



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 01:08 AM UTC

PDB ID : 3N1X / pdb_00003n1x
Title : X-ray Crystal Structure of Toluene/o-Xylene Monooxygenase Hydroxylase
T201C Mutant
Authors : Sazinsky, M.H.; McCormick, M.S.; Lippard, S.J.
Deposited on : 2010-05-17
Resolution : 2.40 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

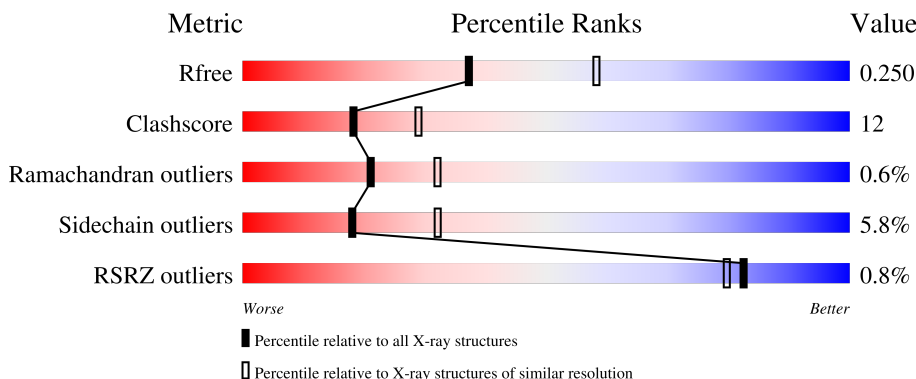
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	498	% 64% 28% 6% .
2	B	330	% 63% 29% 5% ..
3	C	86	55% 38% 5% ..

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7520 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 Toluene o-xylene monooxygenase component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	1	0
			4021	2567	673	754	27			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	CYS	THR	engineered mutation	UNP Q6IV66

- Molecule 2 is a protein called Toluene o-xylene monooxygenase component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	324	Total	C	N	O	S	0	0	0
			2658	1685	469	494	10			

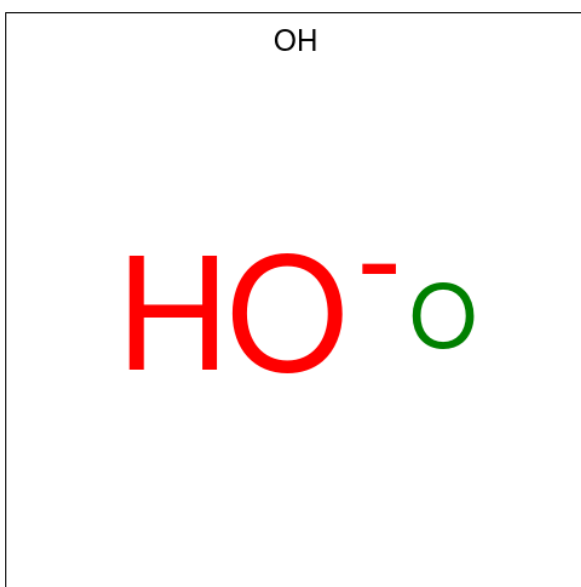
- Molecule 3 is a protein called Toluene o-xylene monooxygenase component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	85	Total	C	N	O	S	0	0	0
			689	432	123	129	5			

- Molecule 4 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Fe	0	0
			2	2		

- Molecule 5 is HYDROXIDE ION (CCD ID: OH) (formula: HO).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O		0	0
			1	1			

