Full wwPDB X-ray Structure Validation Report (i)

Dec 7, 2023 – 10:34 pm GMT

PDB ID	:	1O7J
Title	:	Atomic resolution structure of Erwinia chrysanthemi L-asparaginase
Authors	:	Lubkowski, J.; Dauter, M.; Aghaiypour, K.; Wlodawer, A.; Dauter, Z.
Deposited on	:	2002-11-07
Resolution	:	1.00 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 (i) 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 (i)) were used in the production of this report:

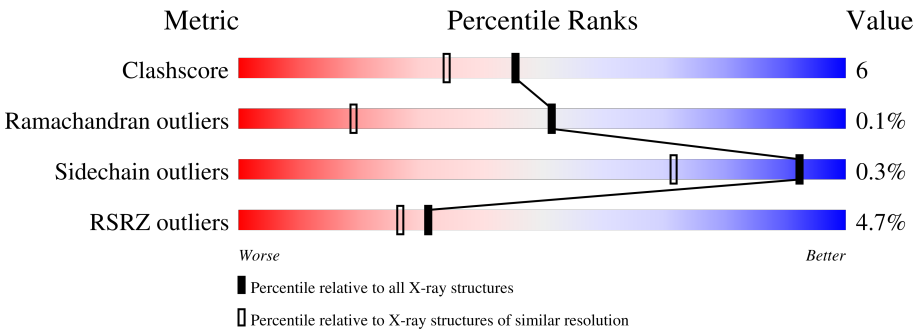
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.00 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))
Clashscore	141614	1117 (1.06-0.94)
Ramachandran outliers	138981	1043 (1.06-0.94)
Sidechain outliers	138945	1045 (1.06-0.94)
RSRZ outliers	127900	1023 (1.06-0.94)

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 <=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	327	6% 88% 10% ••
1	B	327	4% 87% 12% ••
1	C	327	4% 91% 8% ••
1	D	327	5% 91% 8% ••

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
4	EDO	A	1335	-	-	X	-
4	EDO	B	1331	-	-	X	-
4	EDO	B	1332	-	-	X	-
4	EDO	D	1331	-	-	X	-
4	EDO	D	1333	-	-	X	-
4	EDO	D	1334	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 20944 atoms, of which 9378 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.

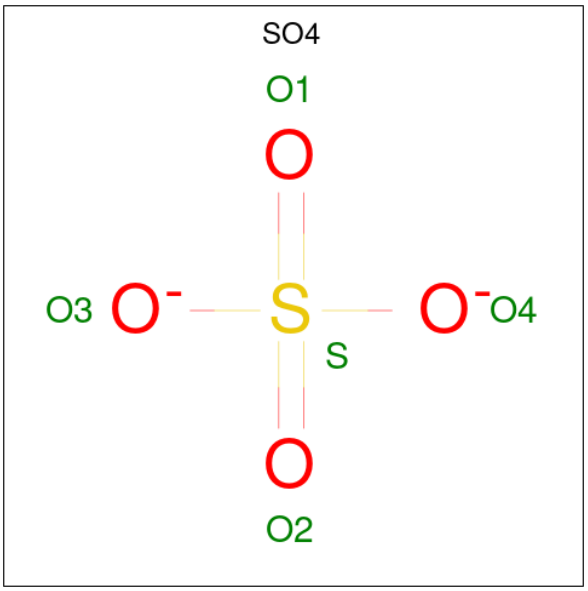
- Molecule 1 is a protein called L-ASPARAGINASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	325	4862	1600	2326	445	480	11	28	20	0
1	B	325	4881	1585	2366	436	484	10	47	18	0
1	C	325	4871	1586	2348	450	478	9	36	17	0
1	D	325	4879	1600	2338	446	486	9	80	21	0

There are 16 discrepancies between the modelled and reference sequences:

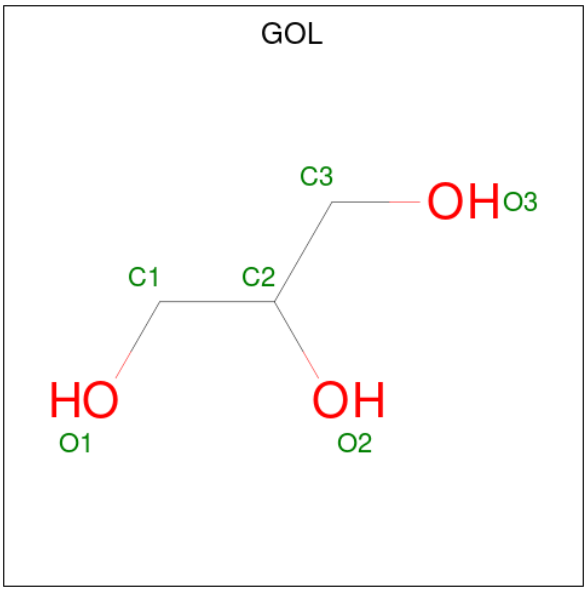
Chain	Residue	Modelled	Actual	Comment	Reference
A	156	ILE	LEU	variant	UNP P06608
A	178	ARG	LYS	variant	UNP P06608
A	267	LEU	MET	variant	UNP P06608
A	274	MET	ILE	variant	UNP P06608
B	156	ILE	LEU	variant	UNP P06608
B	178	ARG	LYS	variant	UNP P06608
B	267	LEU	MET	variant	UNP P06608
B	274	MET	ILE	variant	UNP P06608
C	156	ILE	LEU	variant	UNP P06608
C	178	ARG	LYS	variant	UNP P06608
C	267	LEU	MET	variant	UNP P06608
C	274	MET	ILE	variant	UNP P06608
D	156	ILE	LEU	variant	UNP P06608
D	178	ARG	LYS	variant	UNP P06608
D	267	LEU	MET	variant	UNP P06608
D	274	MET	ILE	variant	UNP P06608

