



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:00 am BST

PDB ID : 6JP4
Title : Crystal structure of the catalytic domain of a multi-domain alginate lyase
Dp0100 from thermophilic bacterium Defluviitalea phaphyphila
Authors : Ji, S.Q.; Dix, S.R.; Aziz, A.; Sedelnikova, S.E.; Li, F.L.; Rice, D.W.
Deposited on : 2019-03-25
Resolution : 2.07 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

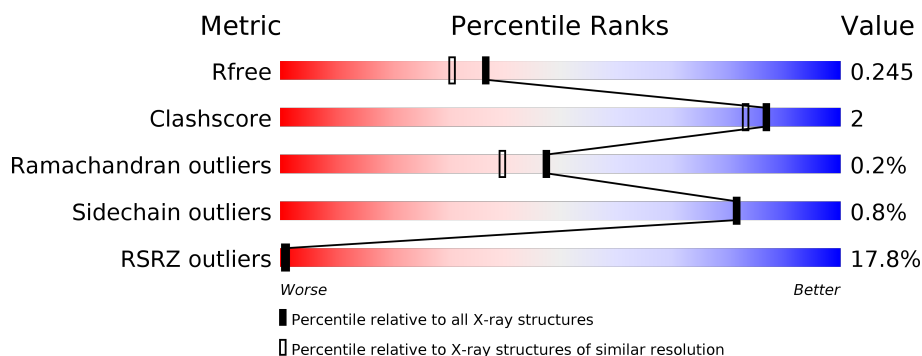
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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 on 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	770	<div> <div></div> <div>93%7%</div> </div>
1	B	770	<div> <div>%</div> <div>93%7%</div> </div>
1	C	770	<div> <div>6%</div> <div>94%6%</div> </div>
1	D	770	<div> <div>64%</div> <div>100%</div> </div>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 22705 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 Alginate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	770	Total	C	N	O	S	0	0	0
			6240	3961	1017	1246	16			
1	B	770	Total	C	N	O	S	0	0	0
			6240	3961	1017	1246	16			
1	C	770	Total	C	N	O	S	0	0	0
			6240	3961	1017	1246	16			
1	D	770	Total	C	N	O		0	0	0
			3080	1540	770	770				

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		

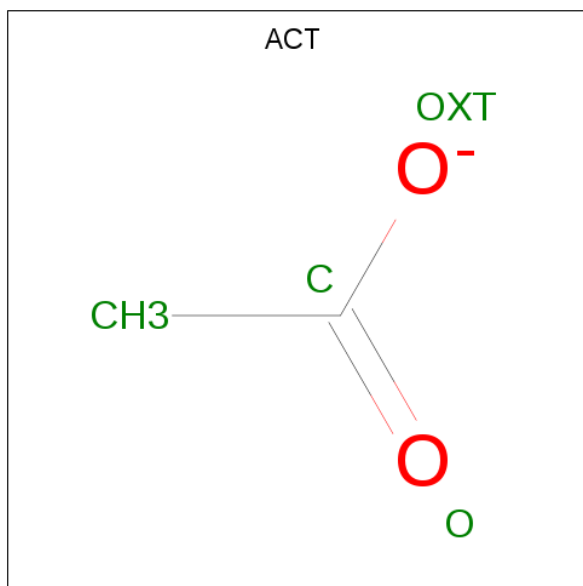
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Ca 2 2	0	0
4	A	2	Total Ca 2 2	0	0
4	C	2	Total Ca 2 2	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



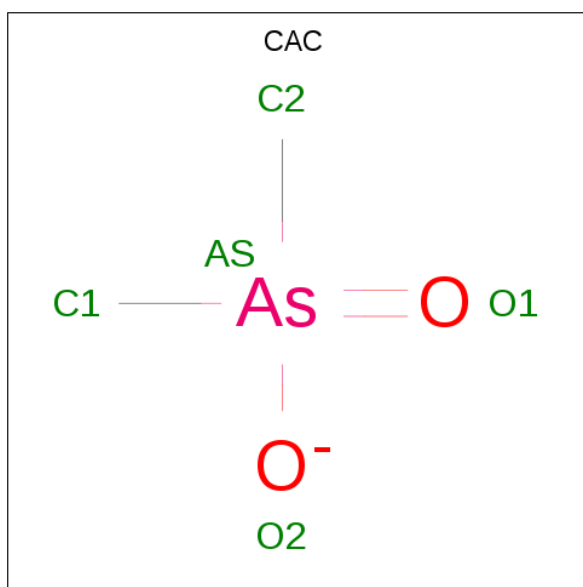
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 7 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	As	C	O	0	0
			5	1	2	2		

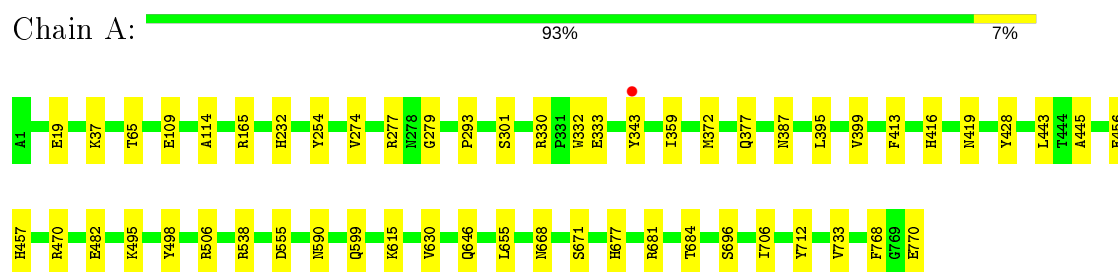
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	490	Total	O	0	0
			490	490		
8	B	267	Total	O	0	0
			267	267		
8	C	74	Total	O	0	0
			74	74		
8	D	1	Total	O	0	0
			1	1		

