



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 11:14 AM EDT

PDB ID : 6TQS
Title : The crystal structure of the MSP domain of human MOSPD2 in complex with the conventional FFAT motif of ORP1.
Authors : McEwen, A.G.; Poussin-Courmontagne, P.; Di Mattia, T.; Wendling, C.; Cavarelli, J.; Tomasetto, C.; Alpy, F.
Deposited on : 2019-12-17
Resolution : 2.25 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:

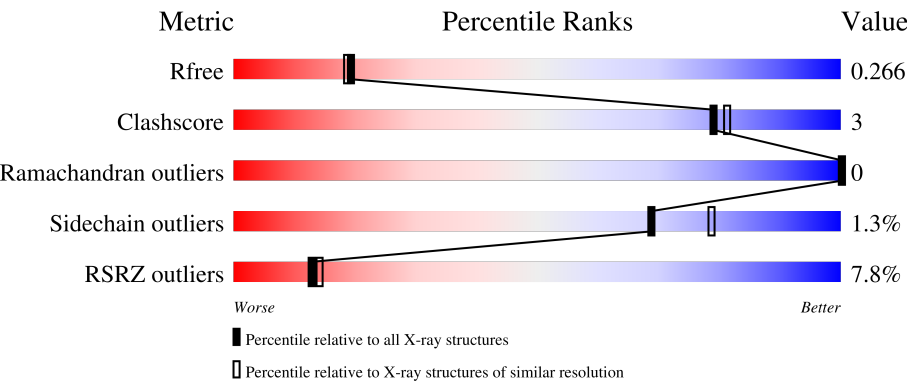
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	216	<div><div>2%</div><div></div><div>56%</div><div>5%</div><div>39%</div></div>
1	B	216	<div><div>7%</div><div></div><div>56%</div><div>6%</div><div>39%</div></div>
1	C	216	<div><div>2%</div><div></div><div>57%</div><div>.</div><div>39%</div></div>
1	D	216	<div><div>%</div><div></div><div>56%</div><div>.</div><div>40%</div></div>
1	E	216	<div><div>3%</div><div></div><div>54%</div><div>6%</div><div>40%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	216	<div><div><div></div><div></div><div></div></div><div>4%55%5%40%</div></div>
2	G	21	<div><div><div></div><div></div><div></div></div><div>29%33%5%62%</div></div>
2	H	21	<div><div><div></div><div></div><div></div></div><div>24%29%5%67%</div></div>
2	I	21	<div><div><div></div><div></div><div></div></div><div>5%33%5%62%</div></div>
2	J	21	<div><div><div></div><div></div><div></div></div><div>33%33%5%62%</div></div>
2	K	21	<div><div><div></div><div></div><div></div></div><div>10%33%67%</div></div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6821 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 Motile sperm domain-containing protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	131	Total	C	N	O	S	0	1	0
			1015	641	177	192	5			
1	B	132	Total	C	N	O	S	0	7	0
			1050	663	185	197	5			
1	C	132	Total	C	N	O	S	0	4	0
			1034	654	180	195	5			
1	D	129	Total	C	N	O	S	0	3	0
			1016	639	181	191	5			
1	E	129	Total	C	N	O	S	0	0	0
			985	622	170	188	5			
1	F	130	Total	C	N	O	S	0	4	0
			1023	645	180	192	6			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	281	MET	-	initiating methionine	UNP Q8NHP6
A	491	HIS	-	expression tag	UNP Q8NHP6
A	492	HIS	-	expression tag	UNP Q8NHP6
A	493	HIS	-	expression tag	UNP Q8NHP6
A	494	HIS	-	expression tag	UNP Q8NHP6
A	495	HIS	-	expression tag	UNP Q8NHP6
A	496	HIS	-	expression tag	UNP Q8NHP6
B	281	MET	-	initiating methionine	UNP Q8NHP6
B	491	HIS	-	expression tag	UNP Q8NHP6
B	492	HIS	-	expression tag	UNP Q8NHP6
B	493	HIS	-	expression tag	UNP Q8NHP6
B	494	HIS	-	expression tag	UNP Q8NHP6
B	495	HIS	-	expression tag	UNP Q8NHP6
B	496	HIS	-	expression tag	UNP Q8NHP6
C	281	MET	-	initiating methionine	UNP Q8NHP6
C	491	HIS	-	expression tag	UNP Q8NHP6
C	492	HIS	-	expression tag	UNP Q8NHP6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	493	HIS	-	expression tag	UNP Q8NHP6
C	494	HIS	-	expression tag	UNP Q8NHP6
C	495	HIS	-	expression tag	UNP Q8NHP6
C	496	HIS	-	expression tag	UNP Q8NHP6
D	281	MET	-	initiating methionine	UNP Q8NHP6
D	491	HIS	-	expression tag	UNP Q8NHP6
D	492	HIS	-	expression tag	UNP Q8NHP6
D	493	HIS	-	expression tag	UNP Q8NHP6
D	494	HIS	-	expression tag	UNP Q8NHP6
D	495	HIS	-	expression tag	UNP Q8NHP6
D	496	HIS	-	expression tag	UNP Q8NHP6
E	281	MET	-	initiating methionine	UNP Q8NHP6
E	491	HIS	-	expression tag	UNP Q8NHP6
E	492	HIS	-	expression tag	UNP Q8NHP6
E	493	HIS	-	expression tag	UNP Q8NHP6
E	494	HIS	-	expression tag	UNP Q8NHP6
E	495	HIS	-	expression tag	UNP Q8NHP6
E	496	HIS	-	expression tag	UNP Q8NHP6
F	281	MET	-	initiating methionine	UNP Q8NHP6
F	491	HIS	-	expression tag	UNP Q8NHP6
F	492	HIS	-	expression tag	UNP Q8NHP6
F	493	HIS	-	expression tag	UNP Q8NHP6
F	494	HIS	-	expression tag	UNP Q8NHP6
F	495	HIS	-	expression tag	UNP Q8NHP6
F	496	HIS	-	expression tag	UNP Q8NHP6