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



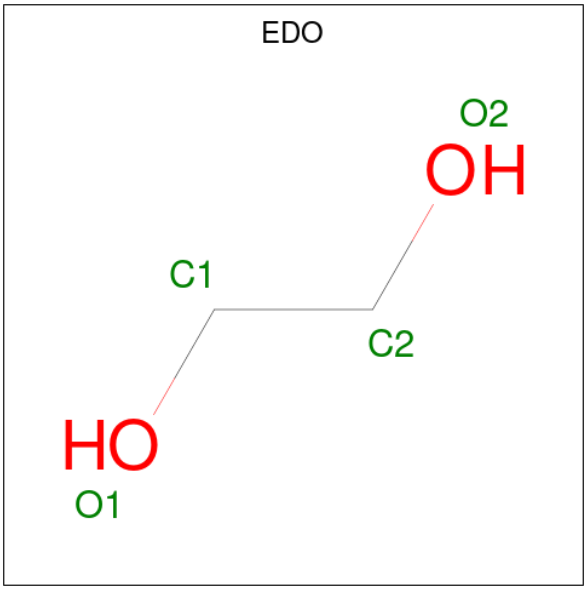
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
2	A	1	5	4	1		0	0
			Total	O	S			
2	A	1	5	4	1		0	0
			Total	O	S			
2	B	1	5	4	1		0	0
			Total	O	S			
2	B	1	5	4	1		0	0
			Total	O	S			
2	C	1	5	4	1		0	0
			Total	O	S			
2	C	1	5	4	1		0	0
			Total	O	S			
2	D	1	5	4	1		0	0
			Total	O	S			
2	D	1	5	4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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

- Molecule 5 is water.

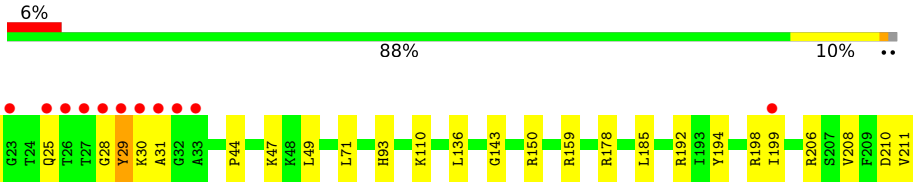
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	348	348	348	0	0
			Total	O		
5	B	310	310	310	0	0
			Total	O		
5	C	355	355	355	0	0
			Total	O		
5	D	347	347	347	0	0

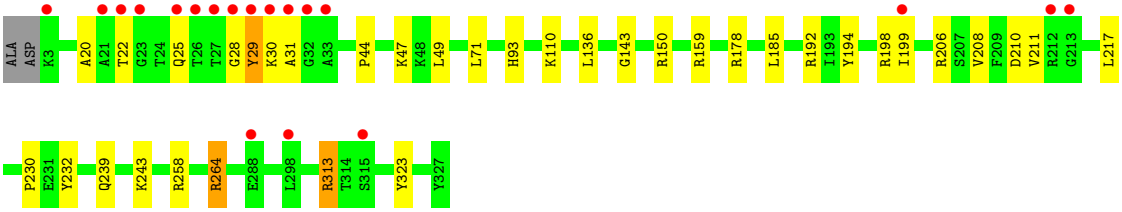
3 Residue-property plots (i)

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: L-ASPARAGINASE

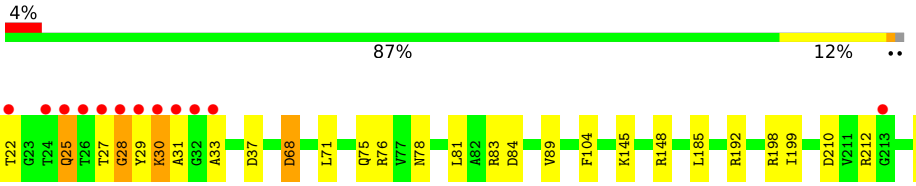
Chain A:

