



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:37 AM UTC

PDB ID : 6QWV / pdb_00006qwv
Title : SARM1 SAM1-2 domains
Authors : Sporny, M.; Isupov, N.M.; Opatowsky, Y.
Deposited on : 2019-03-06
Resolution : 2.47 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

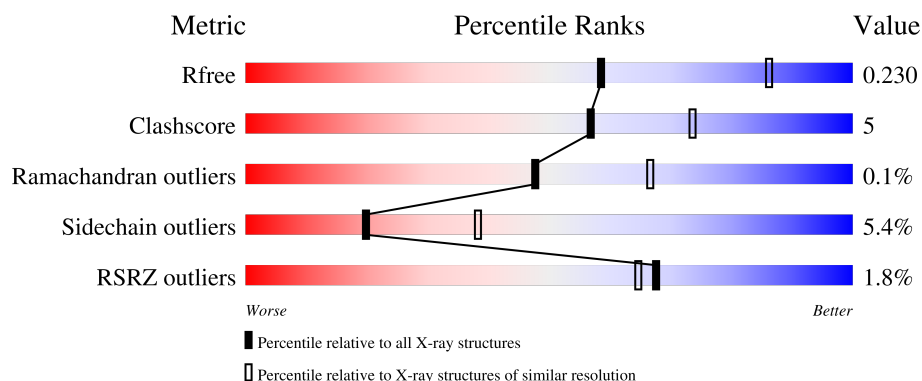
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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.



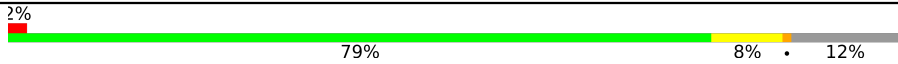
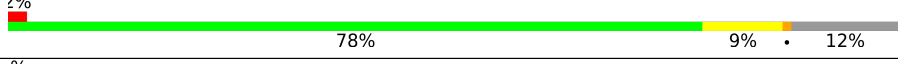
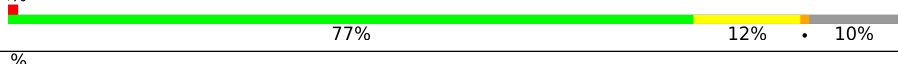
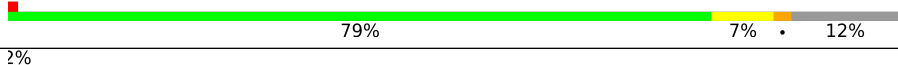
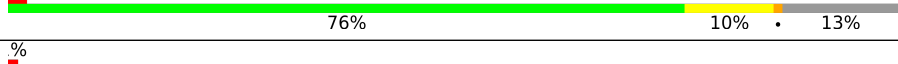
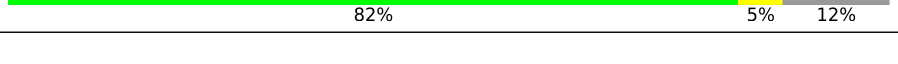
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	164	2% 77% 10% • 13%
1	B	164	4% 77% 17% • •
1	C	164	0% 79% 9% • 10%
1	D	164	74% 14% • 11%
1	E	164	2% 79% 10% • 11%

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Mol	Chain	Length	Quality of chain
1	F	164	
1	G	164	
1	H	164	
1	I	164	
1	J	164	
1	K	164	
1	L	164	
1	M	164	
1	N	164	
1	O	164	
1	P	164	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	D	608	-	-	X	-
2	EDO	E	601	-	-	X	-
2	EDO	O	601	-	-	X	-
4	PEG	D	602	-	-	X	-
5	PGE	B	605	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20654 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 Sterile alpha and TIR motif-containing protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	143	Total	C	N	O	S	0	7	0
			1211	763	220	221	7			
1	B	157	Total	C	N	O	S	0	8	0
			1324	832	241	244	7			
1	C	148	Total	C	N	O	S	0	5	0
			1232	775	221	229	7			
1	D	146	Total	C	N	O	S	0	3	0
			1204	756	215	226	7			
1	E	146	Total	C	N	O	S	0	3	0
			1209	761	219	222	7			
1	F	144	Total	C	N	O	S	0	7	0
			1211	762	219	223	7			
1	G	145	Total	C	N	O	S	0	5	0
			1206	758	217	224	7			
1	H	146	Total	C	N	O	S	0	4	0
			1210	761	217	225	7			
1	I	145	Total	C	N	O	S	0	9	0
			1220	768	218	227	7			
1	J	147	Total	C	N	O	S	0	4	0
			1216	764	219	226	7			
1	K	148	Total	C	N	O	S	0	5	0
			1234	776	224	227	7			
1	L	145	Total	C	N	O	S	0	5	0
			1205	758	216	224	7			
1	M	145	Total	C	N	O	S	0	6	0
			1211	763	218	223	7			
1	N	143	Total	C	N	O	S	0	4	0
			1181	744	210	220	7			
1	O	145	Total	C	N	O	S	0	6	0
			1211	763	218	223	7			
1	P	144	Total	C	N	O	S	0	6	0
			1207	759	220	221	7			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	385	GLY	-	expression tag	UNP Q6SZW1
A	386	SER	-	expression tag	UNP Q6SZW1
B	385	GLY	-	expression tag	UNP Q6SZW1
B	386	SER	-	expression tag	UNP Q6SZW1
C	385	GLY	-	expression tag	UNP Q6SZW1
C	386	SER	-	expression tag	UNP Q6SZW1
D	385	GLY	-	expression tag	UNP Q6SZW1
D	386	SER	-	expression tag	UNP Q6SZW1
E	385	GLY	-	expression tag	UNP Q6SZW1
E	386	SER	-	expression tag	UNP Q6SZW1
F	385	GLY	-	expression tag	UNP Q6SZW1
F	386	SER	-	expression tag	UNP Q6SZW1
G	385	GLY	-	expression tag	UNP Q6SZW1
G	386	SER	-	expression tag	UNP Q6SZW1
H	385	GLY	-	expression tag	UNP Q6SZW1
H	386	SER	-	expression tag	UNP Q6SZW1
I	385	GLY	-	expression tag	UNP Q6SZW1
I	386	SER	-	expression tag	UNP Q6SZW1
J	385	GLY	-	expression tag	UNP Q6SZW1
J	386	SER	-	expression tag	UNP Q6SZW1
K	385	GLY	-	expression tag	UNP Q6SZW1
K	386	SER	-	expression tag	UNP Q6SZW1
L	385	GLY	-	expression tag	UNP Q6SZW1
L	386	SER	-	expression tag	UNP Q6SZW1
M	385	GLY	-	expression tag	UNP Q6SZW1
M	386	SER	-	expression tag	UNP Q6SZW1
N	385	GLY	-	expression tag	UNP Q6SZW1
N	386	SER	-	expression tag	UNP Q6SZW1
O	385	GLY	-	expression tag	UNP Q6SZW1
O	386	SER	-	expression tag	UNP Q6SZW1
P	385	GLY	-	expression tag	UNP Q6SZW1
P	386	SER	-	expression tag	UNP Q6SZW1

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

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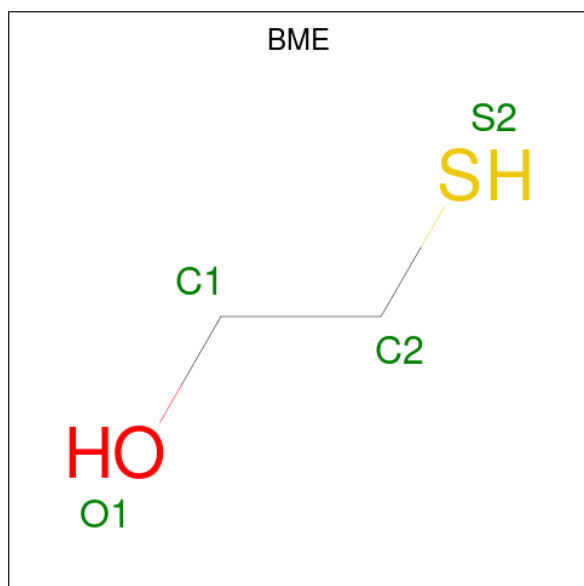
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	I	1	Total	C	O	0	0
			4	2	2		
2	I	1	Total	C	O	0	0
			4	2	2		
2	J	1	Total	C	O	0	0
			4	2	2		
2	J	1	Total	C	O	0	0
			4	2	2		
2	J	1	Total	C	O	0	0
			4	2	2		
2	J	1	Total	C	O	0	0
			4	2	2		
2	J	1	Total	C	O	0	0
			4	2	2		
2	K	1	Total	C	O	0	0
			4	2	2		
2	K	1	Total	C	O	0	0
			4	2	2		
2	K	1	Total	C	O	0	0
			4	2	2		
2	K	1	Total	C	O	0	0
			4	2	2		
2	L	1	Total	C	O	0	0
			4	2	2		
2	L	1	Total	C	O	0	0
			4	2	2		
2	L	1	Total	C	O	0	0
			4	2	2		
2	M	1	Total	C	O	0	0
			4	2	2		
2	M	1	Total	C	O	0	0
			4	2	2		
2	M	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	M	1	Total C O 4 2 2	0	0
2	N	1	Total C O 4 2 2	0	0
2	O	1	Total C O 4 2 2	0	0
2	O	1	Total C O 4 2 2	0	0
2	O	1	Total C O 4 2 2	0	0
2	P	1	Total C O 4 2 2	0	0
2	P	1	Total C O 4 2 2	0	0
2	P	1	Total C O 4 2 2	0	0

- Molecule 3 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C_2H_6OS).



