



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:39 AM UTC

PDB ID : 6JP4 / pdb_00006jp4
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 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

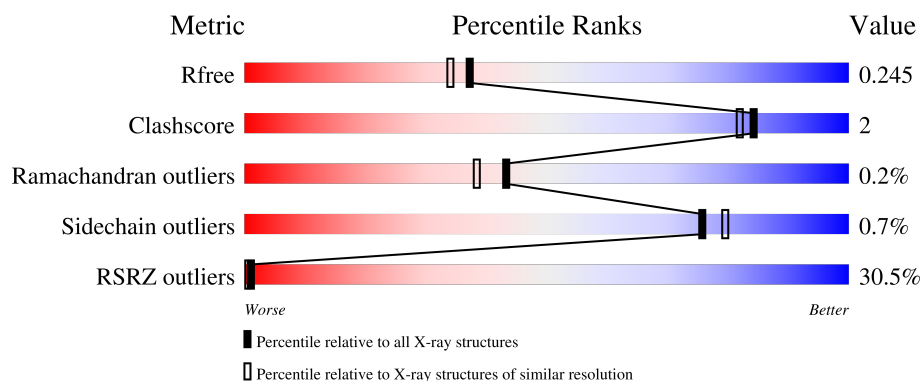
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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}	180053	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (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 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	770	2% 92% 8%
1	B	770	5% 92% 8%
1	C	770	20% 93% 7%
1	D	770	94% 99% .

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
7	CAC	A	812	-	X	-	-

2 Entry composition

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 (CCD ID: MN) (formula: Mn).

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

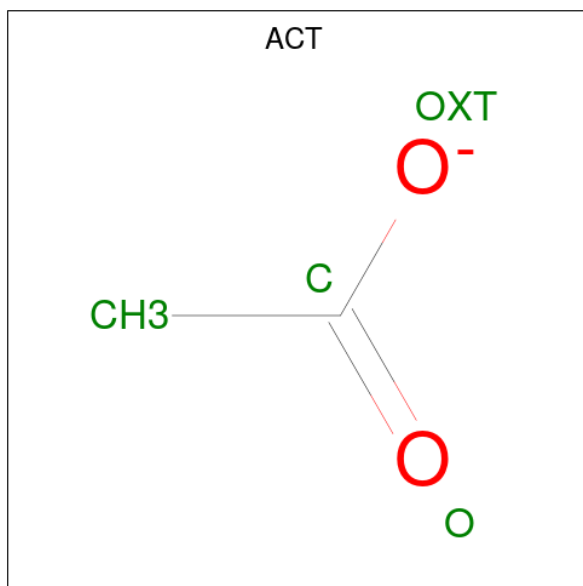
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



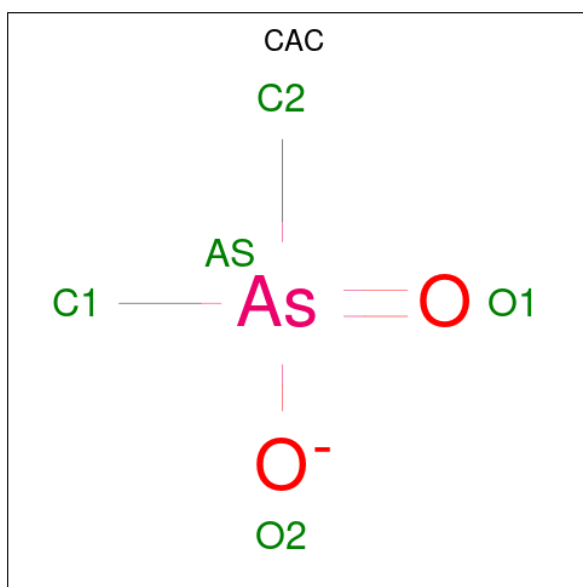
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: 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 (CCD ID: 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		

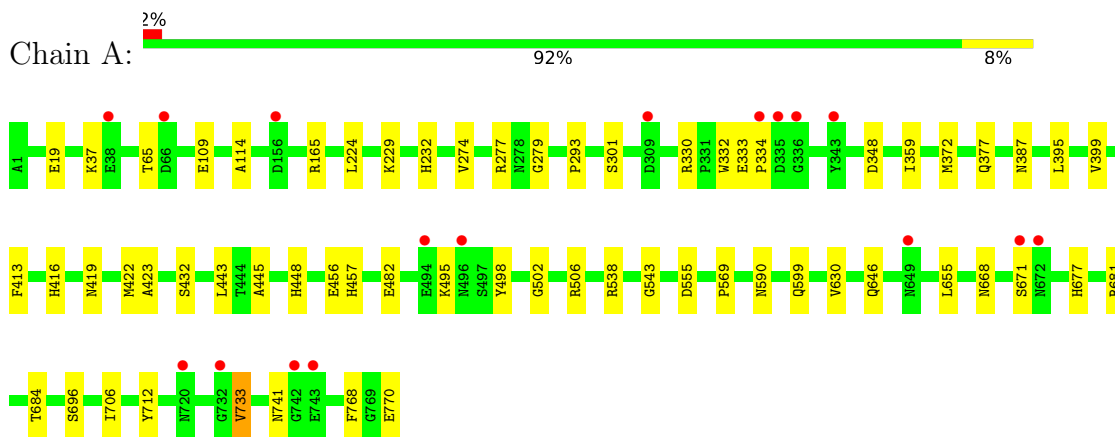
- Molecule 8 is water.

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		

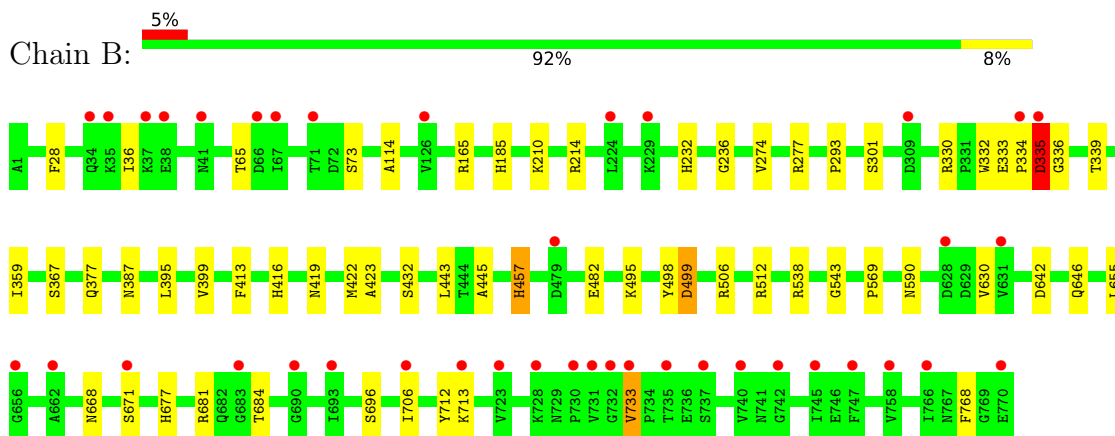
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

