2	A	20	0	9	0	0
2	B	20	0	9	0	0
2	C	10	0	5	0	0
2	D	10	0	5	0	0
3	A	72	0	0	0	0
3	B	73	0	0	0	0
3	C	85	0	0	2	0
3	D	65	0	0	1	0
All	All	6992	0	6612	117	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 9.

All (117) 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:197[B]:VAL:HG13	1:A:241:LEU:HD13	1.34	1.08
1:C:280:LYS:HE3	1:C:281:TYR:CE2	1.94	1.02
1:D:186:MET:CE	1:D:191:PHE:HA	1.90	1.01
1:A:197[B]:VAL:CG1	1:A:241:LEU:HD13	1.93	0.98
1:B:134:ASN:HB3	1:B:203:ASN:HD22	1.32	0.93
1:A:245:VAL:CG1	1:A:249:PHE:HD2	1.81	0.91
1:A:134:ASN:HB3	1:A:203:ASN:HD22	1.37	0.90
1:A:197[A]:VAL:HG22	1:A:241:LEU:HD13	1.58	0.86
1:D:165:ARG:HA	1:D:274:ASN:HD22	1.41	0.86
1:B:108:GLU:CD	1:B:132:ARG:HH12	1.85	0.82
1:B:108:GLU:OE2	1:B:132:ARG:NH1	2.13	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ASP:CB	1:B:92:PRO:HD2	2.10	0.81
1:C:155:PRO:HD2	1:C:156:GLU:OE1	1.81	0.81
1:A:245:VAL:CG1	1:A:249:PHE:CD2	2.65	0.80
1:C:247:GLN:NE2	1:C:251:VAL:HG21	1.98	0.78
1:C:143:GLU:O	1:C:280:LYS:HE2	1.83	0.76
1:B:200:VAL:O	1:B:227:PRO:O	2.04	0.76
1:D:186:MET:HE2	1:D:191:PHE:HA	1.66	0.76
1:B:91:ASP:CB	1:B:92:PRO:CD	2.65	0.75
1:A:245:VAL:HG11	1:A:249:PHE:CD2	2.20	0.75
1:C:247:GLN:NE2	1:C:251:VAL:CG2	2.51	0.73
1:B:139:LYS:O	1:B:143:GLU:HG3	1.89	0.72
1:B:103:MET:HE1	1:B:112:MET:HE3	1.70	0.72
1:D:186:MET:CE	1:D:191:PHE:CA	2.68	0.72
1:B:134:ASN:CB	1:B:203:ASN:HD22	2.02	0.70
1:A:134:ASN:CB	1:A:203:ASN:HD22	2.06	0.68
1:B:302:HIS:O	1:B:303:HIS:HB2	1.94	0.68
1:B:177:LYS:HA	1:B:260:THR:HG23	1.76	0.67
1:D:186:MET:HE2	1:D:191:PHE:CA	2.24	0.67
1:C:280:LYS:HE3	1:C:281:TYR:HE2	1.54	0.66
1:A:287:ASN:O	1:A:291:ARG:HG3	1.97	0.64
1:B:134:ASN:CB	1:B:203:ASN:ND2	2.60	0.64
1:D:113:PRO:HB2	1:D:114:PRO:HD3	1.80	0.64
1:A:197[B]:VAL:HG12	1:A:224:LEU:HB3	1.78	0.63
1:C:116:MET:HE1	1:C:128:ILE:HG13	1.79	0.63
1:B:302:HIS:O	1:B:303:HIS:CB	2.47	0.62
1:D:143:GLU:HG3	1:D:278:HIS:CD2	2.35	0.62
1:D:165:ARG:HA	1:D:274:ASN:ND2	2.15	0.60
1:C:169:HIS:HD2	1:C:248:ARG:H	1.49	0.59
1:C:137:ASN:ND2	1:C:140:GLU:OE1	2.37	0.57
1:B:137:ASN:HB2	1:B:140:GLU:HB2	1.86	0.57
1:A:208:GLU:O	1:A:212:LEU:HD12	2.05	0.56
1:C:247:GLN:O	1:C:251:VAL:HG23	2.05	0.56
1:B:134:ASN:HB3	1:B:203:ASN:ND2	2.10	0.56
1:C:115:LEU:HD23	1:C:116:MET:CE	2.37	0.55
1:C:157:LEU:C	1:C:159:THR:H	2.15	0.55
1:D:170:ARG:O	1:D:247:GLN:HB2	2.07	0.55
1:C:137:ASN:CG	1:C:140:GLU:OE1	2.50	0.54