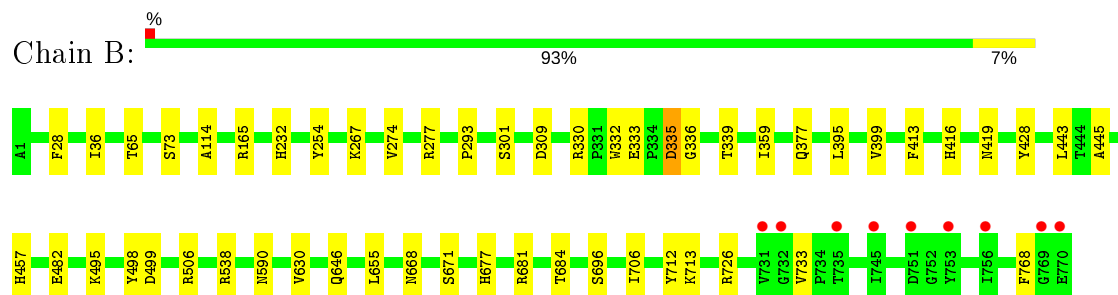
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

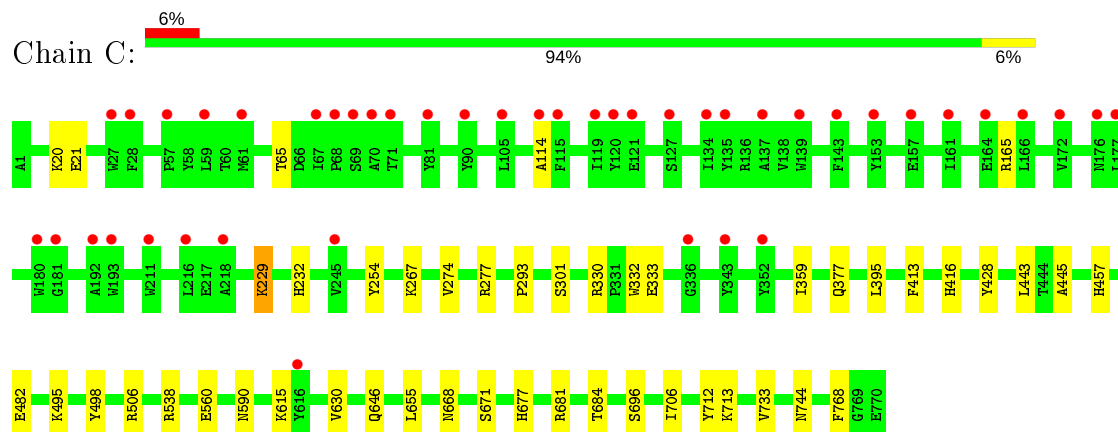
• Molecule 1: Alginate lyase



• Molecule 1: Alginate lyase



• Molecule 1: Alginate lyase



• Molecule 1: Alginate lyase



A1	Y103	H205	H511	D383	A445	V518	N583	F644	I704	I764
T5	R104	L212	S312	W384	E446	A519	N584	M645	D705	I765
Y6	L105	N213	T313	F386	H447	D520	G587	Q646	I706	I766
F9	R106	A219	A314	N387	N448	Q521	A588	L648	S707	I767
S25	A107	L111	K315	N388	N449	F523	F589	M649	D708	F768
L26	T108	T223	L316	N389	V450	L522	N590	M650	E709	G769
W27	L111	Y233	A317	P389	I451	S524	S591	A651	T710	E770
F28	A114	F115	N318	N390	T452	R525	S592	E652	Q711	
T29	F115	D116	L320	R392	A453	R526	G593	M653	Y712	
K30	G117	P118	Q321	N393	N454	V528	Y594	S654	K713	
S31	I119	I118	W322	L394	P456	O529	L595	L655	G714	
D32	E121	F249	F325	L395	H457	Y530	N596	G656	T715	
Q34	G129	P250	N526	F396	V461	S531	A597	D657	I716	
K35	G130	Y254	E332	Q397	S462	L532	R598	T659	A717	
I36	T125	V257	E333	G398	T466	Y533	Q599	T660	L718	
M41	S126	G261	P334	A400	P467	G536	I600	D661	N720	
T46	G128	N266	D335	A401	V468	R537	K602	A662	E721	
E48	G129	T270	G336	E402	S469	R538	D603	T663	T722	
L49	G130	A144	S337	H405	R470	R539	T604	F664	T723	
W50	W139	A144	Y443	Y406	D474	E540	M605	A665	E724	
E51	Y147	A144	T346	H407	D475	Y547	F606	Y666	L725	
T60	D148	A144	T349	Y408	D476	R548	N607	T667	R726	
M61	W149	A144	D350	D409	D477	L549	Q608	G668	T727	
E62	Y149	A144	Q351	H410	F478	R550	G609	E669	K728	
T65	Y153	A144	T352	H411	F479	T551	I610	M670	N729	
D66	L154	A144	S357	E418	D480	Y552	V611	S672	F730	
I67	S155	A144	T358	N419	Q481	G558	G612	N673	V731	
P68	S155	A144	E359	Q420	Q482	A561	L613	N673	G732	
S69	D158	A144	E360	M421	R483	R562	S614	E674	T733	
A70	D158	A144	Q361	M422	E484	A563	K615	L675	P734	
T71	E160	A144	K363	A423	A485	M564	G616	H677	T735	
D72	I161	A144	P364	S426	V486	A565	L625	L686	L736	
S73	I161	A144	D365	G427	V496	A566	L626	S626	E746	
D74	I162	A144	V366	Y428	Y498	V566	L627	T627	F747	
I77	A167	A144	S367	S429	F500	V567	D628	D628	S748	
I87	Y172	A144	T368	N431	S501	F568	V629	G629	V749	
A88	G181	A144	V370	R430	G502	P569	V630	E690	E750	
K89	G194	A144	F371	Y433	I505	S570	V631	E691	D751	
N91	L200	A144	N372	E434	R506	K571	G632	M692	G752	
A92	T201	A144	N373	E435	A507	E572	G633	I693	Y753	
F93	L202	A144	N374	G436	I508	S573	V635	F694	T754	
N94	S203	A144	S375	I437	G509	L574	V636	V695	V755	
Y95	G206	A144	Q302	R438	F510	F575	V636	S696	I756	
L96	T307	A144	D305	T439	P511	D577	K637	N697	Q757	
N97	T308	A144	T378	W441	R512	K578	D638	K698	V758	
T98	S209	A144	V379	Y442	Q513	E579	N639	P699	A759	
G99	D204	A144	F380	L443	F516	G580	E640	I700	E760	
		A144	R381	T444	V517	V582	K641	T701	G761	
		A144	S382				D642	F702	E762	
		A144					T643	A703	D763	