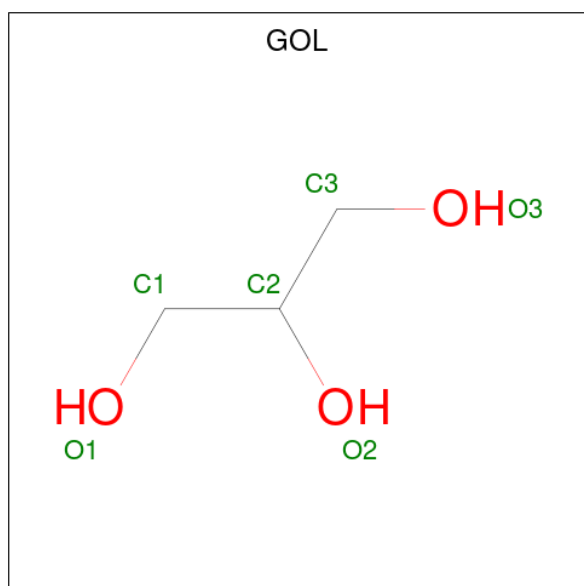
- Molecule 2 is a protein called Oxysterol-binding protein-related protein 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	8	Total	C	N	O	0	0	0
			64	42	8	14			
2	H	7	Total	C	N	O	0	0	0
			56	36	7	13			
2	I	8	Total	C	N	O	0	0	0
			64	42	8	14			
2	J	8	Total	C	N	O	0	0	0
			64	42	8	14			
2	K	7	Total	C	N	O	0	0	0
			59	39	7	13			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	465	GLY	-	cloning artifact	UNP Q9BXW6
G	466	ALA	-	cloning artifact	UNP Q9BXW6
G	467	MET	-	cloning artifact	UNP Q9BXW6
G	468	ARG	-	cloning artifact	UNP Q9BXW6
H	465	GLY	-	cloning artifact	UNP Q9BXW6
H	466	ALA	-	cloning artifact	UNP Q9BXW6
H	467	MET	-	cloning artifact	UNP Q9BXW6
H	468	ARG	-	cloning artifact	UNP Q9BXW6
I	465	GLY	-	cloning artifact	UNP Q9BXW6
I	466	ALA	-	cloning artifact	UNP Q9BXW6
I	467	MET	-	cloning artifact	UNP Q9BXW6
I	468	ARG	-	cloning artifact	UNP Q9BXW6
J	465	GLY	-	cloning artifact	UNP Q9BXW6
J	466	ALA	-	cloning artifact	UNP Q9BXW6
J	467	MET	-	cloning artifact	UNP Q9BXW6
J	468	ARG	-	cloning artifact	UNP Q9BXW6
K	465	GLY	-	cloning artifact	UNP Q9BXW6
K	466	ALA	-	cloning artifact	UNP Q9BXW6
K	467	MET	-	cloning artifact	UNP Q9BXW6
K	468	ARG	-	cloning artifact	UNP Q9BXW6