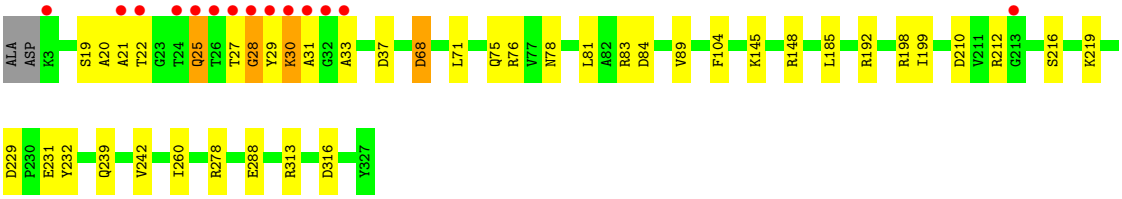




• Molecule 1: L-ASPARAGINASE

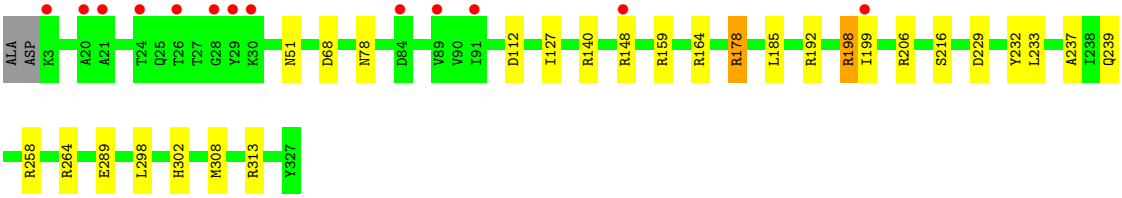
Chain B:





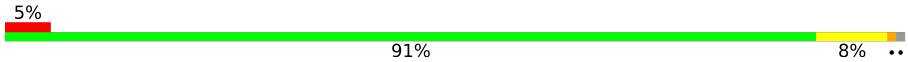
• Molecule 1: L-ASPARAGINASE

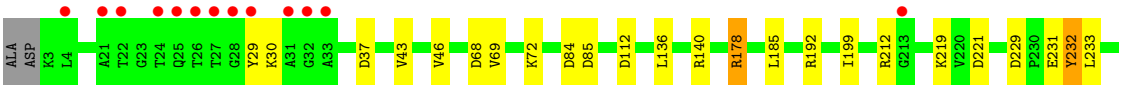
Chain C:



• Molecule 1: L-ASPARAGINASE

Chain D:





Q239
R258
K265
E288
R304
M308
Y323
Y327

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	106.38Å 90.35Å 127.59Å 90.00° 91.40° 90.00°	Depositor
Resolution (Å)	10.00 – 1.00 24.76 – 1.00	Depositor EDS
% Data completeness (in resolution range)	85.6 (10.00-1.00) 82.2 (24.76-1.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.00 (at 1.00Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.110 , 0.128 0.120 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	8.8	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.45 , 60.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.011 for -h,-k,l	Xtriage
F_o,F_c correlation	0.99	EDS
Total number of atoms	20944	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: EDO, SO4, 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	0.74	0/2653	1.27	24/3594 (0.7%)
1	B	0.75	0/2636	1.25	27/3574 (0.8%)
1	C	0.72	1/2636 (0.0%)	1.29	26/3571 (0.7%)
1	D	0.72	0/2662	1.17	26/3606 (0.7%)
All	All	0.74	1/10587 (0.0%)	1.24	103/14345 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	216	SER	CB-OG	-5.50	1.35	1.42