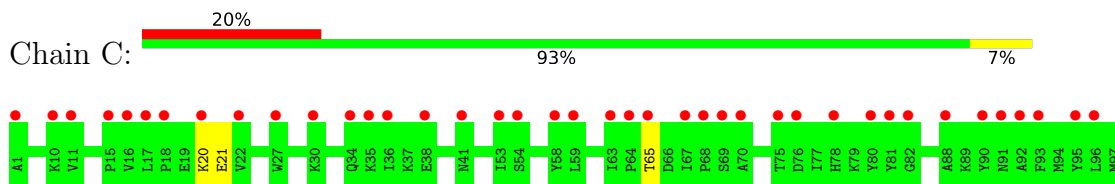
- Molecule 1: Alginate lyase

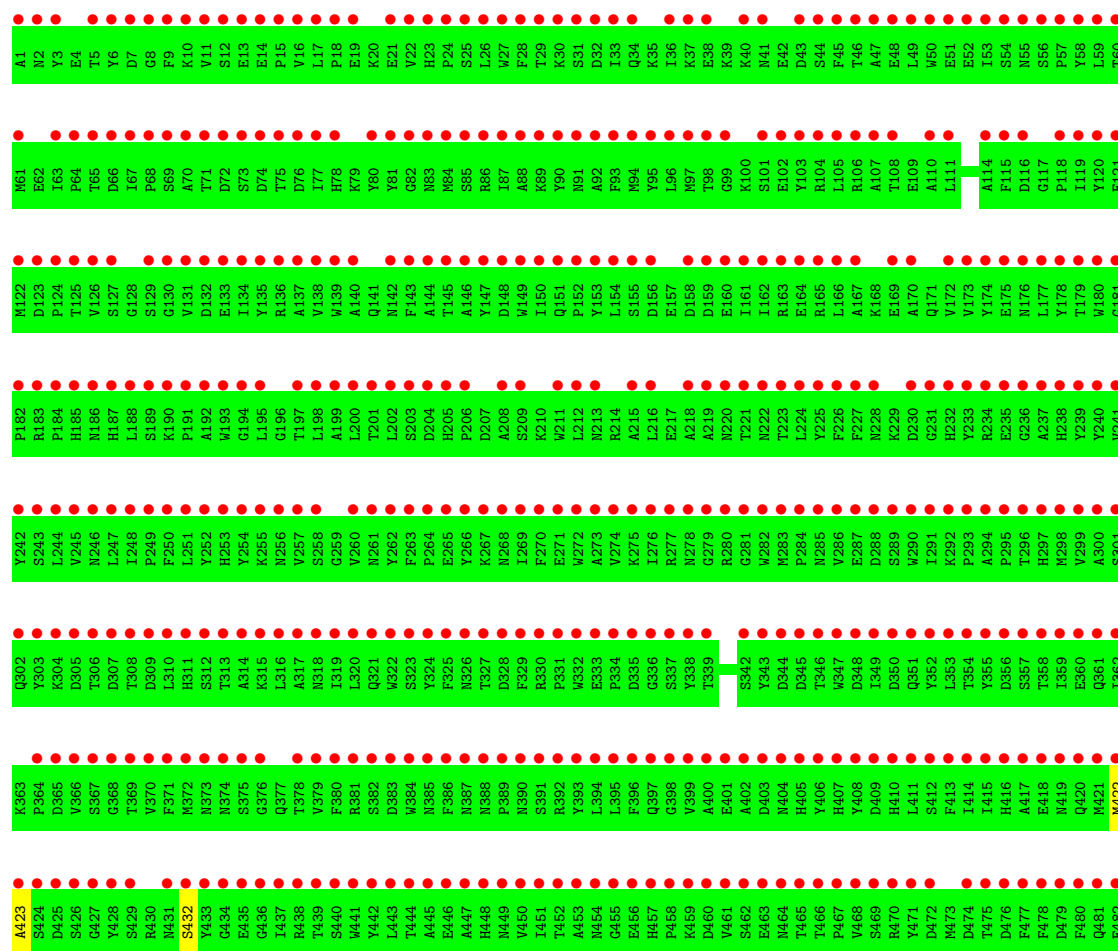


- Molecule 1: Alginate lyase



- Molecule 1: Alginate lyase





V723	K483	G543	D603	T663	W723
E724	E484	E544	T604	F664	E724
L725	A485	G545	M605	A665	L725
R726	V486	N546	F606	Y666	R726
K727	Y487	Y547	M607	T667	K727
N728	D488	R548	Q608	N668	N728
N729	G489	L549	I609	E669	N729
F730	F490	W550	I610	N670	F730
V731	T491	W551	V611	S671	V731
G732	F492	Y552	P612	N672	G732
V733	P493	E553	L613	N673	V733
P734	E494	D564	S614	E674	P734
T735	K495	D565	K615	L675	T735
E736	M496	R566	Y616	Q676	E736
S737	S497	Y567	A617	H677	S737
V738	Y498	G568	D618	F678	V738
V739	D499	Q569	I619	S679	V739
V740	F500	E560	P620	V680	V740
N741	S501	A561	E621	R681	N741
G742	G502	K562	V622	Q682	G742
E743	A503	M563	V623	G683	E743
N744	Q504	A564	D624	T684	N744
I745	I505	A565	L625	S685	I745
E746	R506	W566	S626	L686	E746
F747	A507	V567	T627	D687	F747
S748	I508	F568	D628	Y688	S748
V749	G509	F569	D629	K689	V749
E750	F510	S570	V630	G690	E750
D751	P511	K571	V631	E691	D751
G752	R512	E572	G632	N692	G752
V753	Q513	S573	G633	I693	V753
T754	D514	T574	T634	F694	T754
V755	Y515	F575	V635	V695	V755
I756	F516	L576	V636	S696	I756
Q757	V517	D577	K637	N697	Q757
V758	V518	K578	D638	K698	V758
A759	A519	E579	N639	P699	A759
E760	D520	G580	E640	I700	E760
G761	Q521	E581	K641	T701	G761
D762	L522	V582	D642	F702	D762
D763	F523	N583	T643	A703	D763
I764	S524	Y584	F644	L704	I764
N765	D525	E585	M645	D705	N765
I766	K526	A586	Q646	I706	I766
N767	E527	G587	Q647	S707	N767
F768	V528	A588	L648	D708	F768
G769	Q529	F589	N649	E709	G769
E770	Y530	N590	N650	T710	E770
	D531	S591	A651	Q711	
	L532	Y592	E652	Y712	
	Y533	G593	N653	K713	
	L534	Y594	S654	G714	
	H535	L595	L655	T715	
	Q536	N596	G656	I716	
	Q537	A597	D657	A717	
	R538	R598	I658	A718	
	G539	Q599	T659	L719	
	E540	I600	T660	N720	
	M541	A601	D661	E721	
	S542	K602	A662	T722	

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 98.90 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.5 (98.90-2.07) 99.5 (98.90-2.07)	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)	0.39 , 66.3	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, CA, MG, MN, CAC, EDO

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	1.01	2/6413 (0.0%)	1.32	10/8727 (0.1%)
1	B	1.00	3/6413 (0.0%)	1.33	13/8727 (0.1%)
1	C	0.97	0/6413	1.31	6/8727 (0.1%)
1	D	1.42	0/3079	1.80	2/3847 (0.1%)
All	All	1.06	5/22318 (0.0%)	1.39	31/30028 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	448	HIS	CE1-NE2	6.84	1.39	1.32
1	A	502	GLY	C-O	5.45	1.29	1.23
1	B	457	HIS	CE1-NE2	5.40	1.38	1.32
1	B	214	ARG	CD-NE	5.29	1.53	1.46
1	B	185	HIS	CE1-NE2	5.13	1.37	1.32