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	261.32Å 394.81Å 112.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	98.90 – 2.07 98.70 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.5 (98.90-2.07) 99.5 (98.70-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.222 , 0.240 0.228 , 0.245	Depositor DCC
R_{free} test set	17175 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22705	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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: MG, CA, MN, EDO, ACT, CAC

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	0.69	0/6413	0.85	4/8727 (0.0%)
1	B	0.67	0/6413	0.83	3/8727 (0.0%)
1	C	0.65	0/6413	0.81	0/8727
1	D	0.87	0/3079	0.87	0/3847
All	All	0.70	0/22318	0.83	7/30028 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	372	MET	CA-CB-CG	-6.10	102.93	113.30
1	B	309	ASP	CB-CA-C	-5.49	99.41	110.40
1	A	770	GLU	CA-C-O	-5.49	108.58	120.10
1	A	470	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	B	726	ARG	NE-CZ-NH1	-5.41	117.60	120.30
1	A	343	TYR	CB-CA-C	-5.30	99.80	110.40
1	B	726	ARG	NE-CZ-NH2	5.14	122.87	120.30

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	6240	0	5798	36	0
1	B	6240	0	5798	27	0
1	C	6240	0	5798	27	0
1	D	3080	0	834	0	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
5	A	8	0	6	1	0
5	B	8	0	6	0	0
5	C	4	0	3	0	0
6	A	20	0	30	0	0
6	B	12	0	18	0	0
6	C	4	0	6	0	0
7	A	5	0	0	2	0
8	A	490	0	0	7	0
8	B	267	0	0	3	0
8	C	74	0	0	1	0
8	D	1	0	0	0	0
All	All	22705	0	18297	86	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 2.

All (86) 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:668:ASN:HD22	1:A:677:HIS:HD2	1.27	0.82
1:A:599:GLN:HE21	7:A:812:CAC:C1	1.96	0.78
1:C:668:ASN:HD22	1:C:677:HIS:HD2	1.32	0.78
1:B:668:ASN:HD22	1:B:677:HIS:HD2	1.32	0.77
1:A:37:LYS:NZ	1:C:744:ASN:HD21	1.93	0.67
1:A:456:GLU:OE1	8:A:901:HOH:O	2.14	0.65
1:B:668:ASN:ND2	1:B:677:HIS:HD2	1.95	0.64
1:C:274:VAL:O	1:C:277:ARG:HG2	1.98	0.64
1:A:668:ASN:ND2	1:A:677:HIS:HD2	1.93	0.64
1:C:330:ARG:HA	1:C:333:GLU:HG2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:668:ASN:ND2	1:C:677:HIS:HD2	1.96	0.63
1:B:330:ARG:HA	1:B:333:GLU:HG2	1.81	0.62
1:A:274:VAL:O	1:A:277:ARG:HG2	2.00	0.62
1:A:330:ARG:HA	1:A:333:GLU:HG2	1.82	0.62
1:B:274:VAL:O	1:B:277:ARG:HG2	2.01	0.60
1:C:560:GLU:HB3	1:C:615:LYS:HD3	1.86	0.57
1:C:114:ALA:O	1:C:165:ARG:HD3	2.06	0.56
1:A:109:GLU:HG2	8:A:1222:HOH:O	2.05	0.56
1:A:677:HIS:HE1	8:A:933:HOH:O	1.90	0.54
1:C:646:GLN:HE21	1:C:681:ARG:HH22	1.57	0.53
1:A:19:GLU:CG	1:B:73:SER:HA	2.38	0.53
1:B:416:HIS:HE1	8:B:975:HOH:O	1.91	0.53
1:A:646:GLN:HE21	1:A:681:ARG:HH22	1.56	0.52
1:A:538:ARG:HH22	1:A:590:ASN:HD22	1.57	0.52
1:B:630:VAL:HG12	1:B:655:LEU:HD12	1.92	0.52
1:C:538:ARG:HH22	1:C:590:ASN:HD22	1.57	0.52
1:B:646:GLN:HE21	1:B:681:ARG:HH22	1.58	0.51
1:B:538:ARG:HH22	1:B:590:ASN:HD22	1.57	0.51
1:A:114:ALA:O	1:A:165:ARG:HD3	2.10	0.50
1:B:114:ALA:O	1:B:165:ARG:HD3	2.12	0.50
1:C:443:LEU:C	1:C:443:LEU:HD12	2.32	0.50
1:A:37:LYS:HZ1	1:C:744:ASN:HD21	1.60	0.49
1:B:443:LEU:C	1:B:443:LEU:HD12	2.33	0.48
1:B:395:LEU:O	1:B:413:PHE:HA	2.14	0.48
1:A:443:LEU:C	1:A:443:LEU:HD12	2.33	0.48
1:B:301:SER:HA	1:B:359:ILE:HD11	1.96	0.48
1:A:395:LEU:O	1:A:413:PHE:HA	2.14	0.47
1:A:445:ALA:HB2	1:A:457:HIS:HB3	1.97	0.47
1:C:630:VAL:HG12	1:C:655:LEU:HD12	1.96	0.47
5:A:806:ACT:CH3	8:A:1210:HOH:O	2.63	0.46
1:C:301:SER:HA	1:C:359:ILE:HD11	1.98	0.46
1:C:395:LEU:O	1:C:413:PHE:HA	2.15	0.46
1:C:733:VAL:CG1	1:C:768:PHE:HB3	2.46	0.46
1:A:630:VAL:HG12	1:A:655:LEU:HD12	1.96	0.46
1:A:495:LYS:HE3	1:A:498:TYR:CE1	2.51	0.45
1:C:445:ALA:HB2	1:C:457:HIS:HB3	1.98	0.45
1:B:335:ASP:OD1	1:B:336:GLY:N	2.50	0.44
1:C:20:LYS:HD2	1:C:21:GLU:N	2.32	0.44
1:A:37:LYS:HZ2	1:C:744:ASN:HD21	1.62	0.44
1:B:706:ILE:HA	1:B:712:TYR:CD1	2.53	0.44
1:C:495:LYS:HE3	1:C:498:TYR:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:GLN:NE2	7:A:812:CAC:C1	2.73	0.44
1:A:293:PRO:HD3	1:A:332:TRP:CZ2	2.53	0.43
1:A:555:ASP:HB2	8:A:1231:HOH:O	2.17	0.43
1:B:339:THR:HG23	8:B:1118:HOH:O	2.17	0.43
1:B:232:HIS:CE1	1:B:399:VAL:HG11	2.54	0.43
1:C:482:GLU:HA	1:C:506:ARG:O	2.19	0.43
1:C:293:PRO:HD3	1:C:332:TRP:CZ2	2.53	0.43
1:B:482:GLU:HA	1:B:506:ARG:O	2.18	0.43
1:A:232:HIS:CE1	1:A:399:VAL:HG11	2.54	0.43
1:C:232:HIS:HD2	1:C:377:GLN:OE1	2.02	0.42
1:B:232:HIS:HD2	1:B:377:GLN:OE1	2.03	0.42
1:B:293:PRO:HD3	1:B:332:TRP:CZ2	2.54	0.42
1:B:495:LYS:HE3	1:B:498:TYR:CE2	2.54	0.42
1:A:482:GLU:HA	1:A:506:ARG:O	2.19	0.42
1:A:301:SER:HA	1:A:359:ILE:HD11	2.01	0.42
1:A:684:THR:HA	1:A:696:SER:OG	2.20	0.42
1:C:684:THR:HA	1:C:696:SER:OG	2.20	0.42
1:B:419:ASN:ND2	8:B:930:HOH:O	2.53	0.42
1:C:706:ILE:HA	1:C:712:TYR:CD1	2.54	0.42
1:A:419:ASN:HA	1:A:419:ASN:HD22	1.65	0.42
1:A:387:ASN:C	1:A:419:ASN:HD21	2.23	0.42
1:C:416:HIS:HE1	8:C:918:HOH:O	2.03	0.42
1:A:232:HIS:HD2	1:A:377:GLN:OE1	2.03	0.42
1:B:28:PHE:CD2	1:B:36:ILE:HD13	2.55	0.42
1:B:733:VAL:CG1	1:B:768:PHE:HB3	2.50	0.42
1:C:229:LYS:HE2	1:C:229:LYS:HB2	1.88	0.41
1:A:733:VAL:CG1	1:A:768:PHE:HB3	2.51	0.41
1:B:445:ALA:HB2	1:B:457:HIS:HB3	2.01	0.41
1:B:684:THR:HA	1:B:696:SER:OG	2.20	0.41
1:A:615:LYS:NZ	8:A:928:HOH:O	2.51	0.41
1:A:706:ILE:HA	1:A:712:TYR:CD1	2.56	0.41
1:A:416:HIS:HE1	8:A:979:HOH:O	2.04	0.41
1:C:668:ASN:ND2	1:C:677:HIS:CD2	2.84	0.41
1:A:19:GLU:HG2	1:B:73:SER:HA	2.03	0.41
1:A:279:GLY:H	1:A:416:HIS:CD2	2.39	0.41