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



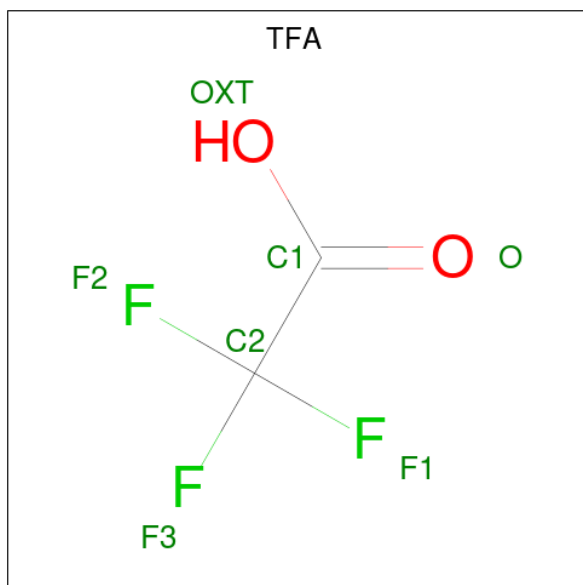
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

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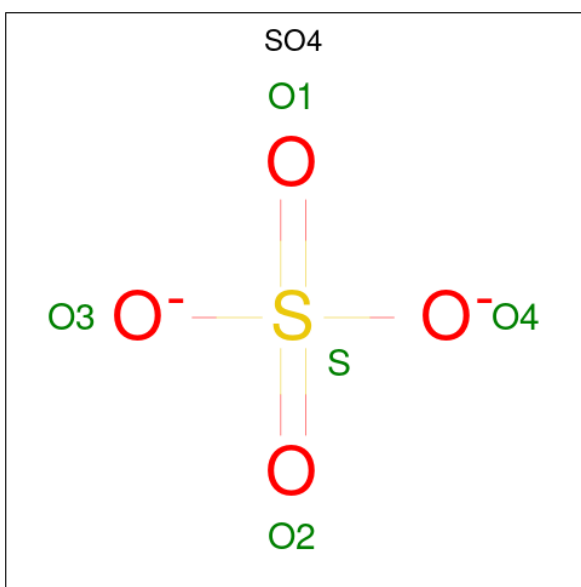
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is trifluoroacetic acid (three-letter code: TFA) (formula: $C_2HF_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	O	0	0
			7	2	3	2		
4	B	1	Total	C	F	O	0	0
			7	2	3	2		
4	C	1	Total	C	F	O	0	0
			7	2	3	2		
4	D	1	Total	C	F	O	0	0
			7	2	3	2		
4	E	1	Total	C	F	O	0	0
			7	2	3	2		
4	F	1	Total	C	F	O	0	0
			7	2	3	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

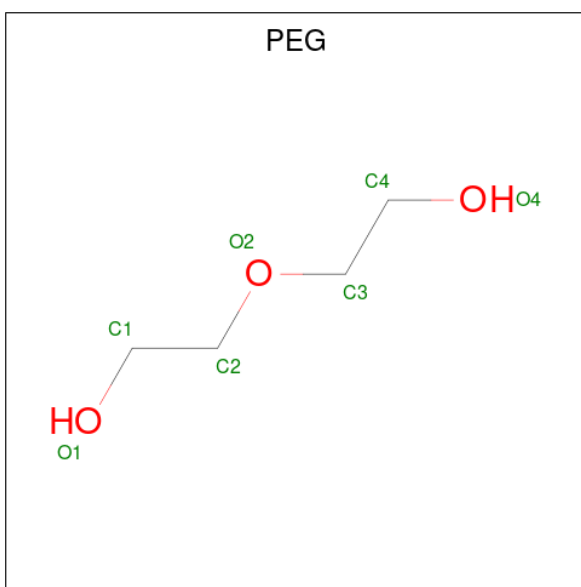


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	1
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