1:C:109[B]:MET:HE1	1:C:249:PHE:CD1	2.42	0.54
1:C:123:ALA:HB1	1:C:126:ILE:HD12	1.90	0.53
1:C:156:GLU:HG2	1:C:157:LEU:N	2.24	0.52
1:D:153:LEU:HD13	1:D:272:ALA:O	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:MET:HE1	1:B:112:MET:CE	2.38	0.52
1:A:245:VAL:HG11	1:A:249:PHE:HD2	1.57	0.51
1:A:112:MET:O	1:A:116:MET:HG2	2.09	0.51
1:D:186:MET:HE3	1:D:191:PHE:HA	1.88	0.51
1:B:220:ARG:CZ	1:B:222:MET:HE1	2.41	0.50
1:B:287:ASN:O	1:B:291:ARG:HG3	2.11	0.50
1:A:245:VAL:HG11	1:A:249:PHE:CE2	2.47	0.49
1:B:165:ARG:CG	1:B:274:ASN:OD1	2.60	0.49
1:D:153:LEU:HD11	1:D:271:ILE:HG23	1.94	0.49
1:D:196:HIS:CE1	1:D:242:ILE:HD11	2.48	0.49
1:A:197[B]:VAL:HG13	1:A:241:LEU:CD1	2.23	0.49
1:A:141:ASP:HB3	1:A:147:VAL:HG23	1.94	0.49
1:C:280:LYS:HE3	1:C:281:TYR:CZ	2.42	0.49
1:B:143:GLU:HG2	1:B:278:HIS:CD2	2.48	0.48
1:C:247:GLN:HE22	1:C:251:VAL:HG21	1.73	0.48
1:D:186:MET:HE2	1:D:191:PHE:CB	2.43	0.48
1:B:303:HIS:O	1:B:303:HIS:CG	2.66	0.48
1:A:173[B]:CYS:SG	1:A:265:PRO:HD2	2.54	0.48
1:C:156:GLU:HG2	1:C:157:LEU:H	1.79	0.48
1:C:164:ARG:NH1	3:C:2028:HOH:O	2.46	0.48
1:D:278:HIS:ND1	1:D:280:LYS:HG3	2.29	0.47
1:A:288:MET:HG2	1:A:291:ARG:NH2	2.30	0.47
1:C:90:MET:HE1	1:C:126:ILE:HD11	1.97	0.47
1:A:95:SER:HB3	1:A:126:ILE:HD11	1.98	0.46
1:A:197[B]:VAL:CG1	1:A:224:LEU:HD23	2.46	0.46
1:D:105:ASP:OD2	1:D:228:HIS:HB3	2.16	0.46
1:C:149:LEU:HD21	1:C:291:ARG:HG2	1.97	0.46
1:C:141:ASP:HB3	1:C:147:VAL:HG23	1.99	0.45
1:C:247:GLN:HE21	1:C:251:VAL:CG2	2.25	0.45
1:D:186:MET:HE1	1:D:191:PHE:HA	1.93	0.45
1:A:277:TRP:CE3	1:A:291:ARG:HD2	2.52	0.45
1:C:192:THR:O	1:C:192:THR:HG22	2.17	0.45
1:A:188:LEU:O	1:A:192:THR:HG23	2.18	0.44
1:D:283:ARG:NH2	3:D:2064:HOH:O	2.40	0.44
1:B:179:HIS:HA	1:B:180:PRO:HD3	1.87	0.44
1:C:109[B]:MET:HE1	1:C:249:PHE:HD1	1.81	0.44
1:C:169:HIS:CD2	1:C:248:ARG:HG2	2.52	0.43
1:D:108:GLU:CD	1:D:132:ARG:HH12	2.25	0.43
1:B:255:VAL:HB	1:B:256:PRO:HD3	2.00	0.43
1:D:149:LEU:HD22	1:D:275:LEU:HD11	2.00	0.43
1:C:127:GLN:NE2	3:C:2015:HOH:O	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:VAL:HB	1:C:227:PRO:HD2	1.99	0.43
1:D:140:GLU:H	1:D:140:GLU:CD	2.27	0.43
1:B:303:HIS:CG	1:D:122:ARG:O	2.72	0.43
1:D:278:HIS:CE1	1:D:280:LYS:HG3	2.53	0.43
1:C:131:LEU:HD13	1:C:131:LEU:N	2.34	0.43
1:C:192:THR:O	1:C:192:THR:CG2	2.65	0.43
1:D:274:ASN:HB2	1:D:276:PHE:CE2	2.54	0.42
1:D:192:THR:O	1:D:192:THR:CG2	2.67	0.42