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	770	GLU	CA-C-O	-7.19	108.58	120.80
1	B	499	ASP	CA-CB-CG	6.56	119.16	112.60
1	A	569	PRO	CA-C-N	6.55	130.64	120.82
1	A	569	PRO	C-N-CA	6.55	130.64	120.82
1	B	335	ASP	CA-CB-CG	6.55	119.15	112.60
1	B	569	PRO	CA-C-N	5.99	129.81	120.82
1	B	569	PRO	C-N-CA	5.99	129.81	120.82
1	C	569	PRO	CA-C-N	5.79	129.50	120.82
1	C	569	PRO	C-N-CA	5.79	129.50	120.82
1	A	334	PRO	CA-C-N	5.70	128.72	120.79
1	A	334	PRO	C-N-CA	5.70	128.72	120.79
1	B	432	SER	CA-C-N	5.66	127.86	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	432	SER	C-N-CA	5.66	127.86	120.28
1	C	432	SER	CA-C-N	5.64	127.84	120.28
1	C	432	SER	C-N-CA	5.64	127.84	120.28
1	A	372	MET	CA-CB-CG	-5.58	102.93	114.10
1	B	543	GLY	CA-C-O	-5.57	118.60	122.22
1	B	334	PRO	CA-C-N	5.38	128.26	120.79
1	B	334	PRO	C-N-CA	5.38	128.26	120.79
1	C	427	GLY	CA-C-N	5.31	128.18	120.79
1	C	427	GLY	C-N-CA	5.31	128.18	120.79
1	A	543	GLY	CA-C-O	-5.22	118.83	122.22
1	D	432	SER	CA-C-N	5.20	127.24	120.28
1	D	432	SER	C-N-CA	5.20	127.24	120.28
1	A	432	SER	CA-C-N	5.17	127.21	120.28
1	A	432	SER	C-N-CA	5.17	127.21	120.28
1	B	236	GLY	CA-C-N	5.12	127.15	120.28
1	B	236	GLY	C-N-CA	5.12	127.15	120.28
1	B	367	SER	CA-C-N	5.10	125.64	119.98
1	B	367	SER	C-N-CA	5.10	125.64	119.98
1	A	348	ASP	CA-CB-CG	5.03	117.63	112.60

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	6240	0	5798	37	0
1	B	6240	0	5798	30	0
1	C	6240	0	5798	29	0
1	D	3080	0	834	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	8	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	94	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 (94) 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
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:A:37:LYS:HZ2	1:C:744:ASN:HD21	1.51	0.58
1:A:229:LYS:NZ	8:A:902:HOH:O	2.30	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:GLU:HG2	8:A:1222:HOH:O	2.05	0.56
1:C:443:LEU:HD12	1:C:443:LEU:C	2.32	0.55
1:A:677:HIS:HE1	8:A:933:HOH:O	1.90	0.54
1:B:443:LEU:C	1:B:443:LEU:HD12	2.33	0.53
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:A:443:LEU:C	1:A:443:LEU:HD12	2.33	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:B:395:LEU:O	1:B:413:PHE:HA	2.14	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:A:387:ASN:C	1:A:419:ASN:HD21	2.23	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:A:741:ASN:CG	8:A:989:HOH:O	2.60	0.45
1:B:335:ASP:OD1	1:B:336:GLY:N	2.50	0.44
1:B:422:MET:O	1:B:423:ALA:C	2.61	0.44
1:C:20:LYS:HD2	1:C:21:GLU:N	2.32	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
1:A:599:GLN:NE2	7:A:812:CAC:C1	2.73	0.44
1:D:422:MET:O	1:D:423:ALA:C	2.61	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:A:422:MET:O	1:A:423:ALA:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:422:MET:O	1:C:423:ALA:C	2.61	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:B:512:ARG:HH21	1:B:642:ASP:CG	2.27	0.42
1:C:387:ASN:C	1:C:419:ASN:HD21	2.26	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:HD22	1:A:419:ASN:HA	1.65	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:B:387:ASN:C	1:B:419:ASN:HD21	2.27	0.41
1:C:229:LYS:HB2	1:C:229:LYS:HE2	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:706:ILE:HA	1:A:712:TYR:CD1	2.56	0.41
1:A:19:GLU:HG2	1:B:73:SER:HA	2.03	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:279:GLY:H	1:A:416:HIS:CD2	2.39	0.41
1:C:512:ARG:HH21	1:C:642:ASP:CG	2.28	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	768/770 (100%)	740 (96%)	27 (4%)	1 (0%)	48	44
1	B	768/770 (100%)	738 (96%)	29 (4%)	1 (0%)	48	44
1	C	768/770 (100%)	736 (96%)	31 (4%)	1 (0%)	48	44
1	D	768/770 (100%)	727 (95%)	39 (5%)	2 (0%)	36	30
All	All	3072/3080 (100%)	2941 (96%)	126 (4%)	5 (0%)	43	38

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%)	84	87
1	B	671/671 (100%)	665 (99%)	6 (1%)	70	74
1	C	671/671 (100%)	665 (99%)	6 (1%)	70	74
All	All	2013/2013 (100%)	1998 (99%)	15 (1%)	76	79

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	THR
1	A	224	LEU
1	A	733	VAL
1	B	65	THR
1	B	210	LYS
1	B	335	ASP
1	B	499	ASP
1	B	713	LYS
1	B	733	VAL
1	C	65	THR
1	C	224	LEU
1	C	229	LYS
1	C	579	GLU
1	C	639	ASN
1	C	713	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	232	HIS
1	A	326	ASN
1	A	416	HIS
1	A	419	ASN
1	A	464	ASN
1	A	481	GLN
1	A	535	HIS
1	A	559	GLN
1	A	590	ASN
1	A	599	GLN
1	A	646	GLN
1	A	677	HIS
1	A	692	ASN
1	A	744	ASN
1	B	41	ASN
1	B	232	HIS
1	B	416	HIS
1	B	419	ASN
1	B	464	ASN
1	B	481	GLN
1	B	535	HIS