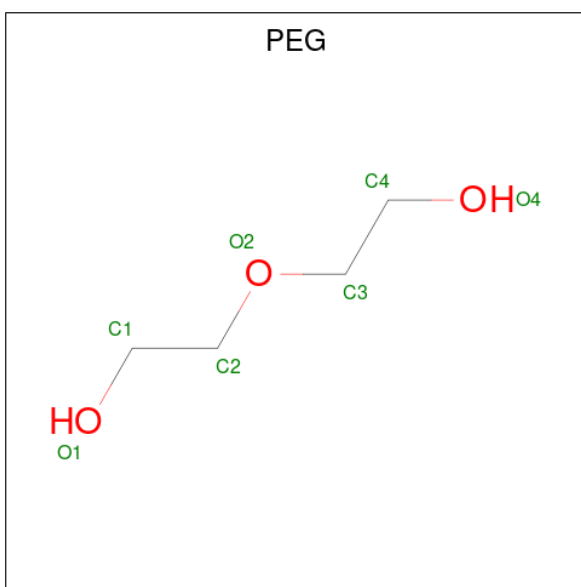
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O S 4 2 1 1	0	0
3	B	1	Total C O S 4 2 1 1	0	0
3	C	1	Total C O S 4 2 1 1	0	0

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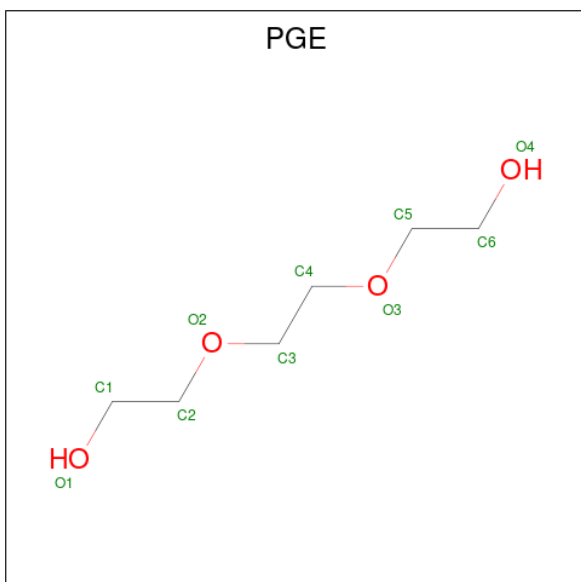
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total 4	C 2	O 1	S 1	0	0
3	E	1	Total 4	C 2	O 1	S 1	0	0
3	F	1	Total 4	C 2	O 1	S 1	0	0
3	G	1	Total 4	C 2	O 1	S 1	0	0
3	H	1	Total 4	C 2	O 1	S 1	0	0
3	I	1	Total 4	C 2	O 1	S 1	0	0
3	J	1	Total 4	C 2	O 1	S 1	0	0
3	K	1	Total 4	C 2	O 1	S 1	0	0
3	L	1	Total 4	C 2	O 1	S 1	0	0
3	M	1	Total 4	C 2	O 1	S 1	0	0
3	N	1	Total 4	C 2	O 1	S 1	0	0
3	O	1	Total 4	C 2	O 1	S 1	0	0
3	P	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	J	1	Total	C	O	0	0
			7	4	3		
4	J	1	Total	C	O	0	0
			7	4	3		
4	K	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			10	6	4		
5	P	1	Total	C	O	0	0
			10	6	4		

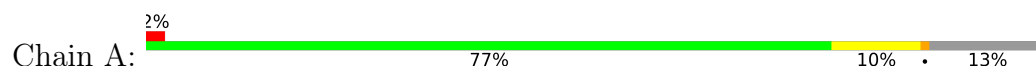
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	42	Total	O	0	0
			42	42		
6	B	62	Total	O	0	0
			62	62		
6	C	86	Total	O	0	0
			86	86		
6	D	77	Total	O	0	0
			77	77		
6	E	45	Total	O	0	0
			45	45		
6	F	37	Total	O	0	0
			37	37		
6	G	37	Total	O	0	0
			37	37		
6	H	43	Total	O	0	0
			43	43		
6	I	62	Total	O	0	0
			62	62		
6	J	84	Total	O	0	0
			84	84		
6	K	62	Total	O	0	0
			62	62		
6	L	50	Total	O	0	0
			50	50		
6	M	62	Total	O	0	0
			62	62		
6	N	25	Total	O	0	0
			25	25		
6	O	52	Total	O	0	0
			52	52		
6	P	45	Total	O	0	0
			45	45		

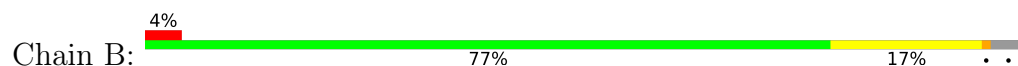
3 Residue-property plots

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: Sterile alpha and TIR motif-containing protein 1



- Molecule 1: Sterile alpha and TIR motif-containing protein 1



- Molecule 1: Sterile alpha and TIR motif-containing protein 1



- Molecule 1: Sterile alpha and TIR motif-containing protein 1

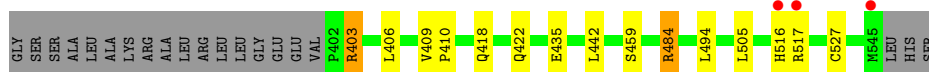
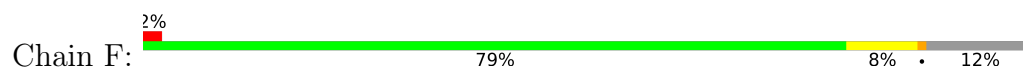


- Molecule 1: Sterile alpha and TIR motif-containing protein 1

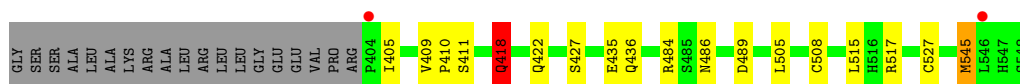
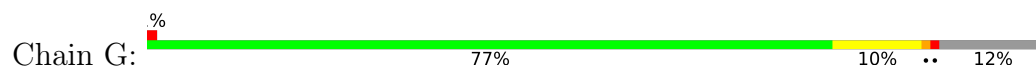




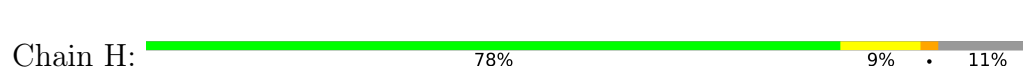
- Molecule 1: Sterile alpha and TIR motif-containing protein 1



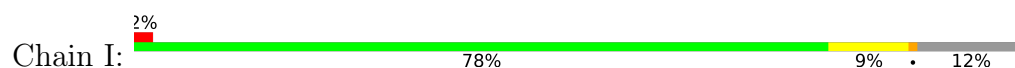
- Molecule 1: Sterile alpha and TIR motif-containing protein 1



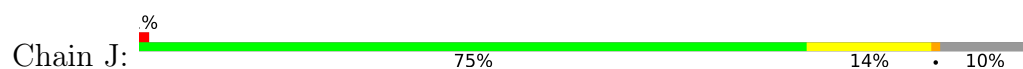
- Molecule 1: Sterile alpha and TIR motif-containing protein 1



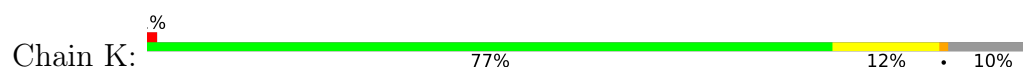
- Molecule 1: Sterile alpha and TIR motif-containing protein 1



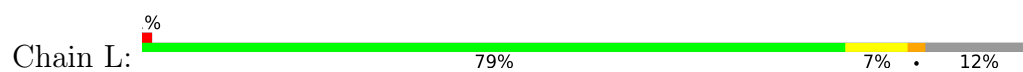
- Molecule 1: Sterile alpha and TIR motif-containing protein 1