1:B:102:ALA:HB2	1:B:131:LEU:HD11	2.01	0.42
1:C:143:GLU:O	1:C:280:LYS:CE	2.63	0.42
1:C:250:ALA:O	1:C:254:GLU:HG3	2.20	0.42
1:C:109[B]:MET:HE2	1:C:109[B]:MET:HB3	1.72	0.42
1:B:165:ARG:HG3	1:B:274:ASN:OD1	2.20	0.42
1:C:173[B]:CYS:SG	1:C:265:PRO:HD2	2.59	0.41
1:B:103:MET:CE	1:B:112:MET:HE3	2.45	0.41
1:C:287:ASN:O	1:C:291:ARG:HG3	2.21	0.41
1:C:223:ARG:HD3	1:C:223:ARG:HA	1.80	0.41
1:B:108:GLU:CD	1:B:132:ARG:NH1	2.65	0.41
1:D:169:HIS:CD2	1:D:271:ILE:HB	2.56	0.41
1:C:140:GLU:O	1:C:144:SER:HB3	2.20	0.40
1:A:153:LEU:HG	1:A:205:GLY:HA3	2.01	0.40
1:A:197[B]:VAL:HG11	1:A:224:LEU:HD23	2.02	0.40
1:A:101:LEU:O	1:A:131:LEU:HD13	2.21	0.40
1:A:248:ARG:O	1:A:252:ARG:HG2	2.21	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	166/218 (76%)	164 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	212/218 (97%)	206 (97%)	6 (3%)	0	100	100
1	C	212/218 (97%)	209 (99%)	3 (1%)	0	100	100
1	D	208/218 (95%)	206 (99%)	2 (1%)	0	100	100
All	All	798/872 (92%)	785 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	174/187 (93%)	169 (97%)	5 (3%)	37	29
1	B	173/187 (92%)	170 (98%)	3 (2%)	53	49
1	C	173/187 (92%)	169 (98%)	4 (2%)	44	38
1	D	176/187 (94%)	174 (99%)	2 (1%)	65	64
All	All	696/748 (93%)	682 (98%)	14 (2%)	48	43

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	LEU
1	A	134	ASN
1	A	137	ASN
1	A	156	GLU
1	A	260	THR
1	B	131	LEU
1	B	137	ASN
1	B	163	GLN
1	C	131	LEU
1	C	139	LYS
1	C	144	SER
1	C	159	THR
1	D	100	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	188	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	203	ASN
1	A	228	HIS
1	B	203	ASN
1	B	228	HIS
1	C	137	ASN
1	C	169	HIS
1	C	203	ASN
1	C	247	GLN
1	D	125	HIS
1	D	127	GLN
1	D	137	ASN
1	D	274	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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	1303	-	10,10,10	1.13	1 (10%)	13,13,13	0.93	0
2	SAL	B	1305	-	10,10,10	1.11	1 (10%)	13,13,13	0.69	0
2	SAL	A	1302	-	10,10,10	1.30	1 (10%)	13,13,13	1.01	1 (7%)
2	SAL	B	1304	-	10,10,10	1.05	0	13,13,13	1.59	3 (23%)
2	SAL	C	1302	-	10,10,10	1.15	0	13,13,13	1.26	2 (15%)
2	SAL	D	1300	-	10,10,10	1.49	2 (20%)	13,13,13	2.66	6 (46%)

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	1303	-	-	0/4/4/4	0/1/1/1
2	SAL	B	1305	-	-	4/4/4/4	0/1/1/1
2	SAL	A	1302	-	-	0/4/4/4	0/1/1/1
2	SAL	B	1304	-	-	0/4/4/4	0/1/1/1
2	SAL	C	1302	-	-	0/4/4/4	0/1/1/1