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	198	ARG	NE-CZ-NH1	18.91	129.75	120.30
1	C	198[A]	ARG	NE-CZ-NH1	16.29	128.44	120.30
1	C	198[B]	ARG	NE-CZ-NH1	16.29	128.44	120.30
1	C	192	ARG	NE-CZ-NH2	-14.28	113.16	120.30
1	A	198	ARG	NE-CZ-NH2	-13.24	113.68	120.30
1	B	192	ARG	NE-CZ-NH2	-11.55	114.53	120.30
1	A	198	ARG	CD-NE-CZ	11.15	139.20	123.60
1	D	140	ARG	NE-CZ-NH1	-9.98	115.31	120.30
1	B	198	ARG	NE-CZ-NH1	9.93	125.26	120.30
1	B	37	ASP	CB-CG-OD1	9.40	126.76	118.30
1	C	313[A]	ARG	NE-CZ-NH2	-9.39	115.60	120.30
1	C	313[B]	ARG	NE-CZ-NH2	-9.39	115.60	120.30
1	A	192	ARG	NE-CZ-NH2	-8.89	115.85	120.30
1	C	140	ARG	NE-CZ-NH1	-8.68	115.96	120.30
1	C	308	MET	CG-SD-CE	-8.62	86.41	100.20
1	B	76	ARG	NE-CZ-NH2	-8.45	116.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	258	ARG	NE-CZ-NH2	-8.35	116.13	120.30
1	B	148	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	B	68	ASP	CB-CG-OD2	-8.30	110.83	118.30
1	A	178	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	D	37	ASP	CB-CG-OD1	8.04	125.54	118.30
1	B	68	ASP	CB-CG-OD1	8.04	125.53	118.30
1	C	206[A]	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	C	206[B]	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	C	206[A]	ARG	CD-NE-CZ	7.99	134.79	123.60
1	C	206[B]	ARG	CD-NE-CZ	7.99	134.79	123.60
1	C	178[A]	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	C	178[B]	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	B	278	ARG	NE-CZ-NH2	7.81	124.21	120.30
1	A	323	TYR	CB-CG-CD1	7.70	125.62	121.00
1	A	178	ARG	CD-NE-CZ	-7.62	112.93	123.60
1	B	288	GLU	OE1-CD-OE2	7.59	132.40	123.30
1	A	264[A]	ARG	NE-CZ-NH1	-7.46	116.57	120.30
1	A	264[B]	ARG	NE-CZ-NH1	-7.46	116.57	120.30
1	C	229	ASP	CB-CG-OD1	7.33	124.90	118.30
1	A	29	TYR	CZ-CE2-CD2	7.24	126.31	119.80
1	B	313	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	C	159	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	D	178	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	B	229	ASP	CB-CG-OD1	6.92	124.53	118.30
1	A	323	TYR	CB-CG-CD2	-6.83	116.90	121.00
1	C	198[A]	ARG	NH1-CZ-NH2	-6.75	111.97	119.40
1	C	198[B]	ARG	NH1-CZ-NH2	-6.75	111.97	119.40
1	A	159	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	B	104	PHE	CB-CG-CD1	6.63	125.44	120.80
1	D	112	ASP	CB-CG-OD2	6.62	124.26	118.30
1	B	192	ARG	CD-NE-CZ	6.62	132.87	123.60
1	B	148	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	A	178	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	B	148	ARG	CD-NE-CZ	-6.47	114.55	123.60
1	D	178	ARG	CD-NE-CZ	-6.39	114.66	123.60
1	A	313[A]	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	313[B]	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	D	192[A]	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	D	192[B]	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	B	278	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	D	84	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	D	192[A]	ARG	NE-CZ-NH2	-6.27	117.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	192[B]	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	A	150	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	D	304	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	C	178[A]	ARG	CD-NE-CZ	-6.17	114.96	123.60
1	C	178[B]	ARG	CD-NE-CZ	-6.17	114.96	123.60
1	D	229	ASP	CB-CG-OD1	6.15	123.83	118.30
1	A	258	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	C	159	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	B	71[A]	LEU	CB-CA-C	6.01	121.61	110.20
1	B	71[B]	LEU	CB-CA-C	6.01	121.61	110.20
1	B	28	GLY	C-N-CA	5.98	136.64	121.70
1	D	140	ARG	NH1-CZ-NH2	5.92	125.92	119.40
1	A	29	TYR	CG-CD2-CE2	-5.87	116.60	121.30
1	A	210	ASP	CB-CG-OD1	5.68	123.41	118.30
1	D	258	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	A	192	ARG	CD-NE-CZ	5.58	131.41	123.60
1	B	231[A]	GLU	OE1-CD-OE2	5.55	129.96	123.30
1	B	231[B]	GLU	OE1-CD-OE2	5.55	129.96	123.30
1	B	83	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	D	212[A]	ARG	C-N-CA	5.50	133.86	122.30
1	D	212[B]	ARG	C-N-CA	5.50	133.86	122.30
1	C	192	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	D	29	TYR	CG-CD1-CE1	-5.47	116.93	121.30
1	A	93	HIS	CA-CB-CG	5.40	122.79	113.60
1	C	148	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	C	229	ASP	CB-CG-OD2	-5.38	113.45	118.30
1	D	308	MET	CG-SD-CE	-5.38	91.59	100.20
1	C	68	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	31	ALA	CA-C-N	5.35	126.90	116.20
1	A	29	TYR	CA-CB-CG	-5.33	103.27	113.40
1	D	232[A]	TYR	CB-CG-CD1	5.31	124.18	121.00
1	D	232[B]	TYR	CB-CG-CD1	5.31	124.18	121.00
1	D	229	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	C	258	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	D	112	ASP	CB-CG-OD1	-5.19	113.63	118.30
1	D	29	TYR	CA-CB-CG	-5.17	103.57	113.40
1	B	316[A]	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	316[B]	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	31	ALA	O-C-N	-5.14	114.47	123.20
1	A	194	TYR	CB-CG-CD1	5.11	124.07	121.00
1	B	210[A]	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	B	210[B]	ASP	CB-CG-OD2	-5.09	113.72	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	323	TYR	CB-CG-CD1	5.08	124.05	121.00
1	D	323	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	D	85	ASP	CB-CG-OD2	-5.03	113.78	118.30

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	2536	2326	2582	39	2
1	B	2515	2366	2540	32	3
1	C	2523	2348	2571	21	0
1	D	2541	2338	2575	41	0
2	A	10	0	0	0	0
2	B	10	0	0	1	0
2	C	10	0	0	0	0
2	D	10	0	0	1	0
3	A	6	0	8	0	0
3	D	6	0	8	0	0
4	A	16	0	14	14	0
4	B	10	0	10	8	0
4	D	13	0	12	21	0
5	A	348	0	0	9	4
5	B	310	0	0	8	5
5	C	355	0	0	8	2
5	D	347	0	0	6	3
All	All	11566	9378	10320	132	11

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 6.