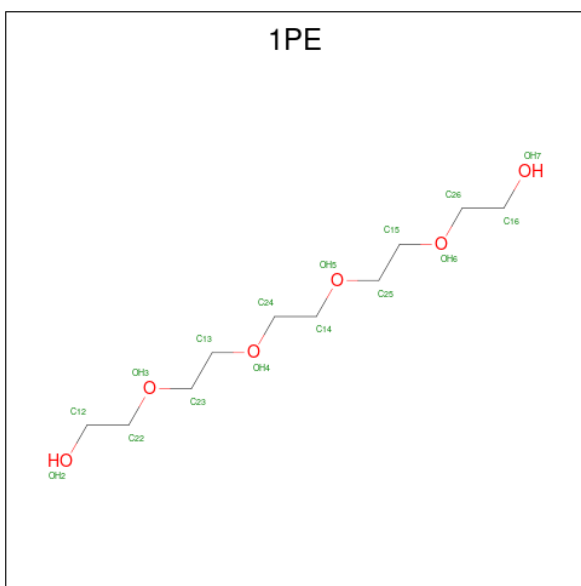
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			7	4	3		

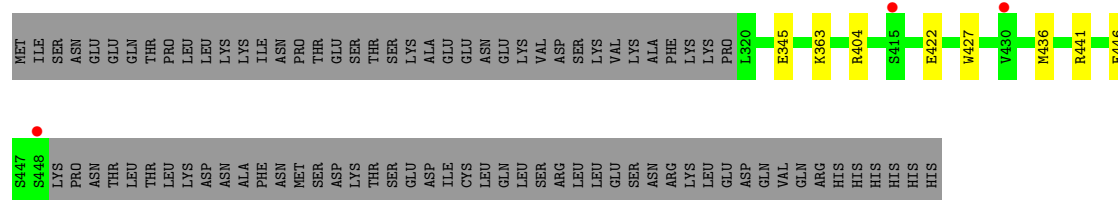
- Molecule 8 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



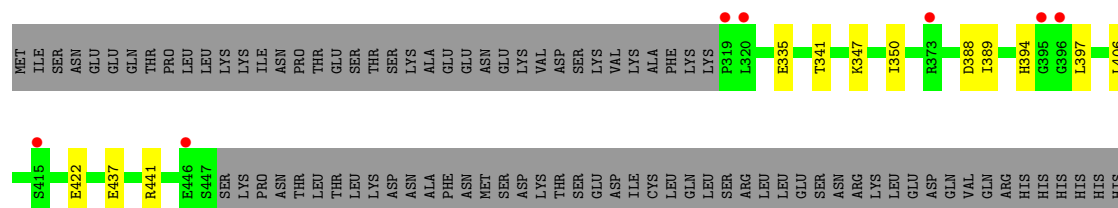
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	F	1	Total	C	O	0	0
			16	10	6		

- Molecule 9 is water.

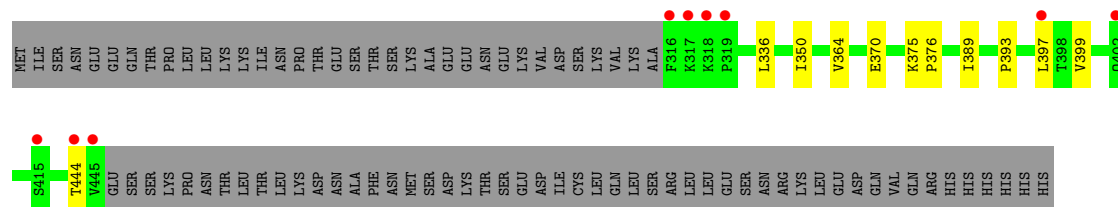
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	56	Total 56	O 56	0	0
9	B	20	Total 20	O 20	0	0
9	C	71	Total 71	O 71	0	0
9	D	32	Total 32	O 32	0	0
9	E	42	Total 42	O 42	0	0
9	F	47	Total 47	O 47	0	0
9	I	1	Total 1	O 1	0	0
9	K	1	Total 1	O 1	0	0



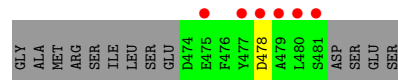
- Molecule 1: Motile sperm domain-containing protein 2