2	SAL	D	1300	-	-	0/4/4/4	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1305	SAL	C1-C1'	2.61	1.55	1.49
2	D	1300	SAL	O2-C2	2.38	1.41	1.36
2	D	1300	SAL	C1-C1'	-2.34	1.44	1.49
2	A	1303	SAL	C1-C1'	2.26	1.54	1.49
2	A	1302	SAL	C1-C1'	2.25	1.54	1.49

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1300	SAL	C6-C1-C2	5.40	124.94	118.15
2	D	1300	SAL	C2-C1-C1'	-4.66	115.23	120.00
2	D	1300	SAL	C3-C2-C1	-4.06	115.66	119.89
2	C	1302	SAL	C6-C1-C2	3.21	122.18	118.15
2	B	1304	SAL	O1'-C1'-C1	-3.03	114.73	121.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1300	SAL	O1'-C1'-C1	-2.75	115.39	121.97
2	D	1300	SAL	O2'-C1'-O1'	2.30	128.29	123.35
2	A	1302	SAL	O2-C2-C1	-2.26	117.52	121.71
2	B	1304	SAL	C2-C1-C1'	2.18	122.24	120.00
2	D	1300	SAL	C4-C5-C6	-2.17	117.56	120.24
2	C	1302	SAL	C3-C2-C1	-2.05	117.75	119.89
2	B	1304	SAL	O2-C2-C1	-2.04	117.93	121.71

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1305	SAL	C2-C1-C1'-O1'
2	B	1305	SAL	C2-C1-C1'-O2'
2	B	1305	SAL	C6-C1-C1'-O2'
2	B	1305	SAL	C6-C1-C1'-O1'

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	211/218 (96%)	0.19	6 (2%) 55 62	10, 24, 36, 45	2 (0%)
1	B	213/218 (97%)	0.36	11 (5%) 33 38	14, 25, 38, 53	1 (0%)
1	C	212/218 (97%)	0.26	8 (3%) 44 50	10, 26, 43, 51	2 (0%)
1	D	209/218 (95%)	0.37	8 (3%) 44 50	14, 28, 40, 46	1 (0%)
All	All	845/872 (96%)	0.30	33 (3%) 43 50	10, 26, 40, 53	6 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	94	ALA	4.8
1	D	92	PRO	3.8
1	A	136	GLY	3.5
1	C	155	PRO	3.2
1	A	135	ALA	3.2
1	B	135	ALA	3.1
1	B	134	ASN	3.0
1	C	154	LEU	2.9
1	D	93	PHE	2.8
1	D	121	GLN	2.8
1	D	153	LEU	2.7
1	C	93	PHE	2.7
1	D	91	ASP	2.7
1	A	93	PHE	2.6
1	B	303	HIS	2.6
1	B	94	ALA	2.6
1	D	135	ALA	2.5
1	C	158	GLN	2.4
1	B	91	ASP	2.4
1	A	301	ALA	2.4
1	C	94	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	137	ASN	2.4
1	B	200	VAL	2.3
1	C	160	GLY	2.2
1	B	203	ASN	2.2
1	A	134	ASN	2.1
1	B	281	TYR	2.1
1	C	134	ASN	2.1
1	B	302	HIS	2.1
1	A	141	ASP	2.1
1	C	157	LEU	2.0
1	D	270	ASP	2.0
1	B	159	THR	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	SAL	B	1305	10/10	0.83	0.13	56,57,59,60	0
2	SAL	C	1302	10/10	0.87	0.12	27,29,32,33	0
2	SAL	A	1303	10/10	0.88	0.11	37,38,41,42	0
2	SAL	D	1300	10/10	0.94	0.07	16,20,23,25	0
2	SAL	B	1304	10/10	0.97	0.05	12,16,20,21	0
2	SAL	A	1302	10/10	0.97	0.05	12,16,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.