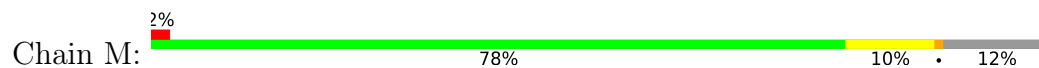
- Molecule 1: Sterile alpha and TIR motif-containing protein 1



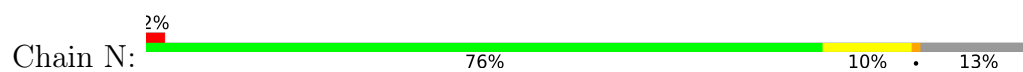
- Molecule 1: Sterile alpha and TIR motif-containing protein 1



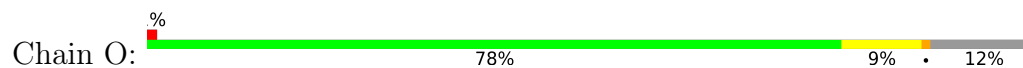
- Molecule 1: Sterile alpha and TIR motif-containing protein 1



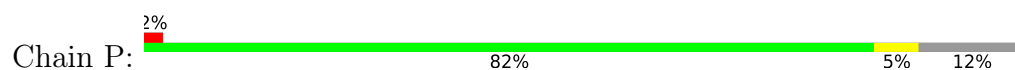
- Molecule 1: Sterile alpha and TIR motif-containing protein 1



- Molecule 1: Sterile alpha and TIR motif-containing protein 1



- Molecule 1: Sterile alpha and TIR motif-containing protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	252.25Å 252.25Å 49.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.40 – 2.47 56.40 – 2.47	Depositor EDS
% Data completeness (in resolution range)	99.1 (56.40-2.47) 99.1 (56.40-2.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.189 , 0.230 0.189 , 0.230	Depositor DCC
R_{free} test set	1333 reflections (1.07%)	wwPDB-VP
Wilson B-factor (Å ²)	51.7	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.011 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20654	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: PGE, BME, EDO, PEG

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	0.57	0/1254	1.08	1/1687 (0.1%)
1	B	0.63	0/1372	1.11	1/1846 (0.1%)
1	C	0.66	0/1271	1.10	1/1713 (0.1%)
1	D	0.67	0/1236	1.11	1/1665 (0.1%)
1	E	0.63	0/1242	1.08	1/1674 (0.1%)
1	F	0.58	0/1256	1.06	2/1692 (0.1%)
1	G	0.58	0/1244	1.06	2/1674 (0.1%)
1	H	0.62	0/1245	1.10	2/1679 (0.1%)
1	I	0.63	0/1270	1.12	3/1711 (0.2%)
1	J	0.69	0/1252	1.09	2/1686 (0.1%)
1	K	0.65	0/1273	1.07	1/1715 (0.1%)
1	L	0.60	0/1244	1.12	2/1675 (0.1%)
1	M	0.62	0/1252	1.10	2/1687 (0.1%)
1	N	0.57	0/1215	1.08	1/1637 (0.1%)
1	O	0.60	0/1252	1.08	2/1687 (0.1%)
1	P	0.62	0/1248	1.11	0/1680
All	All	0.62	0/20126	1.09	24/27108 (0.1%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	414	GLU	CB-CG-CD	10.73	130.85	112.60
1	B	508	CYS	CB-CA-C	-7.62	96.29	110.01
1	C	431	GLU	CB-CG-CD	7.57	125.47	112.60
1	M	402	PRO	CA-N-CD	-7.22	101.89	112.00
1	A	545	MET	N-CA-C	-6.62	105.35	113.50
1	I	544	GLU	CB-CG-CD	6.60	123.83	112.60
1	N	517	ARG	CG-CD-NE	-6.41	97.89	112.00
1	J	484	ARG	CB-CG-CD	6.36	125.92	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	508	CYS	CB-CA-C	-6.19	99.35	110.37
1	M	508	CYS	CB-CA-C	-6.14	98.96	110.01
1	L	517	ARG	CB-CG-CD	6.00	125.10	111.30
1	I	508	CYS	CB-CA-C	-5.97	99.26	110.01
1	F	406	LEU	O-C-N	-5.93	118.80	121.53
1	H	403	ARG	CB-CA-C	5.91	116.90	108.68
1	H	416	GLU	CB-CG-CD	5.89	122.62	112.60
1	G	418	GLN	CB-CG-CD	5.81	122.47	112.60
1	I	543	ARG	CB-CG-CD	5.75	124.53	111.30
1	K	508	CYS	CB-CA-C	-5.70	99.75	110.01
1	F	484	ARG	CG-CD-NE	-5.22	100.52	112.00
1	O	508	CYS	CB-CA-C	-5.20	100.65	110.01
1	O	543	ARG	CB-CG-CD	5.11	123.05	111.30
1	J	484	ARG	CG-CD-NE	-5.11	100.76	112.00
1	E	508	CYS	CB-CA-C	-5.07	100.88	110.01
1	G	508	CYS	CB-CA-C	-5.02	100.98	110.01

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	1211	0	1225	12	0
1	B	1324	0	1339	23	0
1	C	1232	0	1231	13	0
1	D	1204	0	1194	23	0
1	E	1209	0	1207	14	0
1	F	1211	0	1215	11	0
1	G	1206	0	1207	6	0
1	H	1210	0	1208	15	0
1	I	1220	0	1229	11	0
1	J	1216	0	1214	14	0
1	K	1234	0	1238	20	0
1	L	1205	0	1201	6	0
1	M	1211	0	1222	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	1181	0	1182	8	0
1	O	1211	0	1222	15	0
1	P	1207	0	1217	7	0
2	A	8	0	12	3	0
2	B	16	0	24	1	0
2	C	12	0	18	2	0
2	D	24	0	36	9	0
2	E	4	0	6	5	0
2	F	4	0	6	0	0
2	I	8	0	12	1	0
2	J	24	0	36	3	0
2	K	16	0	24	0	0
2	L	12	0	18	1	0
2	M	16	0	24	2	0
2	N	4	0	6	0	0
2	O	12	0	18	4	0
2	P	12	0	18	0	0
3	A	4	0	5	0	0
3	B	4	0	5	0	0
3	C	4	0	5	0	0
3	D	4	0	5	1	0
3	E	4	0	5	0	0
3	F	4	0	5	0	0
3	G	4	0	5	0	0
3	H	4	0	5	1	0
3	I	4	0	5	0	0
3	J	4	0	5	1	0
3	K	4	0	5	0	0
3	L	4	0	5	0	0
3	M	4	0	5	0	0
3	N	4	0	5	1	0
3	O	4	0	5	0	0
3	P	4	0	5	0	0
4	B	7	0	10	1	0
4	D	7	0	10	8	0
4	J	14	0	20	2	0
4	K	7	0	10	2	0
5	B	10	0	14	8	0
5	P	10	0	14	1	0
6	A	42	0	0	1	0
6	B	62	0	0	3	0
6	C	86	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	77	0	0	0	0
6	E	45	0	0	1	0
6	F	37	0	0	0	0
6	G	37	0	0	1	0
6	H	43	0	0	0	0
6	I	62	0	0	1	0
6	J	84	0	0	1	0
6	K	62	0	0	2	0
6	L	50	0	0	2	0
6	M	62	0	0	1	0
6	N	25	0	0	1	0
6	O	52	0	0	0	0
6	P	45	0	0	0	0
All	All	20654	0	19967	181	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 5.