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	768/770 (100%)	740 (96%)	27 (4%)	1 (0%)	51	45
1	B	768/770 (100%)	738 (96%)	29 (4%)	1 (0%)	51	45
1	C	768/770 (100%)	736 (96%)	31 (4%)	1 (0%)	51	45
1	D	768/770 (100%)	727 (95%)	39 (5%)	2 (0%)	41	32
All	All	3072/3080 (100%)	2941 (96%)	126 (4%)	5 (0%)	47	39

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	671	SER
1	B	671	SER
1	C	671	SER
1	D	671	SER
1	D	711	GLN

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	671/671 (100%)	668 (100%)	3 (0%)	91	91
1	B	671/671 (100%)	664 (99%)	7 (1%)	76	75
1	C	671/671 (100%)	665 (99%)	6 (1%)	78	78
All	All	2013/2013 (100%)	1997 (99%)	16 (1%)	81	81

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

Mol	Chain	Res	Type
1	A	65	THR
1	A	254	TYR
1	A	428	TYR
1	B	65	THR
1	B	254	TYR
1	B	267	LYS
1	B	335	ASP
1	B	428	TYR
1	B	499	ASP
1	B	713	LYS
1	C	65	THR
1	C	229	LYS
1	C	254	TYR
1	C	267	LYS
1	C	428	TYR
1	C	713	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	222	ASN
1	A	232	HIS
1	A	318	ASN
1	A	416	HIS
1	A	419	ASN
1	A	464	ASN
1	A	535	HIS
1	A	559	GLN
1	A	590	ASN
1	A	596	ASN
1	A	599	GLN
1	A	646	GLN
1	A	668	ASN
1	A	677	HIS
1	A	692	ASN
1	A	711	GLN
1	A	744	ASN
1	A	767	ASN
1	B	222	ASN
1	B	232	HIS