All (132) 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:C:78:ASN:ND2	5:C:2097:HOH:O	1.65	1.29
1:B:19:SER:O	1:B:30:LYS:HE2	1.34	1.27
1:B:75[A]:GLN:HG3	5:B:2073:HOH:O	1.30	1.26
2:B:1329:SO4:O3	5:B:2307:HOH:O	1.63	1.13
1:D:72:LYS:HZ1	4:D:1334:EDO:H22	1.08	1.07
1:B:239:GLN:HG3	5:B:2233:HOH:O	1.53	1.06
1:C:51[A]:ASN:OD1	5:C:2066:HOH:O	1.76	1.02
1:D:72:LYS:NZ	4:D:1334:EDO:H22	1.80	0.97
1:A:243:LYS:HZ3	4:A:1334:EDO:H11	1.31	0.95
1:D:72:LYS:HZ3	4:D:1331:EDO:C2	1.78	0.95
1:B:212:ARG:HH11	4:B:1332:EDO:H11	1.29	0.94
1:D:72:LYS:NZ	4:D:1331:EDO:C2	2.32	0.92
1:D:72:LYS:HZ1	4:D:1334:EDO:C2	1.82	0.91
1:B:20:ALA:HB2	1:B:29:TYR:HB3	1.52	0.90
1:D:72:LYS:CE	4:D:1333:EDO:C1	2.49	0.90
1:D:72:LYS:CE	4:D:1333:EDO:H11	2.01	0.90
1:B:19:SER:O	1:B:30:LYS:CE	2.20	0.89
1:A:49:LEU:HD11	1:A:136[B]:LEU:CD1	2.04	0.88
1:D:72:LYS:HE3	4:D:1333:EDO:H11	1.58	0.85
1:D:46[A]:VAL:CG1	1:D:136[A]:LEU:HD23	2.07	0.85
1:D:232[B]:TYR:HD2	5:D:2278:HOH:O	1.62	0.82
1:B:78:ASN:HB3	4:B:1332:EDO:H12	1.61	0.81
1:D:46[A]:VAL:HG13	1:D:136[A]:LEU:HD23	1.60	0.81
1:A:49:LEU:CD1	1:A:136[B]:LEU:HD12	2.10	0.81
1:B:75[A]:GLN:CG	5:B:2073:HOH:O	2.00	0.81
1:D:72:LYS:NZ	4:D:1334:EDO:C2	2.41	0.80
1:C:232:TYR:CE1	1:C:233[B]:LEU:HD13	2.19	0.77
1:D:68[B]:ASP:OD1	5:D:2081:HOH:O	2.01	0.77
1:A:239[A]:GLN:HG3	5:A:2273:HOH:O	1.85	0.77
1:D:72:LYS:HE2	4:D:1333:EDO:O1	1.87	0.74
1:A:49:LEU:HD11	1:A:136[B]:LEU:HD11	1.69	0.73
1:D:69:VAL:HG22	4:D:1331:EDO:H11	1.71	0.72
1:A:49:LEU:HD11	1:A:136[B]:LEU:HD12	1.70	0.72
2:D:1329:SO4:O1	5:D:2344:HOH:O	2.09	0.70
1:D:232[B]:TYR:CD2	5:D:2278:HOH:O	2.40	0.69
1:A:264[B]:ARG:NH2	5:A:2284:HOH:O	2.23	0.69
1:D:233:LEU:HD12	5:D:2263:HOH:O	1.92	0.69
1:D:72:LYS:CE	4:D:1333:EDO:O1	2.41	0.69
1:D:72:LYS:HE2	4:D:1333:EDO:C1	2.21	0.68
1:B:212:ARG:NH1	4:B:1332:EDO:H11	2.07	0.67
1:B:212:ARG:HD2	4:B:1331:EDO:H11	1.77	0.67
1:B:68:ASP:OD1	5:B:2065:HOH:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75[B]:GLN:HE22	4:B:1331:EDO:H12	1.61	0.66
1:A:243:LYS:NZ	4:A:1335:EDO:C1	2.59	0.65
1:A:49:LEU:CD1	1:A:136[B]:LEU:CD1	2.71	0.65
1:D:46[A]:VAL:HG13	1:D:136[A]:LEU:CD2	2.26	0.65
1:A:49:LEU:HD12	1:A:136[B]:LEU:HD12	1.79	0.64
1:A:243:LYS:HZ3	4:A:1333:EDO:C2	2.11	0.64
1:A:243:LYS:HZ2	4:A:1335:EDO:C1	2.10	0.64
1:B:20:ALA:HB2	1:B:29:TYR:CB	2.25	0.64
1:B:185:LEU:HD21	1:B:199[B]:ILE:HG23	1.80	0.64
1:B:260[B]:ILE:HD11	5:B:2271:HOH:O	1.97	0.64
1:C:198[A]:ARG:NH2	5:C:2233:HOH:O	1.66	0.63
1:B:21:ALA:HB3	1:B:25:GLN:OE1	1.98	0.63
1:B:22:THR:OG1	1:B:25:GLN:HG2	1.99	0.62
1:B:232[B]:TYR:OH	1:D:219[B]:LYS:HE3	2.00	0.62
1:C:239:GLN:NE2	5:C:2278:HOH:O	2.33	0.61
1:A:243:LYS:NZ	4:A:1335:EDO:H12	2.14	0.61
1:A:28:GLY:HA3	5:A:2020:HOH:O	1.99	0.61
1:C:185:LEU:HD21	1:C:199[B]:ILE:HG23	1.82	0.60
1:D:46[A]:VAL:HG12	1:D:136[A]:LEU:HD23	1.82	0.60
1:B:145:LYS:HG2	5:B:2139:HOH:O	2.02	0.59
1:A:22:THR:HG23	1:A:25[A]:GLN:HE21	1.67	0.59
1:B:232[B]:TYR:OH	1:D:221:ASP:OD2	2.18	0.59