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Mol	Chain	Res	Type
1	B	559	GLN
1	B	590	ASN
1	B	599	GLN
1	B	646	GLN
1	B	668	ASN
1	B	677	HIS
1	B	692	ASN
1	B	744	ASN
1	C	41	ASN
1	C	232	HIS
1	C	416	HIS
1	C	419	ASN
1	C	464	ASN
1	C	481	GLN
1	C	535	HIS
1	C	559	GLN
1	C	590	ASN
1	C	599	GLN
1	C	646	GLN
1	C	668	ASN
1	C	677	HIS
1	C	692	ASN
1	C	720	ASN
1	C	744	ASN
1	C	765	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	A	807	-	3,3,3	0.28	0	2,2,2	0.22	0
6	EDO	B	807	-	3,3,3	0.13	0	2,2,2	0.07	0
6	EDO	B	809	-	3,3,3	0.09	0	2,2,2	0.09	0
6	EDO	C	806	-	3,3,3	0.08	0	2,2,2	0.12	0
5	ACT	C	805	-	3,3,3	0.97	0	3,3,3	0.89	0
7	CAC	A	812	-	2,4,4	2.67	2 (100%)	4,6,6	1.88	2 (50%)
6	EDO	A	810	-	3,3,3	0.08	0	2,2,2	0.21	0
6	EDO	B	808	-	3,3,3	0.24	0	2,2,2	0.14	0
5	ACT	A	805	-	3,3,3	1.26	0	3,3,3	0.54	0
5	ACT	A	806	-	3,3,3	0.88	0	3,3,3	0.91	0
5	ACT	B	805	-	3,3,3	0.85	0	3,3,3	1.01	0
6	EDO	A	809	-	3,3,3	0.09	0	2,2,2	0.13	0
6	EDO	A	811	-	3,3,3	0.17	0	2,2,2	0.30	0
5	ACT	B	806	-	3,3,3	1.14	0	3,3,3	0.67	0
6	EDO	A	808	-	3,3,3	0.07	0	2,2,2	0.11	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
6	EDO	A	807	-	-	0/1/1/1	-
6	EDO	B	807	-	-	0/1/1/1	-
6	EDO	B	809	-	-	0/1/1/1	-
6	EDO	C	806	-	-	1/1/1/1	-
6	EDO	A	810	-	-	1/1/1/1	-
6	EDO	B	808	-	-	0/1/1/1	-
6	EDO	A	809	-	-	0/1/1/1	-
6	EDO	A	811	-	-	0/1/1/1	-
6	EDO	A	808	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	812	CAC	AS-C2	2.76	1.96	1.90
7	A	812	CAC	AS-C1	2.58	1.96	1.90

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	812	CAC	O1-AS-C1	-2.56	108.31	111.50
7	A	812	CAC	O1-AS-C2	-2.02	108.99	111.50

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 [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	770/770 (100%)	-0.06	17 (2%) 62 64	22, 33, 56, 87	0
1	B	770/770 (100%)	0.54	40 (5%) 33 32	26, 44, 76, 120	0
1	C	770/770 (100%)	1.26	156 (20%) 3 2	41, 60, 89, 115	0
1	D	770/770 (100%)	3.72	726 (94%) 0 0	60, 90, 129, 146	0
All	All	3080/3080 (100%)	1.36	939 (30%) 1 0	22, 55, 112, 146	0

All (939) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	233	TYR	8.7
1	D	270	PHE	8.0
1	D	272	TRP	7.7
1	D	303	TYR	7.6
1	D	402	ALA	7.0
1	D	250	PHE	7.0
1	D	475	THR	7.0
1	D	234	ARG	6.8
1	D	239	TYR	6.8
1	D	384	TRP	6.8
1	D	294	ALA	6.7
1	D	680	VAL	6.7
1	D	546	ASN	6.7
1	D	433	TYR	6.6
1	D	405	HIS	6.5
1	D	26	LEU	6.4
1	D	406	TYR	6.4
1	D	492	PHE	6.4
1	D	566	TRP	6.4
1	D	249	PRO	6.3
1	D	338	TYR	6.3

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Mol	Chain	Res	Type	RSRZ
1	D	682	GLN	6.2
1	D	223	THR	6.2
1	D	478	PHE	6.2
1	D	442	TYR	6.2
1	D	408	TYR	6.1
1	D	258	SER	6.1
1	D	482	GLU	6.1
1	D	339	THR	6.1
1	D	322	TRP	6.1
1	D	266	TYR	6.1
1	D	487	TYR	6.0
1	D	248	ILE	6.0
1	D	667	THR	5.9
1	D	241	VAL	5.9
1	D	411	LEU	5.9
1	D	567	VAL	5.9
1	D	362	ILE	5.8
1	D	435	GLU	5.8
1	D	295	PRO	5.8
1	D	186	ASN	5.8
1	D	379	VAL	5.8
1	D	125	THR	5.8
1	D	343	TYR	5.8
1	D	87	ILE	5.8
1	D	290	TRP	5.8
1	D	240	TYR	5.7
1	D	242	TYR	5.7
1	D	282	TRP	5.7
1	D	337	SER	5.7
1	D	312	SER	5.6
1	D	550	TRP	5.6
1	D	428	TYR	5.6
1	D	616	TYR	5.6
1	D	219	ALA	5.6
1	D	717	ALA	5.6
1	D	184	PRO	5.6
1	C	70	ALA	5.6
1	D	730	PRO	5.6
1	D	226	PHE	5.5
1	D	375	SER	5.5
1	D	320	LEU	5.5
1	D	129	SER	5.5