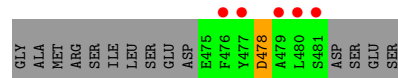
- Molecule 1: Motile sperm domain-containing protein 2



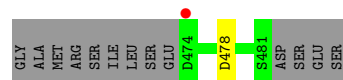
- Molecule 2: Oxysterol-binding protein-related protein 1



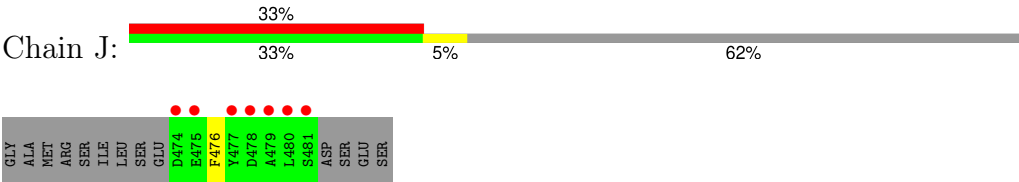
- Molecule 2: Oxysterol-binding protein-related protein 1



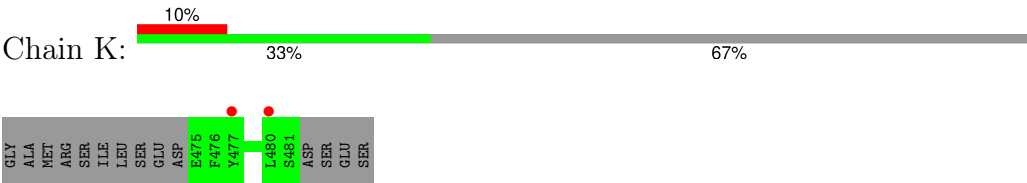
- Molecule 2: Oxysterol-binding protein-related protein 1



● Molecule 2: Oxysterol-binding protein-related protein 1



● Molecule 2: Oxysterol-binding protein-related protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	126.87Å 126.87Å 184.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	70.64 – 2.25 109.88 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (70.64-2.25) 100.0 (109.88-2.25)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.25Å)	Xtriage
Refinement program	PHENIX dev-3644	Depositor
R, R_{free}	0.217 , 0.260 0.225 , 0.266	Depositor DCC
R_{free} test set	2057 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	48.1	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6821	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.76% 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: SO4, TFA, CL, PEG, 1PE, GOL

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	0.25	0/1039	0.42	0/1406
1	B	0.25	0/1076	0.41	0/1459
1	C	0.25	0/1067	0.43	0/1445
1	D	0.25	0/1042	0.42	0/1409
1	E	0.25	0/1006	0.43	0/1365
1	F	0.25	0/1044	0.43	0/1414
2	G	0.25	0/65	0.36	0/87
2	H	0.24	0/57	0.35	0/76
2	I	0.25	0/65	0.34	0/87
2	J	0.25	0/65	0.35	0/87
2	K	0.24	0/60	0.35	0/80
All	All	0.25	0/6586	0.42	0/8915