1:D:231[A]:GLU:OE2	1:D:265:LYS:NZ	2.35	0.59
1:B:30:LYS:O	1:B:30:LYS:CG	2.51	0.59
1:A:208[B]:VAL:HG22	1:A:313[B]:ARG:NH1	2.17	0.58
1:C:264[A]:ARG:NH2	5:C:2292:HOH:O	2.35	0.58
1:A:243:LYS:HD2	4:A:1335:EDO:H11	1.85	0.58
1:B:75[B]:GLN:HE22	4:B:1330:EDO:H11	1.68	0.58
1:A:232[B]:TYR:HD2	5:A:2265:HOH:O	1.88	0.57
1:D:185:LEU:HD21	1:D:199[B]:ILE:HG23	1.87	0.57
1:D:233:LEU:CD1	5:D:2263:HOH:O	2.50	0.57
4:A:1335:EDO:H22	5:A:2348:HOH:O	2.05	0.56
1:D:72:LYS:HZ1	4:D:1333:EDO:C2	2.18	0.56
1:D:72:LYS:HZ2	4:D:1331:EDO:C2	2.17	0.56
1:D:231[A]:GLU:OE2	1:D:265:LYS:CE	2.54	0.55
1:A:71[B]:LEU:HG	1:A:217:LEU:HD21	1.88	0.55
1:C:289:GLU:HG3	5:C:2311:HOH:O	2.06	0.55
1:D:72:LYS:HE2	4:D:1333:EDO:H11	1.79	0.54
1:D:72:LYS:NZ	4:D:1334:EDO:O2	2.41	0.54
1:D:72:LYS:NZ	4:D:1333:EDO:O1	2.42	0.53
1:A:30:LYS:O	1:A:30:LYS:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208[B]:VAL:HG22	1:A:313[B]:ARG:CZ	2.40	0.52
1:A:243:LYS:NZ	4:A:1335:EDO:H11	2.26	0.51
1:A:185:LEU:HD21	1:A:199[B]:ILE:HG23	1.92	0.51
1:C:112:ASP:OD1	5:C:2147:HOH:O	2.19	0.51
1:C:178[B]:ARG:HH22	1:D:178:ARG:NH2	2.09	0.51
1:A:208[B]:VAL:CG2	1:A:313[B]:ARG:CZ	2.89	0.50
1:A:71[B]:LEU:HD21	1:A:211:VAL:HB	1.93	0.50
1:A:20:ALA:HB2	1:A:29:TYR:HB3	1.93	0.50
1:D:69:VAL:CG2	4:D:1331:EDO:H11	2.41	0.49
1:A:110:LYS:NZ	5:A:2125:HOH:O	2.47	0.48
1:A:44:PRO:O	1:A:47:LYS:HG2	2.13	0.48
1:C:164:ARG:CZ	1:C:298[B]:LEU:CD2	2.92	0.48
4:A:1335:EDO:C2	5:A:2348:HOH:O	2.62	0.47
1:A:243:LYS:HZ2	4:A:1335:EDO:H12	1.75	0.47
1:D:43:VAL:O	1:D:46[A]:VAL:HG22	2.15	0.47
1:A:243:LYS:CD	4:A:1335:EDO:H11	2.45	0.46
1:C:164:ARG:NH2	1:C:298[B]:LEU:CD2	2.79	0.46
1:D:231[A]:GLU:OE2	1:D:265:LYS:HE2	2.16	0.45
1:A:232[A]:TYR:OH	1:C:237:ALA:HA	2.17	0.45
1:B:22:THR:OG1	1:B:25:GLN:CG	2.65	0.45
1:B:22:THR:H	1:B:25:GLN:HG3	1.82	0.45
1:A:243:LYS:NZ	4:A:1331:EDO:H12	2.31	0.44
1:D:72:LYS:NZ	4:D:1333:EDO:C1	2.80	0.44
1:A:22:THR:HG23	1:A:25[A]:GLN:NE2	2.30	0.44
1:A:22:THR:OG1	1:A:25[A]:GLN:HG3	2.17	0.44
1:A:143:GLY:HA3	5:A:2158:HOH:O	2.17	0.44
1:A:243:LYS:NZ	4:A:1334:EDO:H11	2.17	0.44
1:B:30:LYS:O	1:B:30:LYS:HG2	2.18	0.43
1:C:298[B]:LEU:HD12	1:C:302[B]:HIS:HB3	2.00	0.43
1:B:30:LYS:HG3	1:B:33:ALA:HB2	2.00	0.43
1:B:232[B]:TYR:OH	1:D:219[B]:LYS:CE	2.66	0.43
1:B:232[B]:TYR:HD2	5:B:2232:HOH:O	2.01	0.43
1:D:43:VAL:O	1:D:43:VAL:HG23	2.19	0.43
1:D:72:LYS:HE3	4:D:1333:EDO:C1	2.28	0.43
1:C:164:ARG:CZ	1:C:298[B]:LEU:HD21	2.49	0.42
1:A:239[A]:GLN:NE2	5:A:2271:HOH:O	2.52	0.42
1:C:198[A]:ARG:NE	5:C:2233:HOH:O	2.50	0.42
1:A:230:PRO:HB2	1:A:232[A]:TYR:CD2	2.55	0.42
1:A:243:LYS:HZ3	4:A:1335:EDO:H12	1.84	0.41
1:B:27:THR:O	1:B:27:THR:OG1	2.33	0.41
1:B:212:ARG:HH11	4:B:1331:EDO:H11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1331:EDO:H11	4:B:1332:EDO:H11	1.89	0.41
1:C:127:ILE:HD13	1:D:136[A]:LEU:CD1	2.50	0.40
1:C:178[B]:ARG:HH11	1:C:178[B]:ARG:HD3	1.69	0.40
1:B:81:LEU:HD21	1:B:89[B]:VAL:HG13	2.03	0.40
1:B:219[A]:LYS:HG2	1:B:242:VAL:HG12	2.04	0.40

