



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 12:21 PM UTC

PDB ID : 1Y7H / pdb_00001y7h
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 : 2.52 Å(reported)

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

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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

<https://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)

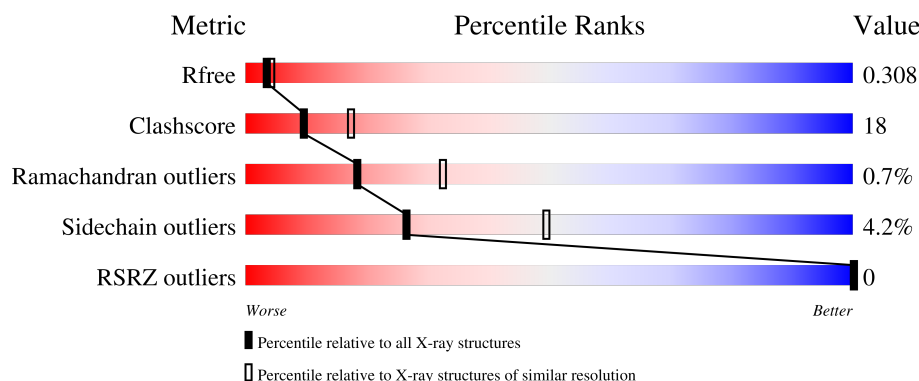
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

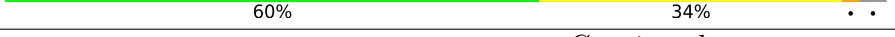
The reported resolution of this entry is 2.52 Å.

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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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	268	 63% 30% . .
1	B	268	 57% 38% . .
1	C	268	 59% 35% . .
1	D	268	 60% 34% . .

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Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	E	268	59%35%
1	F	268	64%29%
1	G	268	59%34%
1	H	268	57%37%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16579 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
1	A	257	Total	C	N	O	S	Se	0	0	0
			2031	1310	330	377	5	9			
1	B	259	Total	C	N	O	S	Se	0	0	0
			2051	1323	333	381	5	9			
1	C	257	Total	C	N	O	S	Se	0	0	0
			2031	1310	330	377	5	9			
1	D	259	Total	C	N	O	S	Se	0	0	0
			2051	1323	333	381	5	9			
1	E	258	Total	C	N	O	S	Se	0	0	0
			2043	1319	331	379	5	9			
1	F	258	Total	C	N	O	S	Se	0	0	0
			2042	1317	331	380	5	9			
1	G	257	Total	C	N	O	S	Se	0	0	0
			2031	1310	330	377	5	9			
1	H	259	Total	C	N	O	S	Se	0	0	0
			2051	1323	333	381	5	9			

There are 136 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	-	cloning artifact	UNP Q6RYA0
A	262	GLU	-	cloning artifact	UNP Q6RYA0
A	263	HIS	-	cloning artifact	UNP Q6RYA0
A	264	HIS	-	cloning artifact	UNP Q6RYA0