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1015	0	1034	7	0
1	B	1050	0	1049	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1034	0	1053	7	0
1	D	1016	0	1031	6	0
1	E	985	0	982	6	0
1	F	1023	0	1027	5	0
2	G	64	0	50	1	0
2	H	56	0	39	1	0
2	I	64	0	50	2	0
2	J	64	0	50	1	0
2	K	59	0	48	0	0
3	A	18	0	24	1	0
3	B	6	0	8	0	0
3	C	6	0	8	1	0
4	A	7	0	0	0	0
4	B	7	0	0	0	0
4	C	7	0	0	0	0
4	D	7	0	0	0	0
4	E	7	0	0	0	0
4	F	7	0	0	0	0
5	A	5	0	0	0	0
5	C	5	0	0	0	0
5	E	10	0	0	0	0
5	F	5	0	0	0	0
6	A	1	0	0	0	0
7	C	7	0	10	0	0
8	F	16	0	22	0	0
9	A	56	0	0	1	0
9	B	20	0	0	0	0
9	C	71	0	0	0	0
9	D	32	0	0	0	0
9	E	42	0	0	0	0
9	F	47	0	0	0	0
9	I	1	0	0	0	0
9	K	1	0	0	0	0
All	All	6821	0	6485	36	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (36) 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:418:THR:H	3:A:504:GOL:H32	1.61	0.65
1:C:439:ARG:H	3:C:601:GOL:H12	1.71	0.55
1:B:372:TYR:HA	1:B:393[A]:PRO:HA	1.90	0.53
1:D:404[A]:ARG:HE	2:J:476:PHE:HZ	1.58	0.52
1:A:318:LYS:NZ	9:A:601:HOH:O	2.44	0.51
1:F:399:VAL:HG12	1:F:444[B]:THR:HG22	1.93	0.50
1:A:336:LEU:HD21	1:A:350:ILE:HG12	1.94	0.49
1:C:365:ARG:HG2	2:I:478:ASP:HA	1.93	0.49
1:C:365:ARG:NE	2:I:478:ASP:OD1	2.46	0.48
1:E:341:THR:HG21	1:E:347:LYS:HE3	1.95	0.48
1:B:365:ARG:HG2	2:H:478:ASP:HA	1.96	0.48
1:A:365:ARG:HG2	2:G:478:ASP:HA	1.95	0.48
1:F:393:PRO:HG3	1:F:397:LEU:HD13	1.95	0.48
1:C:347:LYS:HE3	1:C:390:VAL:HG13	1.97	0.47
1:A:347:LYS:HE3	1:A:390:VAL:HG13	1.97	0.47
1:E:394:HIS:HB2	1:E:397:LEU:HD12	1.96	0.47
1:A:433[B]:ASN:ND2	1:D:345:GLU:OE2	2.46	0.46
1:B:347:LYS:HE3	1:B:390:VAL:HG13	1.98	0.46
1:D:422:GLU:OE1	1:D:422:GLU:N	2.44	0.46
1:B:394[A]:HIS:HB2	1:B:397:LEU:HD12	1.98	0.45
1:B:341:THR:HG22	1:D:436:MET:SD	2.56	0.44
1:B:341:THR:HG21	1:B:347:LYS:HD3	1.99	0.44
1:E:335:GLU:OE2	1:E:441:ARG:NE	2.45	0.44
1:F:364:VAL:HG21	1:F:389:ILE:HD13	1.99	0.44
1:E:406:LEU:HD11	1:E:437:GLU:HB3	1.99	0.43
1:E:350:ILE:HB	1:E:389:ILE:HB	2.01	0.43
1:F:336:LEU:HD21	1:F:350:ILE:HG12	2.00	0.42
1:C:404:ARG:HH12	1:C:439:ARG:HH11	1.67	0.42
1:A:364:VAL:HG21	1:A:389:ILE:HD13	2.00	0.42
1:B:364:VAL:HG11	1:B:374:VAL:HG11	2.02	0.42
1:D:363:LYS:HE2	1:D:427:TRP:CD2	2.55	0.42
1:C:379:SER:OG	1:C:380:SER:N	2.51	0.41
1:F:375:LYS:HA	1:F:376:PRO:HA	1.81	0.41
1:E:422:GLU:OE1	1:E:422:GLU:N	2.49	0.41
1:C:350:ILE:HB	1:C:389:ILE:HB	2.02	0.41
1:D:345:GLU:H	1:D:345:GLU:HG2	1.79	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	130/216 (60%)	126 (97%)	4 (3%)	0	100	100
1	B	137/216 (63%)	131 (96%)	6 (4%)	0	100	100
1	C	134/216 (62%)	130 (97%)	4 (3%)	0	100	100
1	D	130/216 (60%)	126 (97%)	4 (3%)	0	100	100
1	E	127/216 (59%)	122 (96%)	5 (4%)	0	100	100
1	F	131/216 (61%)	126 (96%)	5 (4%)	0	100	100
2	G	6/21 (29%)	6 (100%)	0	0	100	100
2	H	5/21 (24%)	5 (100%)	0	0	100	100
2	I	6/21 (29%)	6 (100%)	0	0	100	100
2	J	6/21 (29%)	6 (100%)	0	0	100	100
2	K	5/21 (24%)	5 (100%)	0	0	100	100
All	All	817/1401 (58%)	789 (97%)	28 (3%)	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	116/197 (59%)	113 (97%)	3 (3%)	46	55
1	B	116/197 (59%)	114 (98%)	2 (2%)	60	71
1	C	117/197 (59%)	117 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	115/197 (58%)	112 (97%)	3 (3%)	46	55
1	E	110/197 (56%)	109 (99%)	1 (1%)	78	86
1	F	115/197 (58%)	114 (99%)	1 (1%)	78	86
2	G	6/18 (33%)	6 (100%)	0	100	100
2	H	5/18 (28%)	4 (80%)	1 (20%)	1	0
2	I	6/18 (33%)	6 (100%)	0	100	100
2	J	6/18 (33%)	6 (100%)	0	100	100
2	K	6/18 (33%)	6 (100%)	0	100	100
All	All	718/1272 (56%)	707 (98%)	11 (2%)	69	75