All (11) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:2211:HOH:O	5:B:2212:HOH:O[2_655]	1.32	0.88
5:A:2107:HOH:O	5:C:2253:HOH:O[4_556]	1.35	0.85
5:B:2250:HOH:O	5:D:2243:HOH:O[4_545]	1.56	0.64
1:B:216:SER:HG	1:B:216:SER:HG[2_655]	1.10	0.50
5:A:2222:HOH:O	5:B:2083:HOH:O[3_455]	1.73	0.47
5:A:2004:HOH:O	5:C:2039:HOH:O[3_555]	1.77	0.43
1:A:206:ARG:NH2	1:B:84:ASP:O[3_455]	1.81	0.39
1:A:206:ARG:HH21	1:B:84:ASP:O[3_455]	1.31	0.29
5:B:2080:HOH:O	5:D:2241:HOH:O[3_545]	1.99	0.21
5:A:2222:HOH:O	5:B:2019:HOH:O[3_455]	2.02	0.18
5:D:2098:HOH:O	5:D:2251:HOH:O[2_555]	2.13	0.07

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	343/327 (105%)	335 (98%)	8 (2%)	0	100	100
1	B	341/327 (104%)	328 (96%)	12 (4%)	1 (0%)	41	14
1	C	340/327 (104%)	333 (98%)	7 (2%)	0	100	100
1	D	344/327 (105%)	337 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1368/1308 (105%)	1333 (97%)	34 (2%)	1 (0%)	51 19

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	28	GLY

5.3.2 Protein sidechains (i)

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	282/264 (107%)	282 (100%)	0	100 100
1	B	280/264 (106%)	278 (99%)	2 (1%)	84 58
1	C	279/264 (106%)	279 (100%)	0	100 100
1	D	282/264 (107%)	281 (100%)	1 (0%)	91 70
All	All	1123/1056 (106%)	1120 (100%)	3 (0%)	92 71

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	25	GLN
1	B	30	LYS
1	D	30	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	239	GLN

5.3.3 RNA (i)

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)

22 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	EDO	A	1335	4	3,3,3	0.58	0	2,2,2	0.24	0
2	SO4	B	1328	-	4,4,4	0.62	0	6,6,6	0.46	0
4	EDO	B	1330	4	2,2,3	0.50	0	1,1,2	0.06	0
2	SO4	C	1329	-	4,4,4	0.35	0	6,6,6	0.50	0
4	EDO	A	1331	4	2,2,3	0.48	0	1,1,2	0.18	0
4	EDO	D	1331	4	2,2,3	0.52	0	1,1,2	0.15	0
3	GOL	A	1330	-	5,5,5	0.71	0	5,5,5	0.44	0
4	EDO	D	1334	4	3,3,3	0.61	0	2,2,2	0.45	0
2	SO4	B	1329	-	4,4,4	0.93	0	6,6,6	1.81	3 (50%)
4	EDO	D	1332	4	2,2,3	0.30	0	1,1,2	0.60	0
2	SO4	C	1328	-	4,4,4	0.35	0	6,6,6	0.27	0
4	EDO	B	1332	4	3,3,3	0.56	0	2,2,2	0.26	0
4	EDO	A	1333	4	2,2,3	0.33	0	1,1,2	0.14	0
3	GOL	D	1330	-	5,5,5	0.48	0	5,5,5	1.06	1 (20%)
4	EDO	B	1331	4	2,2,3	0.57	0	1,1,2	0.00	0
2	SO4	A	1329	-	4,4,4	0.94	0	6,6,6	1.16	1 (16%)
2	SO4	A	1328	-	4,4,4	0.46	0	6,6,6	0.45	0
4	EDO	D	1333	4	2,2,3	0.50	0	1,1,2	0.07	0
2	SO4	D	1328	-	4,4,4	0.53	0	6,6,6	0.31	0
2	SO4	D	1329	-	4,4,4	0.99	0	6,6,6	1.01	0
4	EDO	A	1332	4	2,2,3	0.65	0	1,1,2	0.34	0
4	EDO	A	1334	4	2,2,3	0.12	0	1,1,2	1.11	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
3	GOL	A	1330	-	-	0/4/4/4	-
4	EDO	A	1335	4	-	1/1/1/1	-
4	EDO	B	1332	4	-	0/1/1/1	-
4	EDO	D	1334	4	-	1/1/1/1	-
3	GOL	D	1330	-	-	1/4/4/4	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1329	SO4	O4-S-O3	-2.79	97.14	109.06
2	B	1329	SO4	O4-S-O2	-2.43	96.63	109.31
2	A	1329	SO4	O3-S-O2	-2.41	96.73	109.31
2	B	1329	SO4	O3-S-O2	2.19	120.72	109.31
3	D	1330	GOL	O2-C2-C3	2.03	118.07	109.12

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1334	EDO	O1-C1-C2-O2
4	A	1335	EDO	O1-C1-C2-O2
3	D	1330	GOL	O2-C2-C3-O3

There are no ring outliers.