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Mol	Chain	Res	Type	RSRZ
1	D	124	PRO	5.5
1	D	197	THR	5.5
1	D	426	SER	5.4
1	D	204	ASP	5.4
1	D	518	VAL	5.4
1	D	415	ILE	5.4
1	D	759	ALA	5.4
1	D	374	ASN	5.4
1	D	477	PHE	5.4
1	D	547	TYR	5.4
1	D	371	PHE	5.4
1	D	188	LEU	5.3
1	D	533	TYR	5.3
1	D	232	HIS	5.3
1	D	220	ASN	5.3
1	D	273	ALA	5.3
1	D	399	VAL	5.3
1	D	738	VAL	5.3
1	D	243	SER	5.3
1	D	244	LEU	5.3
1	D	27	TRP	5.3
1	D	179	THR	5.3
1	D	666	TYR	5.3
1	D	276	ILE	5.3
1	D	257	VAL	5.2
1	D	58	TYR	5.2
1	D	373	ASN	5.2
1	D	247	LEU	5.2
1	D	144	ALA	5.1
1	D	7	ASP	5.1
1	D	625	LEU	5.1
1	D	604	THR	5.1
1	B	731	VAL	5.1
1	D	461	VAL	5.1
1	D	631	VAL	5.1
1	D	70	ALA	5.1
1	D	286	VAL	5.1
1	D	528	VAL	5.1
1	D	329	PHE	5.1
1	D	370	VAL	5.1
1	D	284	PRO	5.1
1	D	407	HIS	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	343	TYR	5.0
1	D	653	ASN	5.0
1	D	191	PRO	5.0
1	D	92	ALA	5.0
1	D	131	VAL	5.0
1	D	468	VAL	5.0
1	D	479	ASP	5.0
1	D	237	ALA	5.0
1	D	747	PHE	5.0
1	D	766	ILE	5.0
1	D	552	TYR	5.0
1	D	332	TRP	5.0
1	D	367	SER	5.0
1	D	77	ILE	5.0
1	D	760	GLU	4.9
1	D	542	SER	4.9
1	D	238	HIS	4.9
1	D	684	THR	4.9
1	D	628	ASP	4.9
1	D	366	VAL	4.9
1	D	416	HIS	4.9
1	D	192	ALA	4.9
1	D	200	LEU	4.9
1	D	491	THR	4.9
1	D	490	PHE	4.9
1	D	434	GLY	4.9
1	D	400	ALA	4.8
1	D	453	ALA	4.8
1	D	611	VAL	4.8
1	D	723	VAL	4.8
1	D	358	THR	4.8
1	D	444	THR	4.8
1	D	161	ILE	4.8
1	D	285	ASN	4.8
1	D	622	VAL	4.8
1	D	383	ASP	4.8
1	D	347	TRP	4.8
1	D	380	PHE	4.8
1	D	705	ASP	4.8
1	D	107	ALA	4.8
1	D	324	TYR	4.7
1	D	382	SER	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	167	ALA	4.7
1	D	404	ASN	4.7
1	D	549	LEU	4.7
1	D	67	ILE	4.7
1	D	683	GLY	4.7
1	D	606	PHE	4.7
1	D	309	ASP	4.7
1	D	187	HIS	4.7
1	D	534	LEU	4.7
1	D	376	GLY	4.7
1	D	396	PHE	4.7
1	D	515	TYR	4.7
1	D	236	GLY	4.7
1	D	532	LEU	4.7
1	D	563	MET	4.7
1	D	72	ASP	4.7
1	D	71	THR	4.6
1	D	369	THR	4.6
1	D	111	LEU	4.6
1	D	706	ILE	4.6
1	D	501	SER	4.6
1	D	50	TRP	4.6
1	D	181	GLY	4.6
1	D	574	ILE	4.6
1	D	619	ILE	4.6
1	D	283	MET	4.6
1	D	130	GLY	4.6
1	D	352	TYR	4.6
1	D	648	LEU	4.6
1	D	481	GLN	4.6
1	D	91	ASN	4.6
1	D	469	SER	4.6
1	D	60	THR	4.5
1	D	274	VAL	4.5
1	D	114	ALA	4.5
1	D	437	ILE	4.5
1	D	228	ASN	4.5
1	D	668	ASN	4.5
1	D	570	SER	4.5
1	D	466	THR	4.5
1	D	6	TYR	4.5
1	D	471	TYR	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	162	ILE	4.5
1	D	360	GLU	4.5
1	D	460	ASP	4.5
1	D	467	PRO	4.5
1	D	49	LEU	4.5
1	D	609	ILE	4.5
1	D	506	ARG	4.5
1	D	74	ASP	4.5
1	D	98	THR	4.5
1	D	281	GLY	4.5
1	D	206	PRO	4.5
1	D	583	ASN	4.5
1	D	421	MET	4.4
1	D	126	VAL	4.4
1	D	323	SER	4.4
1	D	149	TRP	4.4
1	D	252	TYR	4.4
1	D	221	THR	4.4
1	D	306	THR	4.4
1	D	293	PRO	4.4
1	D	712	TYR	4.4
1	D	193	TRP	4.4
1	D	346	THR	4.4
1	D	378	THR	4.4
1	D	568	PHE	4.4
1	D	758	VAL	4.4
1	D	610	ILE	4.4
1	D	401	GLU	4.4
1	D	90	TYR	4.3
1	D	95	TYR	4.3
1	D	584	TYR	4.3
1	D	336	GLY	4.3
1	D	735	THR	4.3
1	D	511	PRO	4.3
1	D	34	GLN	4.3
1	D	662	ALA	4.3
1	D	310	LEU	4.3
1	D	704	LEU	4.3
1	D	764	ILE	4.3
1	D	398	GLY	4.3
1	D	41	ASN	4.3
1	D	139	TRP	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	124	PRO	4.3
1	D	480	PHE	4.3
1	D	269	ILE	4.3
1	D	436	GLY	4.3
1	D	741	ASN	4.3
1	D	57	PRO	4.3
1	D	121	GLU	4.3
1	D	263	PHE	4.3
1	D	517	VAL	4.3
1	D	649	ASN	4.3
1	D	513	GLN	4.3
1	D	594	TYR	4.3
1	D	209	SER	4.3
1	D	115	PHE	4.2
1	D	514	ASP	4.2
1	D	447	ALA	4.2
1	D	703	ALA	4.2
1	D	185	HIS	4.2
1	D	278	ASN	4.2
1	D	697	ASN	4.2
1	D	46	THR	4.2
1	D	627	THR	4.2
1	D	18	PRO	4.2
1	D	174	TYR	4.2
1	D	199	ALA	4.2
1	D	725	LEU	4.2
1	D	451	ILE	4.2
1	D	357	SER	4.2
1	D	493	PRO	4.2
1	D	422	MET	4.2
1	D	500	PHE	4.2
1	D	521	GLN	4.2
1	D	450	VAL	4.2
1	D	731	VAL	4.2
1	D	180	TRP	4.2
1	D	761	GLY	4.2
1	D	359	ILE	4.2
1	D	612	PRO	4.2
1	C	343	TYR	4.2
1	D	262	TYR	4.2
1	C	1	ALA	4.2
1	D	423	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	108	THR	4.1
1	D	701	THR	4.1
1	D	135	TYR	4.1
1	D	498	TYR	4.1
1	D	530	TYR	4.1
1	D	595	LEU	4.1
1	D	279	GLY	4.1
1	D	754	THR	4.1
1	D	441	TRP	4.1
1	D	88	ALA	4.1
1	D	630	VAL	4.1
1	D	452	THR	4.1
1	D	134	ILE	4.1
1	D	275	LYS	4.1
1	D	291	ILE	4.1
1	D	334	PRO	4.1
1	D	564	ALA	4.1
1	D	651	ALA	4.1
1	D	516	PHE	4.1
1	D	523	PHE	4.1
1	D	520	ASP	4.1
1	D	663	THR	4.1