All (181) 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:K:516:HIS:CE1	1:K:547:HIS:HB2	1.93	1.04
1:K:516:HIS:CE1	1:K:547:HIS:CB	2.45	0.99
1:O:512:ARG:HH22	2:O:601:EDO:H22	1.28	0.98
1:B:402:PRO:HB2	5:B:605:PGE:H32	1.52	0.89
1:A:465[A]:ARG:HH12	2:A:603:EDO:H21	1.38	0.89
1:G:486:ASN:OD1	1:G:489:ASP:HB2	1.76	0.84
1:K:516:HIS:CE1	1:K:547:HIS:HB3	2.13	0.83
1:K:537:ARG:HH11	1:K:537:ARG:HG2	1.43	0.81
1:D:465:ARG:HD2	2:D:608:EDO:H22	1.64	0.80
1:L:414:GLU:HG3	6:L:737:HOH:O	1.82	0.80
1:K:537:ARG:HH11	1:K:537:ARG:CG	1.95	0.79
1:K:537:ARG:HG2	1:K:537:ARG:NH1	1.98	0.77
1:C:497:ARG:HH12	3:D:603:BME:H11	1.51	0.75
1:O:512:ARG:NH2	2:O:601:EDO:H22	2.02	0.75
1:B:404:PRO:HD2	5:B:605:PGE:H6	1.68	0.74
1:H:521[B]:GLN:HA	1:H:521[B]:GLN:OE1	1.85	0.74
1:I:449:GLU:HG3	2:I:601:EDO:H21	1.70	0.73
1:D:413:LYS:HG3	1:D:416:GLU:OE2	1.89	0.73
1:B:465[A]:ARG:HG2	1:C:442:LEU:HD11	1.71	0.73
1:E:522:GLN:HG3	2:E:601:EDO:H22	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:516:HIS:ND1	1:K:547:HIS:HB3	2.06	0.71
5:B:605:PGE:H2	6:B:751:HOH:O	1.90	0.70
1:J:413:LYS:HG2	1:J:416:GLU:OE1	1.91	0.70
1:B:465[A]:ARG:CG	1:C:442:LEU:HD11	2.23	0.69
1:A:465[A]:ARG:HH12	2:A:603:EDO:C2	2.05	0.69
6:I:717:HOH:O	4:J:601:PEG:H32	1.92	0.68
1:E:522:GLN:CG	2:E:601:EDO:H22	2.25	0.67
1:B:412:TRP:CH2	5:B:605:PGE:H52	2.30	0.66
1:G:418:GLN:HG3	6:G:732:HOH:O	1.95	0.66
1:D:465:ARG:CD	2:D:608:EDO:H22	2.25	0.65
1:M:489:ASP:OD1	6:M:701:HOH:O	2.15	0.63
1:G:515:LEU:HB3	1:G:545:MET:HE1	1.82	0.62
1:L:489:ASP:OD1	1:L:499[B]:ARG:NH1	2.33	0.61
1:D:463:ARG:HH12	2:D:607:EDO:H11	1.65	0.61
1:B:404:PRO:O	5:B:605:PGE:H4	2.01	0.61
1:D:465:ARG:HD2	2:D:608:EDO:C2	2.31	0.60
1:D:497:ARG:HH12	1:E:509:GLY:HA2	1.66	0.60
1:A:540:THR:O	1:A:543[B]:ARG:HG3	2.02	0.59
1:D:479:TYR:HB2	4:D:602:PEG:C2	2.32	0.59
1:K:401:VAL:N	1:K:402:PRO:CD	2.66	0.59
1:C:401:VAL:N	1:C:402:PRO:CD	2.65	0.59
1:M:509:GLY:HA2	1:N:497:ARG:HH12	1.68	0.58
1:H:406:LEU:N	1:H:407:PRO:HD3	2.18	0.58
1:D:465:ARG:HH11	2:D:608:EDO:H11	1.69	0.58
1:H:406:LEU:HB3	1:O:406:LEU:HD21	1.84	0.58
1:K:484:ARG:N	1:K:484:ARG:HD2	2.19	0.58
1:N:437:GLN:NE2	1:O:465[B]:ARG:NH1	2.52	0.57
1:D:468:ARG:HH21	2:D:608:EDO:H12	1.70	0.57
1:F:516[A]:HIS:HD2	1:F:517[A]:ARG:CZ	2.18	0.57
1:M:479:TYR:HB2	2:M:603:EDO:H12	1.86	0.57
1:O:546:LEU:CD2	1:O:546:LEU:H	2.18	0.57
1:O:515:LEU:HB3	1:O:545:MET:HE1	1.86	0.56
1:J:402:PRO:HD2	1:J:403:ARG:NH1	2.20	0.56
1:K:408:SER:HB2	4:K:603:PEG:H12	1.88	0.56
1:O:546:LEU:H	1:O:546:LEU:HD23	1.71	0.56
1:B:516:HIS:HB2	6:B:743:HOH:O	2.05	0.55
1:C:520:GLU:HB2	1:C:539:LEU:HD11	1.87	0.55
1:D:468:ARG:NH2	2:D:608:EDO:H12	2.22	0.55
1:B:406:LEU:N	1:B:407:PRO:HD3	2.21	0.55
1:D:512:ARG:HH12	2:D:604:EDO:H22	1.72	0.54
1:E:465:ARG:CG	1:F:442:LEU:HD11	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:482[B]:CYS:HB3	3:H:601:BME:H12	1.89	0.54
1:D:480:SER:HA	4:D:602:PEG:C3	2.37	0.54
1:I:468:ARG:HD2	5:P:604:PGE:H22	1.90	0.54
1:A:442:LEU:HD11	1:H:465[A]:ARG:CG	2.38	0.54
1:I:514:LEU:HD22	1:J:537:ARG:HD3	1.91	0.53
1:D:540:THR:HG21	1:E:517[A]:ARG:NH2	2.23	0.53
1:B:500:GLN:HE22	4:B:603:PEG:H42	1.74	0.52
1:E:516:HIS:CE1	1:E:517[A]:ARG:HD2	2.44	0.52
1:C:546:LEU:HB3	2:C:602:EDO:H22	1.92	0.52
1:K:516:HIS:CG	1:K:547:HIS:HB3	2.45	0.52
1:B:479:TYR:HB2	2:B:602:EDO:H21	1.91	0.52
1:D:479:TYR:HB2	4:D:602:PEG:H22	1.91	0.52
1:A:465[A]:ARG:NH1	2:A:603:EDO:H21	2.16	0.52
1:J:445:ARG:HA	2:J:605:EDO:H22	1.91	0.52
1:D:480:SER:HA	4:D:602:PEG:H31	1.90	0.51
1:K:445:ARG:HD2	6:K:720:HOH:O	2.10	0.51
1:I:465[A]:ARG:HG2	1:P:442:LEU:HD11	1.92	0.51
1:M:509:GLY:HA2	1:N:497:ARG:NH1	2.25	0.51
1:C:414:GLU:HG3	6:C:750:HOH:O	2.11	0.51
1:A:442:LEU:HD11	1:H:465[B]:ARG:HG2	1.92	0.50
1:D:479:TYR:HB2	4:D:602:PEG:H21	1.92	0.50
1:F:516[A]:HIS:CD2	1:F:517[A]:ARG:CZ	2.94	0.50
1:K:414:GLU:HG3	6:K:746:HOH:O	2.11	0.50
1:H:521[B]:GLN:OE1	1:H:521[B]:GLN:CA	2.57	0.50
1:K:484:ARG:HD2	1:K:484:ARG:H	1.77	0.50
1:J:479:TYR:HB2	2:J:604:EDO:C2	2.42	0.49
1:B:406:LEU:N	1:B:407:PRO:CD	2.75	0.49
1:E:521:GLN:HE21	2:E:601:EDO:H21	1.77	0.49
1:K:408:SER:H	4:K:603:PEG:H12	1.76	0.49
1:C:543:ARG:HA	6:C:776:HOH:O	2.12	0.49
1:C:540:THR:O	1:C:543:ARG:HG2	2.12	0.49
1:O:546:LEU:HD23	1:O:546:LEU:N	2.27	0.49
1:J:507:SER:HA	3:J:606:BME:H11	1.95	0.49
1:E:465:ARG:HG3	1:F:442:LEU:HD11	1.95	0.49
1:B:414:GLU:O	1:B:418:GLN:HG2	2.13	0.48
1:A:442:LEU:HD11	1:H:465[B]:ARG:CG	2.43	0.48
1:O:512:ARG:HH12	2:O:601:EDO:H22	1.78	0.48
1:L:458:LYS:HG3	6:L:736:HOH:O	2.13	0.48
1:B:402:PRO:HD2	5:B:605:PGE:H12	1.94	0.48
1:J:515:LEU:HB3	1:J:545:MET:HE1	1.95	0.48
1:O:442:LEU:HD11	1:P:465[B]:ARG:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:479:TYR:HB2	2:J:604:EDO:H21	1.96	0.48
1:E:521:GLN:NE2	2:E:601:EDO:H21	2.28	0.48
1:N:409:VAL:N	1:N:410:PRO:CD	2.77	0.48
1:H:406:LEU:N	1:H:407:PRO:CD	2.76	0.48
1:B:515:LEU:O	1:B:518:VAL:HG12	2.15	0.47
1:C:420:TRP:HE1	2:C:604:EDO:H12	1.78	0.47
1:I:465[B]:ARG:CG	1:P:442:LEU:HD11	2.44	0.47
1:J:489:ASP:HB2	6:J:778:HOH:O	2.14	0.47
1:J:412:TRP:CZ2	4:J:602:PEG:H21	2.50	0.47
1:D:499:ARG:NH2	4:D:602:PEG:H12	2.30	0.47
1:H:431:GLU:HG3	1:H:434:ARG:HH22	1.80	0.47
1:E:497:ARG:HG2	6:E:729:HOH:O	2.15	0.46
1:M:431:GLU:HG3	1:M:434[B]:ARG:HH21	1.80	0.46
1:H:406:LEU:HA	1:H:476:PHE:O	2.16	0.46
1:A:409:VAL:N	1:A:410:PRO:CD	2.78	0.46
1:I:465[A]:ARG:CG	1:P:442:LEU:HD11	2.45	0.46
1:M:416:GLU:OE2	2:M:602:EDO:H11	2.16	0.46
1:C:484:ARG:HD3	1:C:484:ARG:HA	1.63	0.46
1:B:458:LYS:HB3	6:B:754:HOH:O	2.17	0.45
1:E:484:ARG:HA	1:E:484:ARG:HD3	1.64	0.45
1:D:540:THR:HG21	1:E:517[A]:ARG:HH22	1.81	0.45
1:F:516[A]:HIS:CD2	1:F:517[A]:ARG:NH2	2.84	0.45
1:K:516:HIS:ND1	1:K:547:HIS:CB	2.74	0.45
1:D:426:PHE:HA	2:D:601:EDO:H11	1.98	0.45
1:K:442:LEU:HD11	1:L:465:ARG:HG2	1.98	0.45
1:F:403:ARG:H	1:F:403:ARG:CD	2.29	0.45
1:G:409:VAL:N	1:G:410:PRO:CD	2.80	0.45
1:N:482[B]:CYS:HB3	3:N:601:BME:H21	1.78	0.45
1:M:409:VAL:N	1:M:410:PRO:CD	2.80	0.44
1:H:431:GLU:HG3	1:H:434:ARG:NH2	2.33	0.44
1:J:409:VAL:N	1:J:410:PRO:CD	2.80	0.44
1:K:409:VAL:N	1:K:410:PRO:CD	2.80	0.44
1:F:403:ARG:H	1:F:403:ARG:HD3	1.82	0.44
1:B:392:ARG:HG2	1:B:394:LEU:HD12	2.00	0.44
1:F:403:ARG:CD	1:F:403:ARG:N	2.80	0.44
1:N:499:ARG:HD2	6:N:709:HOH:O	2.18	0.44
1:H:481:THR:O	1:H:484:ARG:NH1	2.51	0.44
1:F:505:LEU:HD23	1:F:527:CYS:SG	2.58	0.43
1:B:484:ARG:HA	1:B:484:ARG:HD3	1.78	0.43
1:O:409:VAL:N	1:O:410:PRO:CD	2.82	0.43
1:L:409:VAL:N	1:L:410:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:TRP:HB2	5:B:605:PGE:H5	2.01	0.43
1:F:459:SER:OG	1:G:436:GLN:NE2	2.46	0.43
1:J:515:LEU:O	1:J:518:VAL:HG12	2.19	0.43
1:A:442:LEU:HD11	1:H:465[A]:ARG:HG2	2.00	0.43
1:I:458:LYS:HA	1:I:458:LYS:HD2	1.95	0.43
1:B:412:TRP:HH2	5:B:605:PGE:H52	1.81	0.43
1:C:401:VAL:N	1:C:402:PRO:HD2	2.31	0.43
1:B:465[A]:ARG:HG3	1:C:442:LEU:HD11	2.01	0.42
1:I:409:VAL:N	1:I:410:PRO:CD	2.81	0.42
1:I:432[B]:SER:OG	1:I:455:LEU:HA	2.20	0.42
1:D:478:ASN:HA	4:D:602:PEG:O1	2.19	0.42
1:G:505:LEU:HD23	1:G:527:CYS:SG	2.59	0.42
1:O:437:GLN:NE2	1:P:465[A]:ARG:NH2	2.67	0.42
1:A:423:GLN:HB3	6:A:702:HOH:O	2.20	0.42
1:B:403:ARG:H	1:B:403:ARG:HG2	1.68	0.42
1:O:414:GLU:O	1:O:418:GLN:HG2	2.20	0.42
1:J:414:GLU:O	1:J:418:GLN:HG2	2.20	0.42
1:B:547:HIS:O	1:B:548:SER:HB2	2.20	0.41
1:E:522:GLN:HG2	2:E:601:EDO:H22	2.00	0.41
1:O:505:LEU:HD23	1:O:527:CYS:SG	2.60	0.41
1:L:530:HIS:O	2:L:604:EDO:H11	2.20	0.41
1:K:515:LEU:HD23	1:K:515:LEU:HA	1.91	0.41
1:N:515:LEU:O	1:N:518:VAL:HG12	2.19	0.41
1:B:540:THR:O	1:B:543[B]:ARG:HG2	2.20	0.41
1:D:483:ASP:O	4:D:602:PEG:H42	2.20	0.41
1:D:491:LEU:HD11	1:D:505:LEU:HD12	2.03	0.41
1:D:494:LEU:HD12	1:D:494:LEU:HA	1.91	0.41
1:A:414:GLU:O	1:A:418:GLN:HG2	2.21	0.41
1:E:409:VAL:N	1:E:410:PRO:CD	2.84	0.41
1:H:409:VAL:N	1:H:410:PRO:CD	2.85	0.40
1:I:465[B]:ARG:HG2	1:P:442:LEU:HD11	2.02	0.40
1:N:487:LEU:HD21	1:N:515:LEU:HD22	2.02	0.40
1:A:484:ARG:HD3	1:A:484:ARG:HA	1.73	0.40
1:F:409:VAL:N	1:F:410:PRO:CD	2.84	0.40
1:P:505:LEU:HD23	1:P:527:CYS:SG	2.61	0.40
1:J:436:GLN:NE2	1:K:459:SER:OG	2.51	0.40
1:I:484:ARG:HA	1:I:484:ARG:HD3	1.71	0.40
1:O:512:ARG:NH1	2:O:601:EDO:H22	2.37	0.40