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

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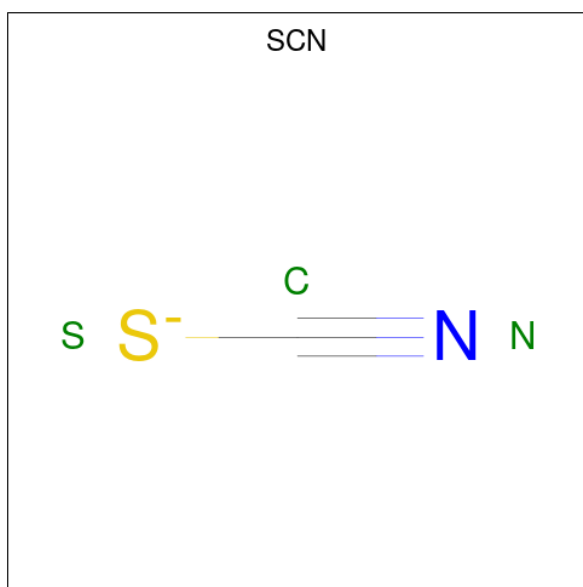
Chain	Residue	Modelled	Actual	Comment	Reference
D	108	MSE	MET	modified residue	UNP Q6RYA0
D	149	MSE	MET	modified residue	UNP Q6RYA0
D	183	MSE	MET	modified residue	UNP Q6RYA0
D	239	MSE	MET	modified residue	UNP Q6RYA0
D	241	MSE	MET	modified residue	UNP Q6RYA0
D	261	LEU	-	cloning artifact	UNP Q6RYA0
D	262	GLU	-	cloning artifact	UNP Q6RYA0
D	263	HIS	-	cloning artifact	UNP Q6RYA0
D	264	HIS	-	cloning artifact	UNP Q6RYA0
D	265	HIS	-	cloning artifact	UNP Q6RYA0
D	266	HIS	-	cloning artifact	UNP Q6RYA0
D	267	HIS	-	cloning artifact	UNP Q6RYA0
D	268	HIS	-	cloning artifact	UNP Q6RYA0
E	63	MSE	MET	modified residue	UNP Q6RYA0
E	66	MSE	MET	modified residue	UNP Q6RYA0
E	85	MSE	MET	modified residue	UNP Q6RYA0
E	91	MSE	MET	modified residue	UNP Q6RYA0
E	108	MSE	MET	modified residue	UNP Q6RYA0
E	149	MSE	MET	modified residue	UNP Q6RYA0
E	183	MSE	MET	modified residue	UNP Q6RYA0
E	239	MSE	MET	modified residue	UNP Q6RYA0
E	241	MSE	MET	modified residue	UNP Q6RYA0
E	261	LEU	-	cloning artifact	UNP Q6RYA0
E	262	GLU	-	cloning artifact	UNP Q6RYA0
E	263	HIS	-	cloning artifact	UNP Q6RYA0
E	264	HIS	-	cloning artifact	UNP Q6RYA0
E	265	HIS	-	cloning artifact	UNP Q6RYA0
E	266	HIS	-	cloning artifact	UNP Q6RYA0
E	267	HIS	-	cloning artifact	UNP Q6RYA0
E	268	HIS	-	cloning artifact	UNP Q6RYA0
F	63	MSE	MET	modified residue	UNP Q6RYA0
F	66	MSE	MET	modified residue	UNP Q6RYA0
F	85	MSE	MET	modified residue	UNP Q6RYA0
F	91	MSE	MET	modified residue	UNP Q6RYA0
F	108	MSE	MET	modified residue	UNP Q6RYA0
F	149	MSE	MET	modified residue	UNP Q6RYA0
F	183	MSE	MET	modified residue	UNP Q6RYA0
F	239	MSE	MET	modified residue	UNP Q6RYA0
F	241	MSE	MET	modified residue	UNP Q6RYA0
F	261	LEU	-	cloning artifact	UNP Q6RYA0
F	262	GLU	-	cloning artifact	UNP Q6RYA0
F	263	HIS	-	cloning artifact	UNP Q6RYA0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	264	HIS	-	cloning artifact	UNP Q6RYA0
F	265	HIS	-	cloning artifact	UNP Q6RYA0
F	266	HIS	-	cloning artifact	UNP Q6RYA0
F	267	HIS	-	cloning artifact	UNP Q6RYA0
F	268	HIS	-	cloning artifact	UNP Q6RYA0
G	63	MSE	MET	modified residue	UNP Q6RYA0
G	66	MSE	MET	modified residue	UNP Q6RYA0
G	85	MSE	MET	modified residue	UNP Q6RYA0
G	91	MSE	MET	modified residue	UNP Q6RYA0
G	108	MSE	MET	modified residue	UNP Q6RYA0
G	149	MSE	MET	modified residue	UNP Q6RYA0
G	183	MSE	MET	modified residue	UNP Q6RYA0
G	239	MSE	MET	modified residue	UNP Q6RYA0
G	241	MSE	MET	modified residue	UNP Q6RYA0
G	261	LEU	-	cloning artifact	UNP Q6RYA0
G	262	GLU	-	cloning artifact	UNP Q6RYA0
G	263	HIS	-	cloning artifact	UNP Q6RYA0
G	264	HIS	-	cloning artifact	UNP Q6RYA0
G	265	HIS	-	cloning artifact	UNP Q6RYA0
G	266	HIS	-	cloning artifact	UNP Q6RYA0
G	267	HIS	-	cloning artifact	UNP Q6RYA0
G	268	HIS	-	cloning artifact	UNP Q6RYA0
H	63	MSE	MET	modified residue	UNP Q6RYA0
H	66	MSE	MET	modified residue	UNP Q6RYA0
H	85	MSE	MET	modified residue	UNP Q6RYA0
H	91	MSE	MET	modified residue	UNP Q6RYA0
H	108	MSE	MET	modified residue	UNP Q6RYA0
H	149	MSE	MET	modified residue	UNP Q6RYA0
H	183	MSE	MET	modified residue	UNP Q6RYA0
H	239	MSE	MET	modified residue	UNP Q6RYA0
H	241	MSE	MET	modified residue	UNP Q6RYA0
H	261	LEU	-	cloning artifact	UNP Q6RYA0
H	262	GLU	-	cloning artifact	UNP Q6RYA0
H	263	HIS	-	cloning artifact	UNP Q6RYA0
H	264	HIS	-	cloning artifact	UNP Q6RYA0
H	265	HIS	-	cloning artifact	UNP Q6RYA0
H	266	HIS	-	cloning artifact	UNP Q6RYA0
H	267	HIS	-	cloning artifact	UNP Q6RYA0
H	268	HIS	-	cloning artifact	UNP Q6RYA0