1	D	626	SER	4.1
1	D	588	ALA	4.0
1	D	103	TYR	4.0
1	D	529	GLN	4.0
1	D	615	LYS	4.0
1	D	535	HIS	4.0
1	D	201	THR	4.0
1	D	235	GLU	4.0
1	D	591	SER	4.0
1	D	548	ARG	4.0
1	D	389	PRO	4.0
1	D	629	ASP	4.0
1	D	325	PHE	4.0
1	C	161	ILE	4.0
1	D	720	ASN	4.0
1	D	335	ASP	4.0
1	D	485	ALA	4.0
1	D	531	ASP	4.0
1	D	73	SER	4.0
1	D	289	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	412	SER	4.0
1	D	36	ILE	4.0
1	D	618	ASP	4.0
1	D	314	ALA	3.9
1	D	56	SER	3.9
1	D	551	THR	3.9
1	D	173	VAL	3.9
1	D	213	ASN	3.9
1	D	458	PRO	3.9
1	D	288	ASP	3.9
1	D	345	ASP	3.9
1	D	536	GLY	3.9
1	D	212	LEU	3.9
1	D	301	SER	3.9
1	C	180	TRP	3.9
1	D	65	THR	3.9
1	D	53	ILE	3.9
1	D	69	SER	3.9
1	C	224	LEU	3.9
1	D	675	LEU	3.9
1	D	715	THR	3.9
1	C	27	TRP	3.9
1	D	68	PRO	3.9
1	D	525	ASP	3.9
1	D	603	ASP	3.9
1	C	114	ALA	3.9
1	D	424	SER	3.9
1	D	462	SER	3.9
1	D	596	ASN	3.9
1	C	193	TRP	3.8
1	D	472	ASP	3.8
1	D	474	ASP	3.8
1	D	432	SER	3.8
1	D	271	GLU	3.8
1	D	326	ASN	3.8
1	D	763	ASP	3.8
1	D	654	SER	3.8
1	D	718	ALA	3.8
1	D	143	PHE	3.8
1	D	752	GLY	3.8
1	D	573	SER	3.8
1	D	431	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	5	THR	3.8
1	D	634	THR	3.8
1	D	364	PRO	3.8
1	D	657	ASP	3.8
1	D	582	VAL	3.8
1	D	9	PHE	3.8
1	D	205	HIS	3.7
1	D	403	ASP	3.7
1	D	638	ASP	3.7
1	D	740	VAL	3.7
1	D	387	ASN	3.7
1	D	600	ILE	3.7
1	C	211	TRP	3.7
1	D	688	TYR	3.7
1	D	296	THR	3.7
1	D	327	THR	3.7
1	D	15	PRO	3.7
1	C	126	VAL	3.7
1	D	755	VAL	3.7
1	D	745	ILE	3.7
1	D	425	ASP	3.7
1	D	557	TYR	3.7
1	C	139	TRP	3.7
1	D	330	ARG	3.7
1	D	361	GLN	3.7
1	C	336	GLY	3.7
1	D	732	GLY	3.7
1	D	66	ASP	3.7
1	D	280	ARG	3.7
1	D	681	ARG	3.7
1	D	321	GLN	3.7
1	D	1	ALA	3.7
1	D	208	ALA	3.7
1	D	565	ALA	3.7
1	C	105	LEU	3.6
1	D	94	MET	3.6
1	D	543	GLY	3.6
1	C	172	VAL	3.6
1	C	245	VAL	3.6
1	D	486	VAL	3.6
1	D	698	LYS	3.6
1	D	505	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	693	ILE	3.6
1	D	751	ASP	3.6
1	D	137	ALA	3.6
1	D	617	ALA	3.6
1	D	734	PRO	3.6
1	D	454	ASN	3.6
1	D	748	SER	3.6
1	D	265	GLU	3.6
1	D	344	ASP	3.6
1	D	386	PHE	3.6
1	D	664	PHE	3.6
1	D	660	THR	3.6
1	C	137	ALA	3.6
1	D	59	LEU	3.6
1	C	153	TYR	3.6
1	C	242	TYR	3.6
1	D	231	GLY	3.6
1	C	615	LYS	3.6
1	D	189	SER	3.6
1	C	731	VAL	3.6
1	D	172	VAL	3.6
1	D	305	ASP	3.6
1	D	409	ASP	3.6
1	D	576	ILE	3.6
1	D	716	ILE	3.6
1	D	613	LEU	3.6
1	D	639	ASN	3.6
1	D	765	ASN	3.6
1	D	25	SER	3.6
1	D	737	SER	3.6
1	D	298	MET	3.5
1	D	541	MET	3.5
1	C	119	ILE	3.5
1	D	308	THR	3.5
1	D	465	THR	3.5
1	C	192	ALA	3.5
1	D	459	LYS	3.5
1	D	195	LEU	3.5
1	D	202	LEU	3.5
1	D	545	GLY	3.5
1	D	101	SER	3.5
1	D	254	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	749	VAL	3.5
1	D	33	ILE	3.5
1	D	445	ALA	3.5
1	D	597	ALA	3.5
1	D	620	PRO	3.5
1	C	194	GLY	3.5
1	D	556	ARG	3.5
1	D	313	THR	3.5
1	C	134	ILE	3.5
1	D	699	PRO	3.5
1	D	655	LEU	3.5
1	D	54	SER	3.5
1	D	524	SER	3.5
1	D	679	SER	3.5
1	D	476	ASP	3.5
1	C	81	TYR	3.5
1	D	390	ASN	3.5
1	D	710	THR	3.5
1	D	24	PRO	3.4
1	D	45	PHE	3.4
1	D	678	PHE	3.4
1	D	702	PHE	3.4
1	D	624	ASP	3.4
1	D	104	ARG	3.4
1	D	494	GLU	3.4
1	D	581	GLU	3.4
1	D	268	ASN	3.4
1	C	99	GLY	3.4
1	C	294	ALA	3.4
1	D	561	ALA	3.4
1	A	335	ASP	3.4
1	D	746	GLU	3.4
1	D	297	HIS	3.4
1	C	135	TYR	3.4
1	D	225	TYR	3.4
1	D	354	THR	3.4
1	D	391	SER	3.4
1	D	652	GLU	3.4
1	D	510	PHE	3.4
1	D	80	TYR	3.4
1	D	97	MET	3.4
1	D	160	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	245	VAL	3.4
1	C	181	GLY	3.4
1	D	31	SER	3.4
1	D	182	PRO	3.4
1	D	537	GLY	3.4
1	D	601	ALA	3.4
1	B	34	GLN	3.4
1	D	105	LEU	3.4
1	D	394	LEU	3.4
1	D	449	ASN	3.3
1	D	470	ARG	3.3
1	D	12	SER	3.3
1	D	16	VAL	3.3
1	D	152	PRO	3.3
1	D	455	GLY	3.3
1	D	63	ILE	3.3
1	D	96	LEU	3.3
1	D	216	LEU	3.3
1	D	395	LEU	3.3
1	C	115	PHE	3.3
1	D	372	MET	3.3
1	D	75	THR	3.3
1	D	119	ILE	3.3
1	D	317	ALA	3.3
1	D	410	HIS	3.3
1	D	658	ILE	3.3
1	C	246	ASN	3.3
1	D	590	ASN	3.3
1	D	744	ASN	3.3
1	D	768	PHE	3.3
1	D	578	LYS	3.3
1	D	659	THR	3.3
1	D	676	GLN	3.3
1	D	22	VAL	3.3
1	C	170	ALA	3.3
1	D	170	ALA	3.3
1	C	91	ASN	3.3
1	D	307	ASP	3.3
1	C	149	TRP	3.2
1	B	656	GLY	3.2
1	D	427	GLY	3.2
1	D	569	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	636	VAL	3.2
1	D	3	TYR	3.2
1	D	178	TYR	3.2
1	D	287	GLU	3.2
1	D	527	GLU	3.2
1	D	222	ASN	3.2