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	148/164 (90%)	146 (99%)	2 (1%)	0	100	100
1	B	163/164 (99%)	159 (98%)	4 (2%)	0	100	100
1	C	151/164 (92%)	147 (97%)	3 (2%)	1 (1%)	18	32
1	D	147/164 (90%)	145 (99%)	2 (1%)	0	100	100
1	E	147/164 (90%)	144 (98%)	3 (2%)	0	100	100
1	F	149/164 (91%)	147 (99%)	2 (1%)	0	100	100
1	G	148/164 (90%)	145 (98%)	3 (2%)	0	100	100
1	H	148/164 (90%)	144 (97%)	4 (3%)	0	100	100
1	I	152/164 (93%)	150 (99%)	2 (1%)	0	100	100
1	J	149/164 (91%)	147 (99%)	2 (1%)	0	100	100
1	K	151/164 (92%)	147 (97%)	4 (3%)	0	100	100
1	L	148/164 (90%)	146 (99%)	2 (1%)	0	100	100
1	M	149/164 (91%)	146 (98%)	3 (2%)	0	100	100
1	N	145/164 (88%)	142 (98%)	2 (1%)	1 (1%)	18	32
1	O	149/164 (91%)	147 (99%)	2 (1%)	0	100	100
1	P	148/164 (90%)	144 (97%)	4 (3%)	0	100	100
All	All	2392/2624 (91%)	2346 (98%)	44 (2%)	2 (0%)	48	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	402	PRO
1	N	405	ILE

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	135/144 (94%)	128 (95%)	7 (5%)	21	39
1	B	148/144 (103%)	138 (93%)	10 (7%)	14	28
1	C	138/144 (96%)	130 (94%)	8 (6%)	18	35
1	D	134/144 (93%)	125 (93%)	9 (7%)	15	29
1	E	134/144 (93%)	126 (94%)	8 (6%)	17	33
1	F	136/144 (94%)	130 (96%)	6 (4%)	25	47
1	G	135/144 (94%)	125 (93%)	10 (7%)	13	24
1	H	135/144 (94%)	127 (94%)	8 (6%)	18	34
1	I	139/144 (96%)	132 (95%)	7 (5%)	22	41
1	J	136/144 (94%)	129 (95%)	7 (5%)	21	40
1	K	138/144 (96%)	128 (93%)	10 (7%)	13	26
1	L	135/144 (94%)	127 (94%)	8 (6%)	18	34
1	M	136/144 (94%)	128 (94%)	8 (6%)	18	34
1	N	132/144 (92%)	123 (93%)	9 (7%)	14	28
1	O	136/144 (94%)	133 (98%)	3 (2%)	45	70
1	P	135/144 (94%)	129 (96%)	6 (4%)	25	47
All	All	2182/2304 (95%)	2058 (94%)	124 (6%)	20	36

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	405	ILE
1	A	411	SER
1	A	422	GLN
1	A	435	GLU
1	A	484	ARG
1	A	494	LEU
1	A	546	LEU
1	B	395	ARG