- Molecule 2 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	S	0	0
			3	1	1	1		
2	B	1	Total	C	N	S	0	0
			3	1	1	1		
2	C	1	Total	C	N	S	0	0
			3	1	1	1		
2	D	1	Total	C	N	S	0	0
			3	1	1	1		
2	E	1	Total	C	N	S	0	0
			3	1	1	1		
2	F	1	Total	C	N	S	0	0
			3	1	1	1		
2	G	1	Total	C	N	S	0	0
			3	1	1	1		
2	H	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total	O	0	0
			19	19		
3	B	27	Total	O	0	0
			27	27		
3	C	30	Total	O	0	0
			30	30		
3	D	25	Total	O	0	0
			25	25		

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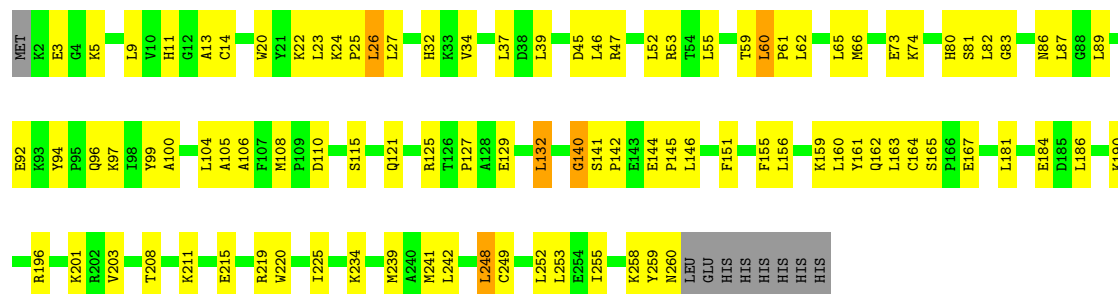
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	28	Total 28	O 28	0	0
3	F	30	Total 30	O 30	0	0
3	G	28	Total 28	O 28	0	0
3	H	37	Total 37	O 37	0	0



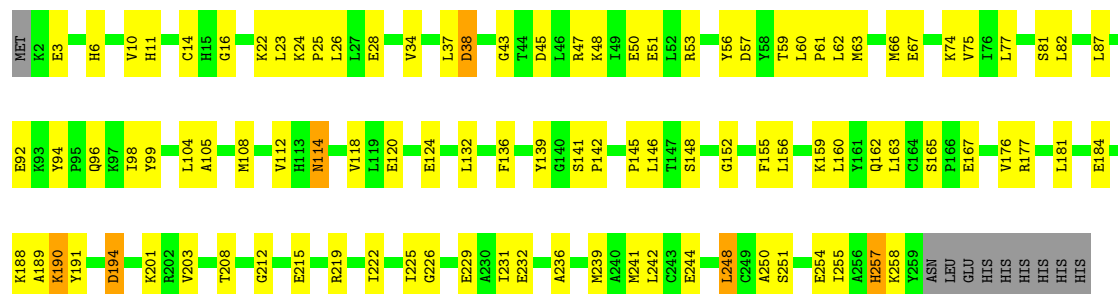
- Molecule 1: salicylic acid-binding protein 2