1	D	443	LEU	3.2
1	D	145	THR	3.2
1	D	253	HIS	3.2
1	D	368	GLY	3.2
1	D	136	ARG	3.2
1	C	770	GLU	3.2
1	C	35	LYS	3.2
1	C	67	ILE	3.2
1	D	166	LEU	3.2
1	D	414	ILE	3.2
1	D	643	THR	3.2
1	D	2	ASN	3.2
1	D	224	LEU	3.2
1	D	319	ILE	3.2
1	D	753	TYR	3.2
1	D	227	PHE	3.2
1	D	644	PHE	3.2
1	A	732	GLY	3.2
1	D	762	GLY	3.2
1	D	331	PRO	3.2
1	D	608	GLN	3.2
1	C	22	VAL	3.1
1	C	167	ALA	3.1
1	D	47	ALA	3.1
1	D	218	ALA	3.1
1	D	586	ALA	3.1
1	D	623	VAL	3.1
1	D	43	ASP	3.1
1	D	353	LEU	3.1
1	D	14	GLU	3.1
1	D	99	GLY	3.1
1	D	264	PRO	3.1
1	D	767	ASN	3.1
1	D	727	VAL	3.1
1	D	739	VAL	3.1
1	B	38	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	85	SER	3.1
1	D	190	LYS	3.1
1	A	742	GLY	3.1
1	C	143	PHE	3.1
1	D	645	MET	3.1
1	D	439	THR	3.1
1	A	720	ASN	3.1
1	D	76	ASP	3.1
1	D	642	ASP	3.1
1	B	126	VAL	3.1
1	D	175	GLU	3.1
1	D	17	LEU	3.1
1	C	101	SER	3.1
1	C	120	TYR	3.1
1	D	646	GLN	3.1
1	D	385	ASN	3.1
1	D	21	GLU	3.1
1	D	116	ASP	3.1
1	D	158	ASP	3.1
1	D	457	HIS	3.1
1	D	665	ALA	3.1
1	D	11	VAL	3.1
1	D	260	VAL	3.1
1	C	58	TYR	3.0
1	D	29	THR	3.0
1	D	246	ASN	3.0
1	D	770	GLU	3.0
1	D	311	HIS	3.0
1	C	154	LEU	3.0
1	D	671	SER	3.0
1	D	464	ASN	3.0
1	C	352	TYR	3.0
1	D	147	TYR	3.0
1	D	575	PHE	3.0
1	D	356	ASP	3.0
1	D	417	ALA	3.0
1	D	159	ASP	3.0
1	D	355	TYR	3.0
1	D	110	ALA	3.0
1	D	512	ARG	3.0
1	D	138	VAL	3.0
1	D	719	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	112	LYS	3.0
1	D	438	ARG	2.9
1	D	38	GLU	2.9
1	D	724	GLU	2.9
1	D	142	ASN	2.9
1	D	692	ASN	2.9
1	D	132	ASP	2.9
1	D	350	ASP	2.9
1	D	708	ASP	2.9
1	D	605	MET	2.9
1	D	757	GLN	2.9
1	D	463	GLU	2.9
1	D	203	SER	2.9
1	D	519	ALA	2.9
1	D	577	ASP	2.9
1	A	334	PRO	2.9
1	D	559	GLN	2.9
1	D	277	ARG	2.9
1	D	393	TYR	2.9
1	D	419	ASN	2.9
1	D	598	ARG	2.9
1	C	20	LYS	2.9
1	D	315	LYS	2.9
1	D	685	SER	2.9
1	D	707	SER	2.9
1	D	256	ASN	2.9
1	C	195	LEU	2.8
1	D	183	ARG	2.8
1	D	351	GLN	2.8
1	D	397	GLN	2.8
1	D	456	GLU	2.8
1	D	553	GLU	2.8
1	D	304	LYS	2.8
1	D	348	ASP	2.8
1	C	216	LEU	2.8
1	D	686	LEU	2.8
1	C	191	PRO	2.8
1	D	497	SER	2.8
1	D	106	ARG	2.8
1	D	538	ARG	2.8
1	D	230	ASP	2.8
1	D	554	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	133	GLU	2.8
1	D	484	GLU	2.8
1	D	540	GLU	2.8
1	D	522	LEU	2.8
1	C	10	LYS	2.8
1	B	770	GLU	2.8
1	D	28	PHE	2.8
1	D	120	TYR	2.8
1	D	89	LYS	2.8
1	B	693	ILE	2.8
1	D	83	ASN	2.7
1	D	176	ASN	2.7
1	C	155	SER	2.7
1	D	429	SER	2.7
1	D	413	PHE	2.7
1	D	154	LEU	2.7
1	B	334	PRO	2.7
1	C	18	PRO	2.7
1	D	44	SER	2.7
1	C	76	ASP	2.7
1	D	742	GLY	2.7
1	D	267	LYS	2.7
1	C	98	THR	2.7
1	D	592	TYR	2.7
1	D	729	ASN	2.7
1	D	164	GLU	2.7
1	D	544	GLU	2.7
1	D	709	GLU	2.7
1	B	67	ILE	2.7
1	D	756	ILE	2.7
1	D	714	GLY	2.7
1	D	769	GLY	2.7
1	B	733	VAL	2.7
1	D	635	VAL	2.7
1	D	365	ASP	2.7
1	D	700	ILE	2.7
1	B	713	LYS	2.7
1	D	194	GLY	2.7
1	D	302	GLN	2.6
1	C	109	GLU	2.6
1	D	140	ALA	2.6
1	D	215	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	251	LEU	2.6
1	D	448	HIS	2.6
1	C	189	SER	2.6
1	D	499	ASP	2.6
1	D	728	LYS	2.6
1	D	349	ILE	2.6
1	B	732	GLY	2.6
1	D	580	GLY	2.6
1	D	504	GLN	2.6
1	D	572	GLU	2.6
1	D	621	GLU	2.6
1	D	607	MET	2.6
1	D	23	HIS	2.6
1	D	602	LYS	2.6
1	D	163	ARG	2.6
1	C	196	GLY	2.6
1	D	690	GLY	2.6
1	C	164	GLU	2.6
1	A	649	ASN	2.6
1	D	673	ASN	2.6
1	D	211	TRP	2.6
1	C	177	LEU	2.6
1	D	177	LEU	2.6
1	D	198	LEU	2.6
1	D	316	LEU	2.6
1	C	589	PHE	2.6
1	C	11	VAL	2.6
1	C	240	TYR	2.6
1	D	695	VAL	2.6
1	D	711	GLN	2.6
1	D	670	ASN	2.6
1	C	30	LYS	2.6
1	D	40	LYS	2.6
1	D	292	LYS	2.6
1	D	661	ASP	2.6
1	C	570	SER	2.6
1	D	151	GLN	2.5
1	A	743	GLU	2.5
1	C	102	GLU	2.5
1	D	585	GLU	2.5
1	C	63	ILE	2.5
1	D	150	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	95	TYR	2.5
1	D	153	TYR	2.5
1	A	496	ASN	2.5
1	D	55	ASN	2.5
1	D	526	LYS	2.5
1	D	123	ASP	2.5
1	D	328	ASP	2.5
1	D	118	PRO	2.5
1	C	34	GLN	2.5
1	C	166	LEU	2.5
1	C	188	LEU	2.5
1	C	198	LEU	2.5
1	D	589	PHE	2.5
1	B	766	ILE	2.5
1	D	509	GLY	2.5
1	D	496	ASN	2.5
1	D	650	ASN	2.5
1	B	309	ASP	2.5
1	D	488	ASP	2.5
1	B	662	ALA	2.5
1	D	333	GLU	2.5
1	D	560	GLU	2.5
1	D	669	GLU	2.5
1	D	93	PHE	2.5
1	C	136	ARG	2.5
1	C	178	TYR	2.5
1	C	209	SER	2.5
1	D	127	SER	2.5
1	D	440	SER	2.5
1	B	747	PHE	2.5
1	C	100	LYS	2.5
1	C	229	LYS	2.5
1	C	90	TYR	2.4
1	B	671	SER	2.4
1	C	402	ALA	2.4