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Mol	Chain	Res	Type
1	B	400	GLU
1	B	403	ARG
1	B	411	SER
1	B	422	GLN
1	B	427[A]	SER
1	B	427[B]	SER
1	B	434[A]	ARG
1	B	434[B]	ARG
1	B	484	ARG
1	C	411[A]	SER
1	C	411[B]	SER
1	C	422	GLN
1	C	431	GLU
1	C	435	GLU
1	C	458	LYS
1	C	484	ARG
1	C	517	ARG
1	D	411	SER
1	D	413	LYS
1	D	446	LEU
1	D	458	LYS
1	D	484	ARG
1	D	497	ARG
1	D	520	GLU
1	D	543	ARG
1	D	548	SER
1	E	411	SER
1	E	422	GLN
1	E	427	SER
1	E	494	LEU
1	E	515	LEU
1	E	517[A]	ARG
1	E	517[B]	ARG
1	E	546	LEU
1	F	403	ARG
1	F	418	GLN
1	F	422	GLN
1	F	435	GLU
1	F	484	ARG
1	F	494	LEU
1	G	405	ILE
1	G	411	SER

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Mol	Chain	Res	Type
1	G	418	GLN
1	G	422	GLN
1	G	427[A]	SER
1	G	427[B]	SER
1	G	435	GLU
1	G	484	ARG
1	G	517	ARG
1	G	545	MET
1	H	400	GLU
1	H	403	ARG
1	H	411[A]	SER
1	H	411[B]	SER
1	H	416	GLU
1	H	422	GLN
1	H	435	GLU
1	H	484	ARG
1	I	411[A]	SER
1	I	411[B]	SER
1	I	413	LYS
1	I	418	GLN
1	I	458	LYS
1	I	544	GLU
1	I	547	HIS
1	J	411[A]	SER
1	J	411[B]	SER
1	J	422	GLN
1	J	435	GLU
1	J	484	ARG
1	J	520	GLU
1	J	543	ARG
1	K	403	ARG
1	K	411	SER
1	K	422	GLN
1	K	434	ARG
1	K	435	GLU
1	K	497	ARG
1	K	515	LEU
1	K	537	ARG
1	K	543[A]	ARG
1	K	543[B]	ARG
1	L	411	SER
1	L	422	GLN

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Mol	Chain	Res	Type
1	L	435	GLU
1	L	458	LYS
1	L	484	ARG
1	L	508	CYS
1	L	517	ARG
1	L	543	ARG
1	M	411	SER
1	M	422	GLN
1	M	472	GLU
1	M	508	CYS
1	M	515	LEU
1	M	520	GLU
1	M	545	MET
1	M	546	LEU
1	N	405	ILE
1	N	411	SER
1	N	422	GLN
1	N	435	GLU
1	N	458	LYS
1	N	484	ARG
1	N	517	ARG
1	N	543	ARG
1	N	546	LEU
1	O	411	SER
1	O	543	ARG
1	O	545	MET
1	P	403	ARG
1	P	411[A]	SER
1	P	411[B]	SER
1	P	418	GLN
1	P	422	GLN
1	P	435	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	437	GLN
1	A	500	GLN
1	B	486	ASN
1	B	500	GLN
1	C	486	ASN
1	C	500	GLN

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Mol	Chain	Res	Type
1	C	547	HIS
1	D	437	GLN
1	D	486	ASN
1	D	500	GLN
1	E	486	ASN
1	E	500	GLN
1	E	521	GLN
1	F	423	GLN
1	F	486	ASN
1	G	418	GLN
1	G	436	GLN
1	I	418	GLN
1	I	437	GLN
1	I	500	GLN
1	J	436	GLN
1	J	437	GLN
1	J	486	ASN
1	K	422	GLN
1	K	436	GLN
1	K	486	ASN
1	K	500	GLN
1	K	516	HIS
1	L	486	ASN
1	L	530	HIS
1	M	436	GLN
1	M	500	GLN
1	N	437	GLN
1	N	486	ASN
1	N	500	GLN
1	O	423	GLN
1	O	436	GLN
1	O	437	GLN
1	O	486	ASN
1	P	423	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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

66 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	EDO	O	601	-	3,3,3	0.11	0	2,2,2	0.38	0
2	EDO	P	605	-	3,3,3	0.08	0	2,2,2	0.31	0
4	PEG	D	602	-	6,6,6	0.34	0	5,5,5	0.37	0
2	EDO	O	604	-	3,3,3	0.14	0	2,2,2	0.27	0
3	BME	K	602	1	3,3,3	0.26	0	2,2,2	0.34	0
3	BME	M	601	1	3,3,3	0.34	0	2,2,2	1.40	0
2	EDO	P	601	-	3,3,3	0.10	0	2,2,2	0.29	0
2	EDO	C	604	-	3,3,3	0.16	0	2,2,2	0.05	0
2	EDO	L	604	-	3,3,3	0.17	0	2,2,2	0.19	0
2	EDO	I	602	-	3,3,3	0.18	0	2,2,2	0.20	0
2	EDO	D	606	-	3,3,3	0.28	0	2,2,2	0.35	0
2	EDO	B	607	-	3,3,3	0.08	0	2,2,2	0.19	0
2	EDO	L	603	-	3,3,3	0.09	0	2,2,2	0.29	0
2	EDO	K	604	-	3,3,3	0.30	0	2,2,2	0.19	0
2	EDO	B	601	-	3,3,3	0.51	0	2,2,2	0.64	0
2	EDO	O	603	-	3,3,3	0.18	0	2,2,2	0.42	0
3	BME	F	602	1	3,3,3	0.16	0	2,2,2	0.45	0
3	BME	I	603	1	3,3,3	0.19	0	2,2,2	0.42	0
2	EDO	A	601	-	3,3,3	0.06	0	2,2,2	0.31	0
2	EDO	C	603	-	3,3,3	0.17	0	2,2,2	0.15	0
2	EDO	D	601	-	3,3,3	0.30	0	2,2,2	0.68	0
2	EDO	D	607	-	3,3,3	0.10	0	2,2,2	0.25	0
2	EDO	J	603	-	3,3,3	0.20	0	2,2,2	0.44	0
2	EDO	A	603	-	3,3,3	0.18	0	2,2,2	0.23	0
2	EDO	B	602	-	3,3,3	0.23	0	2,2,2	0.24	0
3	BME	P	603	1	3,3,3	0.18	0	2,2,2	0.19	0
2	EDO	J	608	-	3,3,3	0.27	0	2,2,2	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BME	B	604	1	3,3,3	0.42	0	2,2,2	0.59	0
3	BME	J	606	1	3,3,3	0.27	0	2,2,2	0.36	0
2	EDO	D	605	-	3,3,3	0.20	0	2,2,2	0.11	0
3	BME	L	602	1	3,3,3	0.14	0	2,2,2	1.05	0
2	EDO	K	605	-	3,3,3	0.50	0	2,2,2	0.58	0
2	EDO	J	607	-	3,3,3	0.09	0	2,2,2	0.20	0
3	BME	D	603	1	3,3,3	0.29	0	2,2,2	1.17	0
4	PEG	J	601	-	6,6,6	0.53	0	5,5,5	0.32	0
5	PGE	B	605	-	9,9,9	0.31	0	8,8,8	0.35	0
2	EDO	F	601	-	3,3,3	0.06	0	2,2,2	0.02	0
2	EDO	M	603	-	3,3,3	0.18	0	2,2,2	0.39	0
3	BME	E	602	1	3,3,3	0.36	0	2,2,2	0.89	0
4	PEG	B	603	-	6,6,6	0.17	0	5,5,5	0.11	0
2	EDO	E	601	-	3,3,3	0.18	0	2,2,2	0.67	0
2	EDO	J	604	-	3,3,3	0.17	0	2,2,2	1.00	0
2	EDO	J	605	-	3,3,3	0.17	0	2,2,2	0.99	0
2	EDO	J	609	-	3,3,3	0.18	0	2,2,2	0.18	0
2	EDO	K	601	-	3,3,3	0.07	0	2,2,2	0.40	0
2	EDO	K	606	-	3,3,3	0.08	0	2,2,2	0.08	0
3	BME	N	601	1	3,3,3	0.31	0	2,2,2	0.37	0
2	EDO	M	602	-	3,3,3	0.23	0	2,2,2	0.27	0
2	EDO	M	604	-	3,3,3	0.28	0	2,2,2	0.61	0
2	EDO	N	602	-	3,3,3	0.08	0	2,2,2	0.34	0
4	PEG	J	602	-	6,6,6	0.56	0	5,5,5	0.27	0
3	BME	A	602	1	3,3,3	0.29	0	2,2,2	0.65	0
2	EDO	P	602	-	3,3,3	0.24	0	2,2,2	0.33	0
3	BME	O	602	1	3,3,3	0.16	0	2,2,2	0.37	0
2	EDO	M	605	-	3,3,3	0.25	0	2,2,2	0.08	0
3	BME	G	601	1	3,3,3	0.27	0	2,2,2	0.46	0
3	BME	C	601	1	3,3,3	0.32	0	2,2,2	0.55	0
5	PGE	P	604	-	9,9,9	0.22	0	8,8,8	0.19	0
2	EDO	C	602	-	3,3,3	0.34	0	2,2,2	0.78	0
2	EDO	B	606	-	3,3,3	0.19	0	2,2,2	0.25	0
3	BME	H	601	1	3,3,3	0.24	0	2,2,2	0.07	0
2	EDO	D	608	-	3,3,3	0.34	0	2,2,2	0.58	0
4	PEG	K	603	-	6,6,6	0.25	0	5,5,5	0.16	0
2	EDO	D	604	-	3,3,3	0.18	0	2,2,2	0.08	0
2	EDO	I	601	-	3,3,3	0.32	0	2,2,2	0.61	0
2	EDO	L	601	-	3,3,3	0.08	0	2,2,2	0.47	0