Chain D: 60% 34%



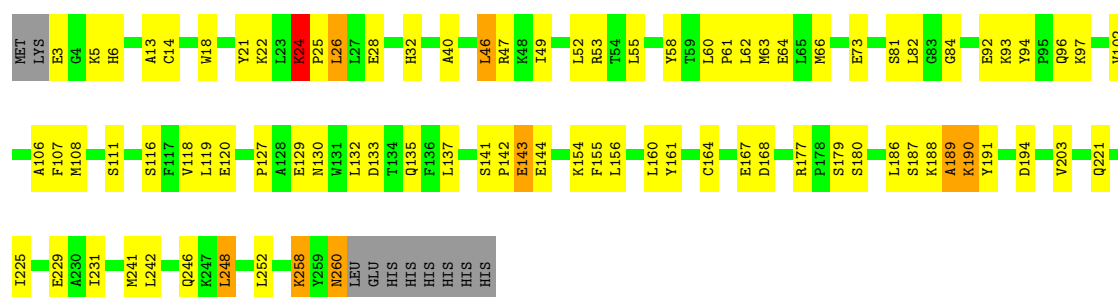
- Molecule 1: salicylic acid-binding protein 2

Chain E: 59% 35%



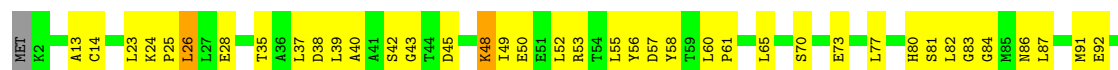
- Molecule 1: salicylic acid-binding protein 2

Chain F: 64% 29%



- Molecule 1: salicylic acid-binding protein 2

Chain G: 59% 34%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	45.63Å 137.74Å 171.21Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	28.17 – 2.52 28.17 – 2.52	Depositor EDS
% Data completeness (in resolution range)	92.3 (28.17-2.52) 97.2 (28.17-2.52)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.67 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.227 , 0.297 0.238 , 0.308	Depositor DCC
R_{free} test set	13694 reflections (9.89%)	wwPDB-VP
Wilson B-factor (Å ²)	18.6	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.388 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16579	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.49	0/2073	0.91	5/2790 (0.2%)
1	B	0.51	0/2094	0.87	1/2819 (0.0%)
1	C	0.50	0/2073	0.86	1/2790 (0.0%)
1	D	0.52	0/2094	0.93	2/2819 (0.1%)
1	E	0.49	0/2086	0.89	1/2808 (0.0%)
1	F	0.49	0/2085	0.84	4/2808 (0.1%)
1	G	0.49	0/2073	0.83	0/2790
1	H	0.49	0/2094	0.89	3/2819 (0.1%)
All	All	0.50	0/16672	0.88	17/22443 (0.1%)

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	THR	N-CA-C	9.01	121.10	111.28
1	D	258	LYS	N-CA-C	6.39	117.94	110.97
1	A	81	SER	CB-CA-C	-5.83	109.84	116.54
1	A	108	MSE	CA-C-N	5.80	125.99	120.31
1	A	108	MSE	C-N-CA	5.80	125.99	120.31

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	2031	0	2013	71	0
1	B	2051	0	2028	79	0
1	C	2031	0	2013	64	0
1	D	2051	0	2028	78	0
1	E	2043	0	2022	78	0
1	F	2042	0	2015	69	0
1	G	2031	0	2013	73	0
1	H	2051	0	2028	72	0
2	A	3	0	0	1	0
2	B	3	0	0	1	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
3	A	19	0	0	1	0
3	B	27	0	0	1	0
3	C	30	0	0	2	0
3	D	25	0	0	0	0
3	E	28	0	0	4	0
3	F	30	0	0	0	0
3	G	28	0	0	1	0
3	H	37	0	0	3	0
All	All	16579	0	16160	577	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 18.