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	433[A]	ASN
1	A	433[B]	ASN
1	A	446	GLU
1	B	366	THR
1	B	406	LEU
1	D	441[A]	ARG
1	D	441[B]	ARG
1	D	446	GLU
1	E	388	ASP
1	F	370	GLU
2	H	478	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	329	HIS
1	C	414	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SO4	E	502	-	4,4,4	0.24	0	6,6,6	0.07	0
3	GOL	A	502	-	5,5,5	0.95	0	5,5,5	1.08	0
4	TFA	B	601	-	6,6,6	0.73	0	9,9,9	0.77	0
5	SO4	C	604[A]	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	E	503	-	4,4,4	0.24	0	6,6,6	0.07	0
8	1PE	F	502	-	15,15,15	0.46	0	14,14,14	0.29	0
4	TFA	D	601	-	6,6,6	0.72	0	9,9,9	0.78	0
3	GOL	A	501	-	5,5,5	0.93	0	5,5,5	1.05	0
4	TFA	F	501	-	6,6,6	0.72	0	9,9,9	0.76	0
3	GOL	A	504	-	5,5,5	0.94	0	5,5,5	1.09	0
4	TFA	E	501	-	6,6,6	0.73	0	9,9,9	0.75	0
4	TFA	A	503	-	6,6,6	0.72	0	9,9,9	0.75	0
3	GOL	C	601	-	5,5,5	0.95	0	5,5,5	1.04	0
7	PEG	C	603	-	6,6,6	0.43	0	5,5,5	0.33	0
5	SO4	A	505	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	F	503	-	4,4,4	0.23	0	6,6,6	0.08	0
3	GOL	B	602	-	5,5,5	0.94	0	5,5,5	1.06	0
4	TFA	C	602	-	6,6,6	0.74	0	9,9,9	0.76	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
3	GOL	A	502	-	-	2/4/4/4	-
4	TFA	B	601	-	-	0/6/6/6	-
8	1PE	F	502	-	-	2/13/13/13	-
4	TFA	D	601	-	-	0/6/6/6	-
3	GOL	A	501	-	-	2/4/4/4	-
4	TFA	F	501	-	-	0/6/6/6	-
3	GOL	A	504	-	-	0/4/4/4	-
4	TFA	E	501	-	-	0/6/6/6	-
4	TFA	A	503	-	-	0/6/6/6	-
3	GOL	C	601	-	-	2/4/4/4	-
7	PEG	C	603	-	-	1/4/4/4	-
3	GOL	B	602	-	-	0/4/4/4	-
4	TFA	C	602	-	-	0/6/6/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	GOL	C1-C2-C3-O3
3	C	601	GOL	C1-C2-C3-O3
8	F	502	1PE	OH7-C16-C26-OH6
3	A	501	GOL	C1-C2-C3-O3
8	F	502	1PE	OH2-C12-C22-OH3
3	A	502	GOL	O2-C2-C3-O3
3	C	601	GOL	O2-C2-C3-O3
7	C	603	PEG	O2-C3-C4-O4
3	A	501	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	504	GOL	1	0
3	C	601	GOL	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	131/216 (60%)	0.08	5 (3%) 40 43	35, 44, 90, 130	0
1	B	132/216 (61%)	0.73	15 (11%) 5 4	48, 84, 125, 154	0
1	C	132/216 (61%)	0.04	4 (3%) 50 53	36, 44, 86, 117	0
1	D	129/216 (59%)	0.22	3 (2%) 60 63	38, 62, 104, 127	0
1	E	129/216 (59%)	0.15	7 (5%) 25 28	34, 54, 103, 140	0
1	F	130/216 (60%)	0.15	9 (6%) 16 18	36, 48, 105, 125	0
2	G	8/21 (38%)	3.01	6 (75%) 0 0	107, 110, 113, 123	0
2	H	7/21 (33%)	2.47	5 (71%) 0 0	113, 117, 127, 146	0