12 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1335	EDO	10	0
4	B	1330	EDO	1	0
4	A	1331	EDO	1	0
4	D	1331	EDO	5	0
4	D	1334	EDO	5	0
2	B	1329	SO4	1	0
4	B	1332	EDO	4	0
4	A	1333	EDO	1	0
4	B	1331	EDO	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1333	EDO	11	0
2	D	1329	SO4	1	0
4	A	1334	EDO	2	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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	325/327 (99%)	0.51	19 (5%)	23	22	7, 11, 27, 46	5 (1%)
1	B	325/327 (99%)	0.57	14 (4%)	35	29	7, 11, 27, 59	7 (2%)
1	C	325/327 (99%)	0.46	13 (4%)	38	31	7, 11, 21, 40	4 (1%)
1	D	325/327 (99%)	0.46	15 (4%)	32	27	7, 11, 23, 44	8 (2%)
All	All	1300/1308 (99%)	0.50	61 (4%)	31	26	7, 11, 25, 59	24 (1%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	29	TYR	9.9
1	B	27	THR	8.9
1	B	30	LYS	8.8
1	B	26	THR	8.5
1	B	28	GLY	7.0
1	B	21	ALA	6.6
1	B	25	GLN	6.6
1	A	31	ALA	5.9
1	A	28	GLY	5.6
1	D	28	GLY	5.4
1	A	29	TYR	5.4
1	A	26	THR	5.4
1	B	22	THR	5.3
1	B	33	ALA	5.3
1	B	24	THR	4.9
1	B	32	GLY	4.7
1	C	26	THR	4.7
1	D	21	ALA	4.6
1	A	30	LYS	4.4
1	A	32	GLY	4.0
1	A	33	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	27	THR	3.5
1	B	3	LYS	3.5
1	D	29	TYR	3.4
1	A	21	ALA	3.4
1	A	315	SER	3.3
1	D	33	ALA	3.2
1	D	22	THR	3.2
1	B	31	ALA	3.1
1	A	22	THR	3.1
1	D	4	LEU	3.0
1	A	3	LYS	2.9
1	C	3	LYS	2.9
1	C	89[A]	VAL	2.9
1	D	288	GLU	2.8
1	D	26	THR	2.8
1	D	27	THR	2.8
1	A	288	GLU	2.8
1	D	31	ALA	2.7
1	C	20	ALA	2.6
1	C	29	TYR	2.6
1	D	213[A]	GLY	2.6
1	C	148	ARG	2.5
1	D	24	THR	2.5
1	A	23	GLY	2.3
1	C	28	GLY	2.3
1	C	24	THR	2.3
1	A	25[A]	GLN	2.3
1	B	213	GLY	2.3
1	C	84	ASP	2.3
1	C	21	ALA	2.2
1	A	213	GLY	2.2
1	A	298[A]	LEU	2.2
1	D	25	GLN	2.2
1	D	32	GLY	2.2
1	D	239	GLN	2.2
1	C	30	LYS	2.2
1	A	199[A]	ILE	2.1
1	C	91[A]	ILE	2.0
1	A	212	ARG	2.0
1	C	199[A]	ILE	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
4	EDO	D	1333	3/4	0.30	0.31	56,56,58,60	0
4	EDO	D	1332	3/4	0.38	0.21	47,47,47,50	0
4	EDO	D	1334	4/4	0.55	0.27	59,60,61,61	0
4	EDO	D	1331	3/4	0.78	0.33	51,51,53,64	0
4	EDO	A	1331	3/4	0.80	0.13	28,28,37,46	0
4	EDO	B	1332	4/4	0.83	0.16	20,23,31,57	0
4	EDO	A	1335	4/4	0.86	0.18	28,38,39,43	0
4	EDO	A	1333	3/4	0.86	0.11	20,20,25,25	0
4	EDO	A	1334	3/4	0.86	0.12	24,24,29,29	0
3	GOL	D	1330	6/6	0.90	0.20	12,24,27,28	0
4	EDO	B	1331	3/4	0.91	0.16	20,20,26,28	0
4	EDO	B	1330	3/4	0.91	0.19	22,22,26,38	0
2	SO4	C	1329	5/5	0.92	0.25	19,19,40,40	0
2	SO4	D	1329	5/5	0.92	0.20	20,25,39,49	0
2	SO4	A	1329	5/5	0.93	0.19	19,27,51,52	0
4	EDO	A	1332	3/4	0.93	0.10	16,16,23,25	0
2	SO4	B	1329	5/5	0.94	0.13	21,24,27,31	0
3	GOL	A	1330	6/6	0.97	0.10	11,13,15,16	0
2	SO4	D	1328	5/5	0.99	0.08	8,9,10,11	0
2	SO4	A	1328	5/5	0.99	0.09	8,9,10,11	0
2	SO4	C	1328	5/5	0.99	0.08	9,9,10,11	0
2	SO4	B	1328	5/5	0.99	0.07	9,9,10,11	0

6.5 Other polymers (i)

There are no such residues in this entry.