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Mol	Chain	Res	Type
1	B	318	ASN
1	B	416	HIS
1	B	419	ASN
1	B	464	ASN
1	B	535	HIS
1	B	559	GLN
1	B	590	ASN
1	B	596	ASN
1	B	599	GLN
1	B	646	GLN
1	B	668	ASN
1	B	677	HIS
1	B	692	ASN
1	B	711	GLN
1	B	744	ASN
1	B	767	ASN
1	C	41	ASN
1	C	222	ASN
1	C	232	HIS
1	C	318	ASN
1	C	416	HIS
1	C	419	ASN
1	C	464	ASN
1	C	535	HIS
1	C	559	GLN
1	C	590	ASN
1	C	599	GLN
1	C	608	GLN
1	C	646	GLN
1	C	668	ASN
1	C	677	HIS
1	C	692	ASN
1	C	711	GLN
1	C	744	ASN
1	C	767	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 12 are monoatomic - leaving 15 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	$\# Z > 2$
6	EDO	C	806	-	3,3,3	0.08	0	2,2,2	0.19	0
7	CAC	A	812	-	0,4,4	0.00	-	0,6,6	0.00	-
6	EDO	B	807	-	3,3,3	0.13	0	2,2,2	0.01	0
6	EDO	A	807	-	3,3,3	0.28	0	2,2,2	0.30	0
5	ACT	A	805	-	1,3,3	3.07	1 (100%)	0,3,3	0.00	-
6	EDO	A	810	-	3,3,3	0.08	0	2,2,2	0.29	0
5	ACT	B	805	-	1,3,3	3.39	1 (100%)	0,3,3	0.00	-
5	ACT	A	806	-	1,3,3	2.93	1 (100%)	0,3,3	0.00	-
6	EDO	B	809	-	3,3,3	0.09	0	2,2,2	0.10	0
5	ACT	B	806	-	1,3,3	3.66	1 (100%)	0,3,3	0.00	-
6	EDO	A	811	-	3,3,3	0.17	0	2,2,2	0.36	0
6	EDO	A	809	-	3,3,3	0.09	0	2,2,2	0.19	0
6	EDO	A	808	-	3,3,3	0.07	0	2,2,2	0.18	0
6	EDO	B	808	-	3,3,3	0.24	0	2,2,2	0.20	0
5	ACT	C	805	-	1,3,3	3.70	1 (100%)	0,3,3	0.00	-

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
6	EDO	C	806	-	-	1/1/1/1	-
6	EDO	A	811	-	-	0/1/1/1	-
6	EDO	B	807	-	-	0/1/1/1	-
6	EDO	A	807	-	-	0/1/1/1	-
6	EDO	A	810	-	-	1/1/1/1	-
6	EDO	B	809	-	-	0/1/1/1	-
6	EDO	A	808	-	-	0/1/1/1	-
6	EDO	B	808	-	-	0/1/1/1	-
6	EDO	A	809	-	-	0/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	805	ACT	CH3-C	3.70	1.53	1.48
5	B	806	ACT	CH3-C	3.66	1.53	1.48
5	B	805	ACT	CH3-C	3.39	1.53	1.48
5	A	805	ACT	CH3-C	3.07	1.52	1.48
5	A	806	ACT	CH3-C	2.93	1.52	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	806	EDO	O1-C1-C2-O2
6	A	810	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	812	CAC	2	0
5	A	806	ACT	1	0

5.7 Other polymers

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 ⓘ

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	770/770 (100%)	0.09	1 (0%) 95 95	22, 33, 56, 87	0
1	B	770/770 (100%)	0.07	9 (1%) 79 80	26, 44, 77, 120	0
1	C	770/770 (100%)	0.33	44 (5%) 23 24	41, 60, 89, 115	0
1	D	770/770 (100%)	3.11	493 (64%) 0 0	60, 90, 129, 146	0
All	All	3080/3080 (100%)	0.90	547 (17%) 1 1	22, 55, 112, 146	0

All (547) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	706	ILE	13.3
1	D	732	GLY	12.9
1	D	731	VAL	12.8
1	D	658	ILE	11.1
1	D	753	TYR	10.5
1	D	769	GLY	10.5
1	D	543	GLY	10.2
1	D	759	ALA	10.0
1	D	758	VAL	9.8
1	D	574	ILE	9.6
1	D	749	VAL	9.0
1	D	733	VAL	9.0
1	D	752	GLY	8.7
1	D	745	ILE	8.6
1	D	564	ALA	8.5
1	D	770	GLU	8.4
1	D	662	ALA	8.3
1	D	533	TYR	8.3
1	D	735	THR	8.3
1	D	548	ARG	8.3
1	D	760	GLU	8.2

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Mol	Chain	Res	Type	RSRZ
1	D	567	VAL	8.1
1	D	683	GLY	7.9
1	D	545	GLY	7.8
1	D	594	TYR	7.8
1	D	597	ALA	7.8
1	D	566	TRP	7.7
1	D	627	THR	7.7
1	D	764	ILE	7.6
1	D	688	TYR	7.6
1	D	600	ILE	7.5
1	D	712	TYR	7.5
1	D	727	VAL	7.5
1	D	690	GLY	7.5
1	D	692	ASN	7.1
1	D	569	PRO	7.1
1	D	622	VAL	7.1
1	D	651	ALA	7.1
1	D	655	LEU	7.0
1	D	563	MET	7.0
1	D	652	GLU	7.0
1	D	730	PRO	7.0
1	D	530	TYR	7.0
1	D	734	PRO	6.9
1	D	638	ASP	6.9
1	D	710	THR	6.9
1	D	599	GLN	6.9
1	D	768	PHE	6.8
1	D	675	LEU	6.7
1	D	670	ASN	6.7
1	D	639	ASN	6.7
1	D	704	LEU	6.7
1	D	580	GLY	6.7
1	D	575	PHE	6.6
1	D	629	ASP	6.6
1	D	593	GLY	6.5
1	D	656	GLY	6.5
1	D	729	ASN	6.4
1	D	596	ASN	6.4
1	D	766	ILE	6.4
1	D	751	ASP	6.4
1	D	610	ILE	6.3
1	D	755	VAL	6.3