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	EDO	O	601	-	-	1/1/1/1	-
2	EDO	P	605	-	-	0/1/1/1	-
4	PEG	D	602	-	-	3/4/4/4	-
2	EDO	O	604	-	-	0/1/1/1	-
3	BME	K	602	1	-	1/1/1/1	-
3	BME	M	601	1	-	0/1/1/1	-
2	EDO	P	601	-	-	1/1/1/1	-
2	EDO	C	604	-	-	1/1/1/1	-
2	EDO	L	604	-	-	1/1/1/1	-
2	EDO	I	602	-	-	1/1/1/1	-
2	EDO	D	606	-	-	0/1/1/1	-
2	EDO	B	607	-	-	0/1/1/1	-
2	EDO	L	603	-	-	1/1/1/1	-
2	EDO	K	604	-	-	1/1/1/1	-
2	EDO	B	601	-	-	1/1/1/1	-
2	EDO	O	603	-	-	1/1/1/1	-
3	BME	F	602	1	-	1/1/1/1	-
3	BME	I	603	1	-	0/1/1/1	-
2	EDO	A	601	-	-	0/1/1/1	-
2	EDO	C	603	-	-	0/1/1/1	-
2	EDO	D	601	-	-	1/1/1/1	-
2	EDO	D	607	-	-	1/1/1/1	-
2	EDO	J	603	-	-	1/1/1/1	-
2	EDO	A	603	-	-	1/1/1/1	-
2	EDO	B	602	-	-	1/1/1/1	-
3	BME	P	603	1	-	1/1/1/1	-
2	EDO	J	608	-	-	1/1/1/1	-
3	BME	B	604	1	-	0/1/1/1	-
3	BME	J	606	1	-	0/1/1/1	-
2	EDO	D	605	-	-	1/1/1/1	-
3	BME	L	602	1	-	0/1/1/1	-
2	EDO	K	605	-	-	1/1/1/1	-
2	EDO	J	607	-	-	1/1/1/1	-
3	BME	D	603	1	-	1/1/1/1	-
4	PEG	J	601	-	-	3/4/4/4	-
5	PGE	B	605	-	-	6/7/7/7	-
2	EDO	F	601	-	-	1/1/1/1	-
2	EDO	M	603	-	-	0/1/1/1	-
3	BME	E	602	1	-	0/1/1/1	-
4	PEG	B	603	-	-	0/4/4/4	-
2	EDO	E	601	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	J	604	-	-	1/1/1/1	-
2	EDO	J	605	-	-	1/1/1/1	-
2	EDO	J	609	-	-	1/1/1/1	-
2	EDO	K	601	-	-	0/1/1/1	-
2	EDO	K	606	-	-	1/1/1/1	-
3	BME	N	601	1	-	1/1/1/1	-
2	EDO	M	602	-	-	1/1/1/1	-
2	EDO	M	604	-	-	0/1/1/1	-
2	EDO	N	602	-	-	1/1/1/1	-
4	PEG	J	602	-	-	2/4/4/4	-
3	BME	A	602	1	-	0/1/1/1	-
2	EDO	P	602	-	-	1/1/1/1	-
3	BME	O	602	1	-	0/1/1/1	-
2	EDO	M	605	-	-	0/1/1/1	-
3	BME	G	601	1	-	0/1/1/1	-
3	BME	C	601	1	-	1/1/1/1	-
5	PGE	P	604	-	-	4/7/7/7	-
2	EDO	C	602	-	-	0/1/1/1	-
2	EDO	B	606	-	-	1/1/1/1	-
3	BME	H	601	1	-	1/1/1/1	-
2	EDO	D	608	-	-	1/1/1/1	-
4	PEG	K	603	-	-	3/4/4/4	-
2	EDO	D	604	-	-	0/1/1/1	-
2	EDO	I	601	-	-	1/1/1/1	-
2	EDO	L	601	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	601	BME	O1-C1-C2-S2
3	N	601	BME	O1-C1-C2-S2
5	B	605	PGE	O2-C3-C4-O3
4	J	601	PEG	O1-C1-C2-O2
4	K	603	PEG	O1-C1-C2-O2
5	P	604	PGE	O2-C3-C4-O3
5	B	605	PGE	C1-C2-O2-C3
3	D	603	BME	O1-C1-C2-S2

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Mol	Chain	Res	Type	Atoms
3	F	602	BME	O1-C1-C2-S2
3	K	602	BME	O1-C1-C2-S2
4	D	602	PEG	O1-C1-C2-O2
4	J	602	PEG	O1-C1-C2-O2
5	P	604	PGE	O1-C1-C2-O2
2	B	606	EDO	O1-C1-C2-O2
2	E	601	EDO	O1-C1-C2-O2
2	J	604	EDO	O1-C1-C2-O2
2	J	608	EDO	O1-C1-C2-O2
2	J	609	EDO	O1-C1-C2-O2
2	N	602	EDO	O1-C1-C2-O2
2	O	603	EDO	O1-C1-C2-O2
5	P	604	PGE	C6-C5-O3-C4
4	K	603	PEG	O2-C3-C4-O4
2	D	605	EDO	O1-C1-C2-O2
2	D	607	EDO	O1-C1-C2-O2
2	I	601	EDO	O1-C1-C2-O2
2	P	601	EDO	O1-C1-C2-O2
3	P	603	BME	O1-C1-C2-S2
5	B	605	PGE	O3-C5-C6-O4
5	B	605	PGE	O1-C1-C2-O2
4	J	601	PEG	C4-C3-O2-C2
5	B	605	PGE	C3-C4-O3-C5
4	D	602	PEG	O2-C3-C4-O4
2	C	604	EDO	O1-C1-C2-O2
4	J	602	PEG	C1-C2-O2-C3
5	P	604	PGE	C1-C2-O2-C3
2	I	602	EDO	O1-C1-C2-O2
2	K	606	EDO	O1-C1-C2-O2
2	L	604	EDO	O1-C1-C2-O2
4	J	601	PEG	C1-C2-O2-C3
2	B	602	EDO	O1-C1-C2-O2
2	J	607	EDO	O1-C1-C2-O2
2	K	605	EDO	O1-C1-C2-O2
2	O	601	EDO	O1-C1-C2-O2
5	B	605	PGE	C6-C5-O3-C4
2	A	603	EDO	O1-C1-C2-O2
2	D	608	EDO	O1-C1-C2-O2
2	J	605	EDO	O1-C1-C2-O2
4	D	602	PEG	C1-C2-O2-C3
4	K	603	PEG	C4-C3-O2-C2
2	B	601	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	D	601	EDO	O1-C1-C2-O2
2	F	601	EDO	O1-C1-C2-O2
2	L	603	EDO	O1-C1-C2-O2
2	K	604	EDO	O1-C1-C2-O2
2	M	602	EDO	O1-C1-C2-O2
2	P	602	EDO	O1-C1-C2-O2
3	H	601	BME	O1-C1-C2-S2
2	J	603	EDO	O1-C1-C2-O2

There are no ring outliers.