1	D	571	LYS	2.4
1	D	392	ARG	2.4
1	C	36	ILE	2.4
1	D	342	SER	2.4
1	C	65	THR	2.4
1	C	82	GLY	2.4
1	D	19	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	169	GLU	2.4
1	C	54	SER	2.4
1	C	272	TRP	2.4
1	D	61	MET	2.4
1	B	37	LYS	2.4
1	B	229	LYS	2.4
1	C	165	ARG	2.4
1	B	224	LEU	2.4
1	C	212	LEU	2.4
1	D	102	GLU	2.4
1	B	683	GLY	2.4
1	D	599	GLN	2.4
1	D	647	GLN	2.4
1	D	148	ASP	2.4
1	D	694	PHE	2.4
1	D	726	ARG	2.4
1	C	15	PRO	2.4
1	C	324	TYR	2.3
1	C	406	TYR	2.3
1	D	81	TYR	2.3
1	C	218	ALA	2.3
1	D	446	GLU	2.3
1	B	690	GLY	2.3
1	C	259	GLY	2.3
1	D	656	GLY	2.3
1	D	32	ASP	2.3
1	D	562	LYS	2.3
1	C	129	SER	2.3
1	C	78	HIS	2.3
1	C	125	THR	2.3
1	D	722	THR	2.3
1	C	233	TYR	2.3
1	D	261	ASN	2.3
1	C	202	LEU	2.3
1	C	593	GLY	2.3
1	D	633	GLY	2.3
1	A	66	ASP	2.3
1	C	335	ASP	2.3
1	D	641	LYS	2.3
1	C	93	PHE	2.3
1	D	614	SER	2.3
1	C	38	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	145	THR	2.3
1	B	335	ASP	2.3
1	C	200	LEU	2.3
1	C	231	GLY	2.3
1	C	251	LEU	2.3
1	C	353	LEU	2.3
1	C	558	GLY	2.3
1	D	82	GLY	2.3
1	D	489	GLY	2.3
1	D	502	GLY	2.3
1	C	571	LYS	2.3
1	D	84	MET	2.3
1	D	122	MET	2.3
1	B	745	ILE	2.3
1	C	53	ILE	2.3
1	D	299	VAL	2.3
1	B	730	PRO	2.3
1	C	586	ALA	2.3
1	C	340	GLY	2.3
1	C	59	LEU	2.3
1	C	244	LEU	2.3
1	D	677	HIS	2.2
1	D	508	ILE	2.2
1	C	16	VAL	2.2
1	C	68	PRO	2.2
1	D	165	ARG	2.2
1	D	318	ASN	2.2
1	D	10	LYS	2.2
1	C	628	ASP	2.2
1	C	205	HIS	2.2
1	D	381	ARG	2.2
1	D	255	LYS	2.2
1	D	672	ASN	2.2
1	D	674	GLU	2.2
1	D	78	HIS	2.2
1	C	616	TYR	2.2
1	C	290	TRP	2.2
1	B	728	LYS	2.2
1	D	483	LYS	2.2
1	D	388	ASN	2.2
1	A	156	ASP	2.2
1	B	706	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	372	MET	2.2
1	C	160	GLU	2.2
1	C	92	ALA	2.2
1	C	96	LEU	2.2
1	B	737	SER	2.2
1	D	86	ARG	2.2
1	D	30	LYS	2.2
1	A	672	ASN	2.2
1	B	41	ASN	2.2
1	C	159	ASP	2.2
1	C	334	PRO	2.1
1	C	162	ILE	2.1
1	D	146	ALA	2.1
1	D	300	ALA	2.1
1	D	507	ALA	2.1
1	C	214	ARG	2.1
1	A	671	SER	2.1
1	D	713	LYS	2.1
1	C	41	ASN	2.1
1	C	103	TYR	2.1
1	C	428	TYR	2.1
1	B	479	ASP	2.1
1	C	309	ASP	2.1
1	D	640	GLU	2.1
1	B	71	THR	2.1
1	B	735	THR	2.1
1	D	64	PRO	2.1
1	A	336	GLY	2.1
1	B	740	VAL	2.1
1	C	117	GLY	2.1
1	C	131	VAL	2.1
1	D	632	GLY	2.1
1	C	140	ALA	2.1
1	C	17	LEU	2.1
1	C	495	LYS	2.1
1	A	38	GLU	2.1
1	D	13	GLU	2.1
1	D	51	GLU	2.1
1	B	66	ASP	2.1
1	C	64	PRO	2.1
1	B	631	VAL	2.1
1	C	88	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	146	ALA	2.1
1	D	155	SER	2.1
1	D	418	GLU	2.1
1	D	156	ASP	2.1
1	D	420	GLN	2.1
1	C	346	THR	2.1
1	C	543	GLY	2.1
1	B	35	LYS	2.1
1	C	574	ILE	2.1
1	D	37	LYS	2.1
1	B	723	VAL	2.1
1	D	733	VAL	2.1
1	A	494	GLU	2.0
1	C	121	GLU	2.0
1	C	341	ALA	2.1
1	D	48	GLU	2.0
1	D	52	GLU	2.0
1	D	579	GLU	2.0
1	C	186	ASN	2.0
1	A	309	ASP	2.0
1	D	555	ASP	2.0
1	C	113	ARG	2.0
1	C	179	THR	2.0
1	C	80	TYR	2.0
1	D	8	GLY	2.0
1	D	593	GLY	2.0
1	C	276	ILE	2.0
1	B	758	VAL	2.0
1	C	623	VAL	2.0
1	C	69	SER	2.0
1	C	301	SER	2.0
1	C	441	TRP	2.0
1	B	628	ASP	2.0
1	C	75	THR	2.0
1	C	118	PRO	2.0
1	B	742	GLY	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EDO	A	810	4/4	0.73	0.27	63,88,90,104	0
6	EDO	C	806	4/4	0.77	0.25	74,77,86,98	0
7	CAC	A	812	5/5	0.77	0.21	46,62,135,159	0
6	EDO	A	811	4/4	0.82	0.22	47,48,52,86	0
3	MG	C	802	1/1	0.84	0.14	72,72,72,72	0
5	ACT	B	806	4/4	0.86	0.22	48,52,60,77	0
6	EDO	B	809	4/4	0.86	0.22	55,61,62,70	0
5	ACT	A	806	4/4	0.87	0.18	53,56,64,67	0
6	EDO	A	809	4/4	0.88	0.18	72,74,74,77	0
6	EDO	B	807	4/4	0.89	0.17	42,46,49,50	0
5	ACT	C	805	4/4	0.89	0.17	60,67,68,70	0
6	EDO	B	808	4/4	0.91	0.14	31,38,44,57	0
5	ACT	A	805	4/4	0.91	0.16	31,40,50,56	0
5	ACT	B	805	4/4	0.92	0.15	33,44,46,64	0
6	EDO	A	808	4/4	0.94	0.13	66,69,75,79	0
6	EDO	A	807	4/4	0.95	0.09	24,25,31,32	0
3	MG	A	802	1/1	0.95	0.07	50,50,50,50	0
3	MG	B	802	1/1	0.96	0.05	56,56,56,56	0
4	CA	C	803	1/1	0.97	0.06	51,51,51,51	0
4	CA	B	804	1/1	0.98	0.04	46,46,46,46	0
2	MN	C	801	1/1	0.98	0.05	51,51,51,51	0
4	CA	C	804	1/1	0.98	0.05	45,45,45,45	0
4	CA	A	804	1/1	0.99	0.02	29,29,29,29	0
4	CA	B	803	1/1	0.99	0.02	30,30,30,30	0
2	MN	B	801	1/1	0.99	0.02	28,28,28,28	0
4	CA	A	803	1/1	0.99	0.02	26,26,26,26	0
2	MN	A	801	1/1	1.00	0.02	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.