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Mol	Chain	Res	Type	RSRZ
1	D	693	ILE	6.2
1	D	767	ASN	6.2
1	D	606	PHE	6.2
1	D	703	ALA	6.2
1	D	26	LEU	6.1
1	D	336	GLY	6.1
1	D	630	VAL	6.1
1	D	595	LEU	6.1
1	D	609	ILE	6.0
1	D	631	VAL	6.0
1	D	294	ALA	6.0
1	D	450	VAL	5.9
1	D	578	LYS	5.9
1	D	512	ARG	5.9
1	D	738	VAL	5.9
1	D	505	ILE	5.9
1	D	532	LEU	5.9
1	D	546	ASN	5.8
1	D	691	GLU	5.8
1	D	684	THR	5.8
1	D	765	ASN	5.8
1	D	714	GLY	5.8
1	D	740	VAL	5.7
1	D	66	ASP	5.7
1	D	550	TRP	5.7
1	D	644	PHE	5.7
1	D	529	GLN	5.7
1	D	478	PHE	5.6
1	D	520	ASP	5.6
1	D	367	SER	5.6
1	D	671	SER	5.5
1	D	303	TYR	5.5
1	D	649	ASN	5.5
1	D	522	LEU	5.4
1	D	121	GLU	5.4
1	D	592	TYR	5.4
1	D	411	LEU	5.4
1	D	279	GLY	5.3
1	D	725	LEU	5.3
1	D	682	GLN	5.3
1	D	549	LEU	5.2
1	D	497	SER	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	126	VAL	5.2
1	D	468	VAL	5.2
1	D	623	VAL	5.2
1	D	668	ASN	5.2
1	D	272	TRP	5.2
1	D	570	SER	5.2
1	D	498	TYR	5.2
1	D	71	THR	5.1
1	D	70	ALA	5.1
1	D	665	ALA	5.1
1	D	312	SER	5.1
1	D	513	GLN	5.1
1	D	589	PHE	5.1
1	D	576	ILE	5.1
1	D	568	PHE	5.1
1	D	635	VAL	5.0
1	D	746	GLU	5.0
1	D	329	PHE	5.0
1	D	672	ASN	5.0
1	D	666	TYR	5.0
1	D	421	MET	5.0
1	D	694	PHE	5.0
1	D	332	TRP	5.0
1	D	509	GLY	5.0
1	D	612	PRO	4.9
1	D	325	PHE	4.9
1	D	379	VAL	4.9
1	D	542	SER	4.9
1	D	544	GLU	4.9
1	D	680	VAL	4.9
1	D	496	ASN	4.9
1	C	115	PHE	4.8
1	D	728	LYS	4.8
1	D	469	SER	4.8
1	D	718	ALA	4.8
1	D	448	HIS	4.8
1	D	528	VAL	4.8
1	D	437	ILE	4.8
1	D	750	GLU	4.8
1	D	310	LEU	4.8
1	D	611	VAL	4.8
1	D	386	PHE	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	664	PHE	4.8
1	D	153	TYR	4.8
1	D	757	GLN	4.8
1	C	70	ALA	4.8
1	D	501	SER	4.8
1	D	270	PHE	4.7
1	D	241	VAL	4.7
1	D	748	SER	4.7
1	B	732	GLY	4.7
1	D	736	GLU	4.7
1	D	719	LEU	4.7
1	D	707	SER	4.7
1	D	359	ILE	4.7
1	D	504	GLN	4.7
1	D	537	GLY	4.6
1	D	551	THR	4.6
1	D	625	LEU	4.6
1	D	677	HIS	4.6
1	D	573	SER	4.6
1	D	701	THR	4.6
1	D	756	ILE	4.6
1	D	436	GLY	4.6
1	D	434	GLY	4.6
1	C	180	TRP	4.6
1	D	717	ALA	4.6
1	D	653	ASN	4.6
1	D	673	ASN	4.6
1	D	477	PHE	4.6
1	D	624	ASP	4.6
1	D	27	TRP	4.5
1	D	636	VAL	4.5
1	D	510	PHE	4.5
1	D	233	TYR	4.5
1	D	632	GLY	4.5
1	D	607	MET	4.5
1	D	281	GLY	4.5
1	B	731	VAL	4.5
1	D	659	THR	4.4
1	D	432	SER	4.4
1	C	172	VAL	4.4
1	D	314	ALA	4.4
1	D	282	TRP	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	461	VAL	4.4
1	D	358	THR	4.4
1	D	626	SER	4.4
1	D	416	HIS	4.3
1	D	313	THR	4.3
1	D	154	LEU	4.3
1	D	435	GLU	4.3
1	D	669	GLU	4.3
1	D	506	ARG	4.3
1	D	144	ALA	4.3
1	D	74	ASP	4.3
1	D	484	GLU	4.3
1	D	368	GLY	4.3
1	D	742	GLY	4.3
1	D	486	VAL	4.3
1	D	322	TRP	4.3
1	D	500	PHE	4.2
1	D	674	GLU	4.2
1	D	406	TYR	4.2
1	D	754	THR	4.2
1	D	326	ASN	4.2
1	D	700	ILE	4.2
1	D	422	MET	4.2
1	D	678	PHE	4.2
1	D	702	PHE	4.2
1	D	705	ASP	4.2
1	D	676	GLN	4.2
1	D	582	VAL	4.2
1	D	541	MET	4.2
1	D	617	ALA	4.2
1	D	508	ILE	4.2
1	D	663	THR	4.1
1	D	645	MET	4.1
1	D	362	ILE	4.1
1	D	619	ILE	4.1
1	D	709	GLU	4.1
1	D	167	ALA	4.1
1	D	538	ARG	4.1
1	D	536	GLY	4.1
1	D	257	VAL	4.0
1	D	715	THR	4.0
1	D	454	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	108	THR	4.0
1	D	73	SER	4.0
1	D	737	SER	4.0
1	D	366	VAL	4.0
1	D	34	GLN	4.0
1	D	387	ASN	4.0
1	D	476	ASP	4.0
1	D	376	GLY	4.0
1	D	634	THR	3.9
1	D	481	GLN	3.9
1	D	647	GLN	3.9
1	D	480	PHE	3.9
1	D	95	TYR	3.9
1	C	119	ILE	3.9
1	D	96	LEU	3.9
1	D	648	LEU	3.9