2	I	8/21 (38%)	1.33	1 (12%) 3 3	59, 74, 97, 107	0
2	J	8/21 (38%)	2.08	7 (87%) 0 0	90, 92, 122, 124	0
2	K	7/21 (33%)	1.37	2 (28%) 0 0	77, 87, 94, 110	0
All	All	821/1401 (58%)	0.32	64 (7%) 13 14	34, 56, 113, 154	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	477	TYR	8.6
1	A	446	GLU	8.1
2	H	480	LEU	6.6
1	F	445[A]	VAL	6.5
2	I	474	ASP	6.3
1	F	316	PHE	6.0
1	F	319	PRO	6.0
1	B	374	VAL	5.6
1	A	447	SER	4.1
1	B	446	GLU	4.1
1	B	316	PHE	4.1
1	B	447	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	394[A]	HIS	4.0
1	C	315	ALA	4.0
1	E	319	PRO	3.9
2	K	480	LEU	3.6
1	B	416	SER	3.6
1	C	316	PHE	3.5
1	D	415	SER	3.4
2	H	481	SER	3.3
1	B	391[A]	VAL	3.3
1	D	448	SER	3.3
1	E	446	GLU	3.3
1	C	446	GLU	3.2
1	F	415	SER	3.1
1	A	445	VAL	3.0
1	F	318	LYS	3.0
1	B	340	SER	2.9
1	E	320	LEU	2.9
1	F	402	GLN	2.8
2	G	480	LEU	2.8
2	J	477	TYR	2.8
1	C	415	SER	2.8
1	B	402	GLN	2.7
2	G	478	ASP	2.7
1	E	395	GLY	2.7
1	F	444[A]	THR	2.6
2	J	481	SER	2.6
2	G	481	SER	2.5
2	K	477	TYR	2.5
1	E	396	GLY	2.5
2	J	475	GLU	2.4
1	B	341	THR	2.4
1	E	415	SER	2.4
2	G	475	GLU	2.3
2	H	477	TYR	2.3
1	B	392[A]	SER	2.3
2	G	479	ALA	2.3
1	A	318	LYS	2.3
2	J	474	ASP	2.2
1	B	430	VAL	2.2
1	B	401	ALA	2.2
1	B	396[A]	GLY	2.2
1	E	373	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	397	LEU	2.2
2	J	478	ASP	2.2
2	H	476	PHE	2.1
1	F	317	LYS	2.1
2	H	479	ALA	2.1
1	A	415	SER	2.1
1	B	345	GLU	2.1
1	D	430	VAL	2.1
2	J	480	LEU	2.0
2	J	479	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
8	1PE	F	502	16/16	0.75	0.26	95,96,98,98	16
3	GOL	B	602	6/6	0.81	0.15	95,100,103,105	0
3	GOL	A	502	6/6	0.81	0.26	65,72,76,76	0
7	PEG	C	603	7/7	0.82	0.18	80,84,86,89	0
3	GOL	C	601	6/6	0.83	0.27	61,63,72,78	0
3	GOL	A	504	6/6	0.84	0.15	74,86,88,88	0
3	GOL	A	501	6/6	0.85	0.36	71,77,82,85	0
5	SO4	F	503	5/5	0.88	0.18	113,114,115,116	0
6	CL	A	506	1/1	0.88	0.13	77,77,77,77	0
5	SO4	A	505	5/5	0.91	0.19	62,64,69,69	5
5	SO4	E	503	5/5	0.91	0.16	117,118,118,119	0
5	SO4	C	604[A]	5/5	0.92	0.20	50,52,61,62	5
5	SO4	E	502	5/5	0.94	0.23	93,97,98,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	TFA	A	503	7/7	0.96	0.17	37,41,44,46	0
4	TFA	D	601	7/7	0.97	0.19	59,63,64,66	0
4	TFA	F	501	7/7	0.98	0.09	38,40,46,46	0
4	TFA	C	602	7/7	0.98	0.10	34,38,40,42	0
4	TFA	E	501	7/7	0.98	0.10	38,41,43,43	0
4	TFA	B	601	7/7	0.99	0.13	52,56,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.