27 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	601	EDO	4	0
4	D	602	PEG	8	0
2	C	604	EDO	1	0
2	L	604	EDO	1	0
2	D	601	EDO	1	0
2	D	607	EDO	1	0
2	A	603	EDO	3	0
2	B	602	EDO	1	0
3	J	606	BME	1	0
3	D	603	BME	1	0
4	J	601	PEG	1	0
5	B	605	PGE	8	0
2	M	603	EDO	1	0
4	B	603	PEG	1	0
2	E	601	EDO	5	0
2	J	604	EDO	2	0
2	J	605	EDO	1	0
3	N	601	BME	1	0
2	M	602	EDO	1	0
4	J	602	PEG	1	0
5	P	604	PGE	1	0
2	C	602	EDO	1	0
3	H	601	BME	1	0
2	D	608	EDO	6	0
4	K	603	PEG	2	0
2	D	604	EDO	1	0
2	I	601	EDO	1	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 ⓘ

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	143/164 (87%)	0.09	4 (2%) 55 51	26, 60, 98, 153	7 (4%)
1	B	157/164 (95%)	-0.32	6 (3%) 44 40	26, 46, 130, 161	8 (5%)
1	C	148/164 (90%)	-0.50	2 (1%) 73 71	21, 45, 84, 173	5 (3%)
1	D	146/164 (89%)	-0.61	0 100 100	24, 43, 77, 127	3 (2%)
1	E	146/164 (89%)	-0.26	3 (2%) 63 60	31, 52, 99, 144	3 (2%)
1	F	144/164 (87%)	-0.19	3 (2%) 63 60	28, 56, 92, 151	7 (4%)
1	G	145/164 (88%)	-0.10	2 (1%) 73 71	32, 61, 111, 176	5 (3%)
1	H	146/164 (89%)	-0.31	0 100 100	29, 54, 105, 146	4 (2%)
1	I	145/164 (88%)	-0.33	3 (2%) 63 60	23, 48, 93, 154	9 (6%)
1	J	147/164 (89%)	-0.62	1 (0%) 84 82	20, 41, 76, 142	4 (2%)
1	K	148/164 (90%)	-0.37	2 (1%) 73 71	21, 47, 103, 179	5 (3%)
1	L	145/164 (88%)	-0.30	2 (1%) 73 71	27, 52, 88, 151	5 (3%)
1	M	145/164 (88%)	-0.28	4 (2%) 55 51	33, 49, 89, 141	6 (4%)
1	N	143/164 (87%)	0.10	4 (2%) 55 51	26, 62, 107, 156	4 (2%)
1	O	145/164 (88%)	-0.36	2 (1%) 73 71	24, 51, 85, 145	6 (4%)
1	P	144/164 (87%)	0.03	3 (2%) 63 60	23, 57, 99, 129	6 (4%)
All	All	2337/2624 (89%)	-0.27	41 (1%) 67 65	20, 51, 100, 179	87 (3%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	546	LEU	4.9
1	M	546	LEU	4.9
1	N	546	LEU	4.8
1	A	543[A]	ARG	4.1
1	P	545	MET	3.8

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Mol	Chain	Res	Type	RSRZ
1	J	402	PRO	3.7
1	F	545	MET	3.3
1	G	546	LEU	3.3
1	L	547	HIS	3.2
1	K	401	VAL	3.2
1	I	547	HIS	3.0
1	M	402	PRO	3.0
1	P	543[A]	ARG	3.0
1	A	405	ILE	2.9
1	B	543[A]	ARG	2.9
1	O	402	PRO	2.8
1	N	404	PRO	2.8
1	G	404	PRO	2.7
1	K	402	PRO	2.6
1	E	517[A]	ARG	2.6
1	A	546	LEU	2.6
1	E	402	PRO	2.6
1	B	548	SER	2.6
1	M	509	GLY	2.6
1	I	545	MET	2.5
1	C	404	PRO	2.5
1	I	546	LEU	2.5
1	N	426	PHE	2.4
1	B	394	LEU	2.4
1	F	516[A]	HIS	2.3
1	B	393	ALA	2.3
1	B	547	HIS	2.2
1	B	396	LEU	2.2
1	F	517[A]	ARG	2.2
1	C	548	SER	2.2
1	A	515	LEU	2.1
1	L	405	ILE	2.1
1	M	545	MET	2.0
1	E	547	HIS	2.0
1	P	481	THR	2.0
1	N	545	MET	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
2	EDO	I	602	4/4	0.67	0.29	52,60,98,107	4
2	EDO	D	606	4/4	0.73	0.25	60,73,83,95	4
2	EDO	K	605	4/4	0.74	0.22	44,45,81,101	4
2	EDO	J	608	4/4	0.77	0.31	82,88,93,118	0
3	BME	M	601	4/4	0.77	0.28	50,56,65,81	4
2	EDO	L	604	4/4	0.78	0.15	80,85,86,92	0
2	EDO	A	601	4/4	0.79	0.18	75,92,101,102	0
2	EDO	K	601	4/4	0.79	0.20	78,79,79,100	0
3	BME	D	603	4/4	0.79	0.22	45,55,60,91	4
3	BME	K	602	4/4	0.79	0.26	52,56,74,81	4
2	EDO	K	604	4/4	0.79	0.18	74,76,98,109	0
2	EDO	J	605	4/4	0.80	0.21	40,47,55,59	4
3	BME	P	603	4/4	0.80	0.29	63,66,74,93	4
3	BME	F	602	4/4	0.81	0.20	48,53,78,81	4
3	BME	G	601	4/4	0.81	0.24	52,82,91,110	4
3	BME	I	603	4/4	0.81	0.24	55,57,59,85	4
2	EDO	C	603	4/4	0.81	0.15	86,92,94,120	0
3	BME	B	604	4/4	0.81	0.31	35,60,68,74	4
2	EDO	B	606	4/4	0.81	0.19	66,88,104,111	0
3	BME	E	602	4/4	0.82	0.23	43,63,70,78	4
2	EDO	J	603	4/4	0.83	0.19	69,74,84,111	0
2	EDO	M	602	4/4	0.83	0.14	72,74,75,79	0
2	EDO	N	602	4/4	0.83	0.28	49,67,68,69	4
2	EDO	C	602	4/4	0.83	0.17	77,86,96,106	0
4	PEG	J	601	7/7	0.83	0.15	37,56,63,67	7
3	BME	H	601	4/4	0.84	0.23	52,62,75,85	4
2	EDO	B	601	4/4	0.84	0.23	69,70,75,108	0
2	EDO	D	605	4/4	0.84	0.17	62,70,93,103	0
2	EDO	P	602	4/4	0.85	0.15	67,92,97,117	0
2	EDO	L	601	4/4	0.85	0.17	64,65,70,76	4
4	PEG	J	602	7/7	0.85	0.18	38,47,59,61	7
2	EDO	D	607	4/4	0.86	0.15	78,87,95,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BME	N	601	4/4	0.86	0.25	49,49,55,76	4
3	BME	J	606	4/4	0.86	0.25	53,53,56,80	4
2	EDO	P	605	4/4	0.86	0.16	77,82,88,95	0
3	BME	L	602	4/4	0.86	0.24	44,45,63,78	4
2	EDO	E	601	4/4	0.87	0.12	72,84,88,108	0
2	EDO	O	603	4/4	0.87	0.16	67,73,103,112	0
2	EDO	O	604	4/4	0.87	0.24	56,57,71,76	4
2	EDO	L	603	4/4	0.87	0.23	53,77,84,86	4
4	PEG	K	603	7/7	0.87	0.16	48,76,85,91	7
2	EDO	D	608	4/4	0.88	0.12	54,66,86,90	0
3	BME	A	602	4/4	0.88	0.20	54,54,72,78	4
2	EDO	M	605	4/4	0.88	0.19	49,52,62,72	4
5	PGE	B	605	10/10	0.88	0.14	37,48,54,54	10
2	EDO	I	601	4/4	0.89	0.14	45,51,52,70	4
2	EDO	F	601	4/4	0.89	0.13	82,88,104,105	0
2	EDO	M	604	4/4	0.89	0.17	62,72,75,84	0
5	PGE	P	604	10/10	0.89	0.18	43,58,75,85	10
2	EDO	D	604	4/4	0.90	0.13	66,84,88,107	0
3	BME	C	601	4/4	0.90	0.19	47,47,59,79	4
4	PEG	B	603	7/7	0.90	0.16	60,70,80,82	7
2	EDO	K	606	4/4	0.90	0.19	54,59,71,72	4
4	PEG	D	602	7/7	0.91	0.27	46,49,67,77	7
2	EDO	M	603	4/4	0.91	0.16	58,61,66,68	0
2	EDO	O	601	4/4	0.92	0.12	75,79,80,87	0
2	EDO	A	603	4/4	0.92	0.16	69,85,87,105	0
2	EDO	J	604	4/4	0.92	0.14	41,44,46,49	4
2	EDO	B	607	4/4	0.93	0.13	64,72,84,91	0
2	EDO	J	609	4/4	0.93	0.14	41,52,57,61	4
2	EDO	J	607	4/4	0.93	0.13	66,71,72,98	0
3	BME	O	602	4/4	0.93	0.18	47,50,53,76	4
2	EDO	B	602	4/4	0.94	0.14	37,40,42,45	4
2	EDO	P	601	4/4	0.95	0.11	67,82,85,92	0
2	EDO	C	604	4/4	0.95	0.18	54,60,61,118	0
2	EDO	D	601	4/4	0.96	0.08	51,54,56,56	0

6.5 Other polymers ⓘ

There are no such residues in this entry.