The worst 5 of 577 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:162:GLN:HE21	1:B:237:ASP:HB2	1.28	0.96
1:C:156:LEU:HD12	1:C:160:LEU:HD12	1.49	0.95
1:E:23:LEU:HD22	1:E:248:LEU:HD13	1.50	0.93
1:H:132:LEU:HD12	1:H:155:PHE:HA	1.53	0.91
1:F:132:LEU:HD12	1:F:155:PHE:HA	1.53	0.88

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	255/268 (95%)	233 (91%)	21 (8%)	1 (0%)	30	47
1	B	257/268 (96%)	229 (89%)	26 (10%)	2 (1%)	16	29
1	C	255/268 (95%)	225 (88%)	28 (11%)	2 (1%)	16	29
1	D	257/268 (96%)	231 (90%)	22 (9%)	4 (2%)	7	13
1	E	256/268 (96%)	239 (93%)	15 (6%)	2 (1%)	16	29
1	F	256/268 (96%)	232 (91%)	23 (9%)	1 (0%)	30	47
1	G	255/268 (95%)	233 (91%)	20 (8%)	2 (1%)	16	29
1	H	257/268 (96%)	234 (91%)	22 (9%)	1 (0%)	30	47
All	All	2048/2144 (96%)	1856 (91%)	177 (9%)	15 (1%)	18	32

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	PHE
1	D	140	GLY
1	E	3	GLU
1	E	257	HIS
1	C	117	PHE

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	219/221 (99%)	210 (96%)	9 (4%)	27	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	208/221 (94%)	204 (98%)	4 (2%)	50	74
1	C	219/221 (99%)	208 (95%)	11 (5%)	22	42
1	D	221/221 (100%)	212 (96%)	9 (4%)	27	50
1	E	220/221 (100%)	211 (96%)	9 (4%)	27	50
1	F	220/221 (100%)	209 (95%)	11 (5%)	22	42
1	G	219/221 (99%)	211 (96%)	8 (4%)	30	54
1	H	221/221 (100%)	209 (95%)	12 (5%)	20	39
All	All	1747/1768 (99%)	1674 (96%)	73 (4%)	26	49

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	143	GLU
1	H	194	ASP
1	G	188	LYS
1	H	59	THR
1	D	26	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	260	ASN
1	H	114	ASN
1	G	113	HIS
1	G	135	GLN
1	H	221	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	SCN	E	295	-	1,2,2	0.41	0	0,1,1	-	-
2	SCN	G	297	-	1,2,2	0.11	0	0,1,1	-	-
2	SCN	D	294	-	1,2,2	0.33	0	0,1,1	-	-
2	SCN	A	291	-	1,2,2	0.16	0	0,1,1	-	-
2	SCN	H	298	-	1,2,2	0.68	0	0,1,1	-	-
2	SCN	F	296	-	1,2,2	0.23	0	0,1,1	-	-
2	SCN	C	293	-	1,2,2	0.07	0	0,1,1	-	-
2	SCN	B	292	-	1,2,2	0.37	0	0,1,1	-	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	291	SCN	1	0
2	B	292	SCN	1	0

5.7 Other polymers [i](#)

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 [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	248/268 (92%)	-1.55	0 100 100	2, 15, 34, 45	0
1	B	250/268 (93%)	-1.52	0 100 100	1, 17, 38, 46	0
1	C	248/268 (92%)	-1.54	0 100 100	1, 15, 34, 43	0
1	D	250/268 (93%)	-1.59	0 100 100	1, 13, 32, 49	0
1	E	249/268 (92%)	-1.58	0 100 100	1, 12, 31, 42	0
1	F	249/268 (92%)	-1.54	0 100 100	3, 17, 35, 47	0
1	G	248/268 (92%)	-1.52	0 100 100	2, 16, 35, 44	0
1	H	250/268 (93%)	-1.55	0 100 100	3, 16, 33, 49	0
All	All	1992/2144 (92%)	-1.55	0 100 100	1, 15, 34, 49	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 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	SCN	B	292	3/3	0.99	0.04	26,26,27,28	0
2	SCN	D	294	3/3	0.99	0.06	40,40,42,43	0
2	SCN	F	296	3/3	0.99	0.04	13,13,16,17	0
2	SCN	G	297	3/3	0.99	0.04	28,28,29,30	0
2	SCN	H	298	3/3	0.99	0.04	28,28,28,30	0
2	SCN	C	293	3/3	1.00	0.03	18,18,19,20	0
2	SCN	A	291	3/3	1.00	0.03	32,32,32,34	0
2	SCN	E	295	3/3	1.00	0.04	26,26,26,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.