1	D	306	THR	3.9
1	D	708	ASP	3.9
1	D	697	ASN	3.9
1	D	370	VAL	3.9
1	D	739	VAL	3.9
1	D	642	ASP	3.9
1	D	661	ASP	3.8
1	D	741	ASN	3.8
1	D	761	GLY	3.8
1	D	667	THR	3.8
1	D	547	TYR	3.8
1	D	311	HIS	3.8
1	D	620	PRO	3.8
1	D	369	THR	3.8
1	D	390	ASN	3.8
1	D	415	ILE	3.8
1	D	605	MET	3.8
1	D	591	SER	3.8
1	D	713	LYS	3.8
1	D	399	VAL	3.8
1	D	561	ALA	3.8
1	D	6	TYR	3.7
1	D	114	ALA	3.7
1	D	337	SER	3.7
1	D	111	LEU	3.7
1	D	579	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	447	ALA	3.7
1	D	590	ASN	3.7
1	D	90	TYR	3.7
1	C	181	GLY	3.7
1	D	380	PHE	3.7
1	D	419	ASN	3.7
1	D	711	GLN	3.7
1	D	747	PHE	3.7
1	D	60	THR	3.7
1	D	720	ASN	3.7
1	D	722	THR	3.7
1	D	518	VAL	3.6
1	D	695	VAL	3.6
1	D	375	SER	3.6
1	D	442	TYR	3.6
1	D	441	TRP	3.6
1	D	618	ASP	3.6
1	D	686	LEU	3.6
1	D	98	THR	3.6
1	D	364	PRO	3.6
1	D	565	ALA	3.6
1	D	373	ASN	3.6
1	D	679	SER	3.5
1	C	69	SER	3.5
1	D	149	TRP	3.5
1	D	744	ASN	3.5
1	D	143	PHE	3.5
1	D	274	VAL	3.5
1	D	417	ALA	3.5
1	D	455	GLY	3.5
1	D	681	ARG	3.5
1	D	685	SER	3.5
1	D	657	ASP	3.5
1	D	613	LEU	3.5
1	D	502	GLY	3.5
1	D	516	PHE	3.4
1	D	49	LEU	3.4
1	D	646	GLN	3.4
1	D	67	ILE	3.4
1	D	161	ILE	3.4
1	B	770	GLU	3.4
1	D	50	TRP	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	521	GLN	3.4
1	D	273	ALA	3.4
1	D	204	ASP	3.3
1	D	374	ASN	3.3
1	D	641	LYS	3.3
1	D	523	PHE	3.3
1	D	92	ALA	3.3
1	D	475	THR	3.3
1	D	129	SER	3.3
1	D	360	GLU	3.3
1	D	519	ALA	3.3
1	D	398	GLY	3.2
1	C	211	TRP	3.2
1	D	444	THR	3.2
1	C	27	TRP	3.2
1	D	637	LYS	3.2
1	D	723	VAL	3.2
1	D	466	THR	3.2
1	D	490	PHE	3.2
1	D	77	ILE	3.2
1	D	439	THR	3.2
1	D	130	GLY	3.2
1	D	309	ASP	3.2
1	D	763	ASP	3.2
1	D	587	GLY	3.1
1	C	67	ILE	3.1
1	D	577	ASP	3.1
1	D	621	GLU	3.1
1	D	107	ALA	3.1
1	D	395	LEU	3.1
1	D	139	TRP	3.1
1	C	114	ALA	3.1
1	D	467	PRO	3.1
1	D	699	PRO	3.1
1	D	433	TYR	3.1
1	D	552	TYR	3.1
1	D	305	ASP	3.1
1	D	633	GLY	3.1
1	D	660	THR	3.1
1	D	716	ILE	3.1
1	C	336	GLY	3.1
1	D	445	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	295	PRO	3.1
1	D	689	LYS	3.1
1	D	420	GLN	3.1
1	D	603	ASP	3.0
1	D	105	LEU	3.0
1	D	248	ILE	3.0
1	D	405	HIS	3.0
1	D	628	ASP	3.0
1	C	177	LEU	3.0
1	D	181	GLY	3.0
1	D	36	ILE	3.0
1	D	724	GLU	3.0
1	D	427	GLY	3.0
1	D	301	SER	3.0
1	D	482	GLU	3.0
1	D	162	ILE	3.0
1	D	557	TYR	3.0
1	D	72	ASP	3.0
1	D	485	ALA	3.0
1	D	349	ILE	2.9
1	D	527	GLU	2.9
1	D	616	TYR	2.9
1	C	105	LEU	2.9
1	D	696	SER	2.9
1	D	721	GLU	2.9
1	D	408	TYR	2.9
1	D	46	THR	2.9
1	D	223	THR	2.9
1	C	81	TYR	2.9
1	D	558	GLY	2.9
1	D	743	GLU	2.9
1	D	372	MET	2.9
1	D	104	ARG	2.9
1	D	614	SER	2.9
1	D	47	ALA	2.8
1	D	650	ASN	2.8
1	D	202	LEU	2.8
1	D	440	SER	2.8
1	D	524	SER	2.8
1	C	68	PRO	2.8
1	D	319	ILE	2.8
1	D	160	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	200	LEU	2.8
1	D	394	LEU	2.8
1	D	317	ALA	2.8
1	D	400	ALA	2.8
1	B	745	ILE	2.8
1	D	604	THR	2.8
1	D	41	ASN	2.8
1	D	351	GLN	2.8
1	D	93	PHE	2.7
1	D	726	ARG	2.7
1	D	69	SER	2.7
1	D	117	GLY	2.7
1	D	31	SER	2.7
1	D	503	LYS	2.7
1	D	598	ARG	2.7
1	D	517	VAL	2.7
1	D	640	GLU	2.7
1	D	65	THR	2.7
1	D	91	ASN	2.7
1	D	212	LEU	2.7
1	D	361	GLN	2.7
1	B	769	GLY	2.7
1	D	94	MET	2.7
1	D	320	LEU	2.7
1	C	120	TYR	2.6
1	C	352	TYR	2.6
1	D	584	TYR	2.6
1	D	87	ILE	2.6
1	C	137	ALA	2.6
1	D	88	ALA	2.6
1	D	219	ALA	2.6
1	D	470	ARG	2.6
1	C	61	MET	2.6
1	C	135	TYR	2.6
1	D	388	ASN	2.6
1	C	153	TYR	2.6
1	D	393	TYR	2.6
1	D	33	ILE	2.6
1	D	479	ASP	2.6
1	D	164	GLU	2.6
1	D	254	TYR	2.6
1	C	193	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	457	HIS	2.6
1	D	413	PHE	2.6
1	D	540	GLU	2.6
1	C	218	ALA	2.6
1	C	161	ILE	2.6
1	D	384	TRP	2.6
1	D	511	PRO	2.6
1	D	474	ASP	2.5
1	C	90	TYR	2.5
1	D	276	ILE	2.5
1	D	452	THR	2.5
1	D	643	THR	2.5
1	D	334	PRO	2.5
1	C	157	GLU	2.5
1	D	588	ALA	2.5
1	D	308	THR	2.5
1	D	392	ARG	2.5
1	D	283	MET	2.5
1	D	389	PRO	2.5
1	D	429	SER	2.5
1	D	266	TYR	2.5
1	D	119	ILE	2.5
1	D	115	PHE	2.5
1	D	315	LYS	2.5
1	D	278	ASN	2.4
1	C	121	GLU	2.4
1	D	410	HIS	2.4
1	D	275	LYS	2.4
1	D	291	ILE	2.4
1	D	396	PHE	2.4
1	C	71	THR	2.4
1	D	430	ARG	2.4
1	D	687	ASP	2.4
1	D	382	SER	2.4
1	D	698	LYS	2.4
1	C	343	TYR	2.4
1	D	172	VAL	2.4
1	C	164	GLU	2.4
1	D	5	THR	2.4
1	D	357	SER	2.4
1	D	402	ALA	2.4
1	A	343	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	128	GLY	2.4
1	D	147	TYR	2.4
1	D	62	GLU	2.3
1	D	260	VAL	2.3
1	B	751	ASP	2.3
1	D	51	GLU	2.3
1	C	216	LEU	2.3
1	C	616	TYR	2.3
1	D	525	ASP	2.3
1	D	213	ASN	2.3
1	D	418	GLU	2.3
1	D	249	PRO	2.3
1	D	99	GLY	2.3
1	D	423	ALA	2.3
1	D	125	THR	2.3
1	D	654	SER	2.3
1	D	443	LEU	2.2
1	D	507	ALA	2.2
1	D	335	ASP	2.2
1	D	462	SER	2.2
1	D	61	MET	2.2
1	D	103	TYR	2.2
1	D	205	HIS	2.2
1	D	343	TYR	2.2
1	D	245	VAL	2.2
1	D	539	GLY	2.2
1	D	762	GLY	2.2
1	D	250	PHE	2.2
1	B	756	ILE	2.2
1	D	601	ALA	2.2
1	D	158	ASP	2.2
1	D	29	THR	2.2
1	C	139	TRP	2.2
1	D	116	ASP	2.2
1	D	608	GLN	2.2
1	D	261	ASN	2.2
1	D	346	THR	2.2
1	D	383	ASP	2.2
1	C	134	ILE	2.1
1	D	409	ASP	2.1
1	C	192	ALA	2.1
1	D	378	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	142	ASN	2.1
1	D	572	GLU	2.1
1	D	428	TYR	2.1
1	C	127	SER	2.1
1	D	155	SER	2.1
1	D	298	MET	2.1
1	C	245	VAL	2.1
1	C	28	PHE	2.1
1	D	194	GLY	2.1
1	D	25	SER	2.0
1	D	412	SER	2.0
1	D	426	SER	2.0
1	D	9	PHE	2.0
1	B	753	TYR	2.0
1	D	352	TYR	2.0
1	D	456	GLU	2.0
1	C	57	PRO	2.0
1	C	166	LEU	2.0
1	C	143	PHE	2.0
1	C	176	ASN	2.0
1	B	735	THR	2.0
1	C	59	LEU	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 carbohydrates 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(\AA^2)	Q<0.9
6	EDO	A	810	4/4	0.31	0.29	63,88,90,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	CAC	A	812	5/5	0.74	0.30	46,62,135,159	0
6	EDO	A	809	4/4	0.74	0.18	72,74,74,77	0
6	EDO	C	806	4/4	0.76	0.22	74,77,86,98	0
3	MG	C	802	1/1	0.81	0.08	72,72,72,72	0
6	EDO	B	809	4/4	0.83	0.29	55,61,62,70	0
6	EDO	A	808	4/4	0.83	0.16	66,69,75,79	0
5	ACT	A	806	4/4	0.87	0.12	53,56,64,67	0
5	ACT	C	805	4/4	0.90	0.12	60,67,68,70	0
6	EDO	B	807	4/4	0.91	0.19	42,46,49,50	0
6	EDO	A	811	4/4	0.91	0.14	47,48,52,86	0
6	EDO	A	807	4/4	0.92	0.16	24,25,31,32	0
3	MG	B	802	1/1	0.92	0.07	56,56,56,56	0
5	ACT	B	806	4/4	0.93	0.14	48,52,60,77	0
4	CA	C	803	1/1	0.94	0.11	51,51,51,51	0
6	EDO	B	808	4/4	0.94	0.12	31,38,44,57	0
5	ACT	B	805	4/4	0.95	0.15	33,44,46,64	0
3	MG	A	802	1/1	0.95	0.04	50,50,50,50	0
2	MN	C	801	1/1	0.96	0.14	51,51,51,51	0
5	ACT	A	805	4/4	0.96	0.18	31,40,50,56	0
4	CA	C	804	1/1	0.97	0.14	45,45,45,45	0
4	CA	A	804	1/1	0.98	0.18	29,29,29,29	0
4	CA	B	804	1/1	0.99	0.15	46,46,46,46	0
2	MN	A	801	1/1	0.99	0.20	24,24,24,24	0
4	CA	A	803	1/1	0.99	0.18	26,26,26,26	0
4	CA	B	803	1/1	0.99	0.16	30,30,30,30	0
2	MN	B	801	1/1	0.99	0.19	28,28,28,28	0

6.5 Other polymers ⓘ

There are no such residues in this entry.