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	S	0	0
			5	4	1		

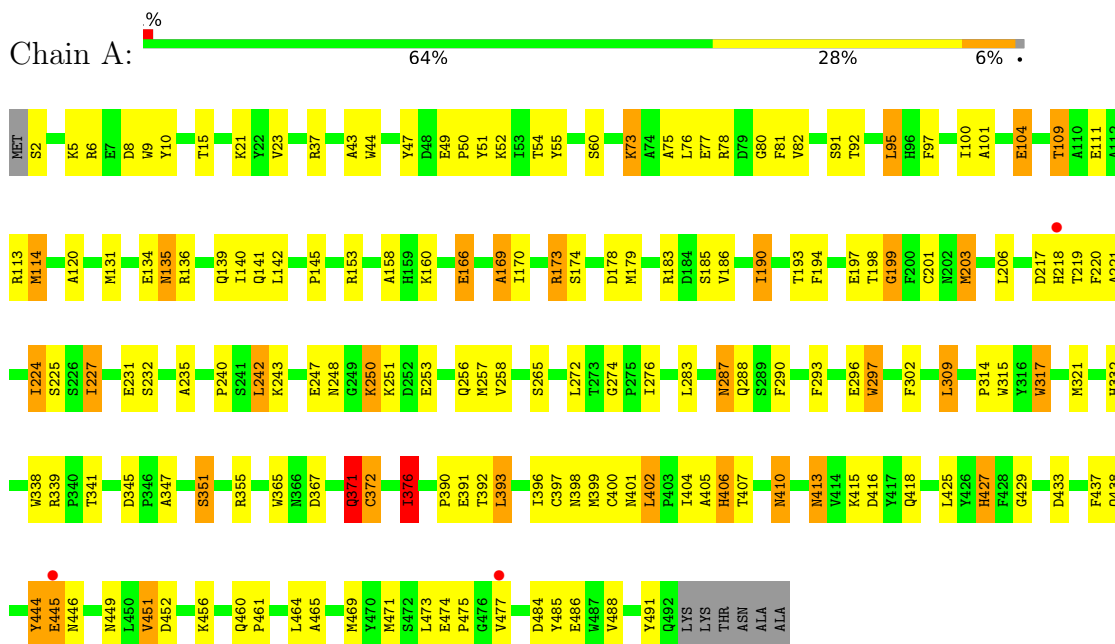
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	73	Total	O	0	0
			73	73		
8	B	62	Total	O	0	0
			62	62		
8	C	5	Total	O	0	0
			5	5		

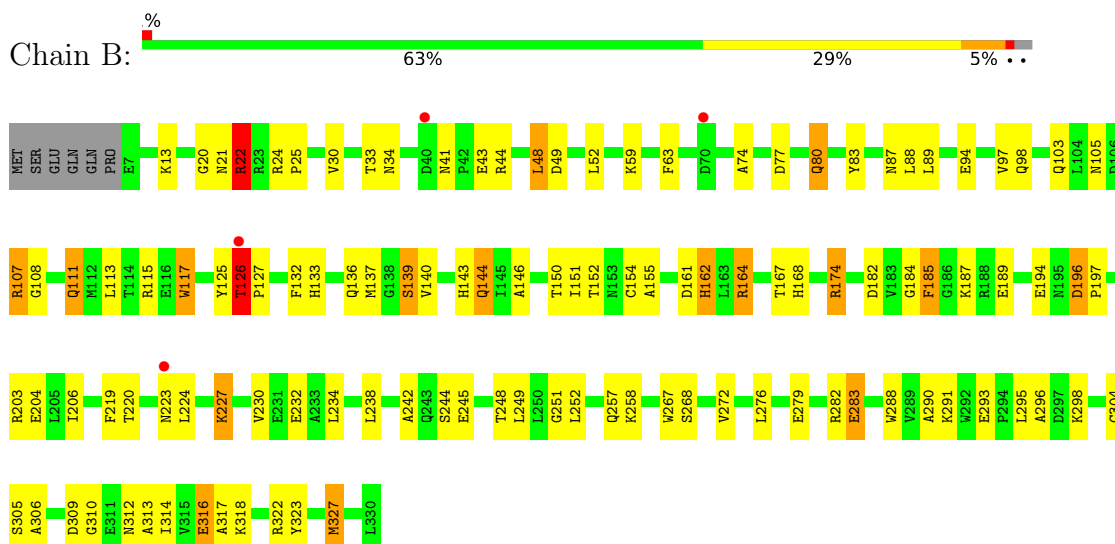
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

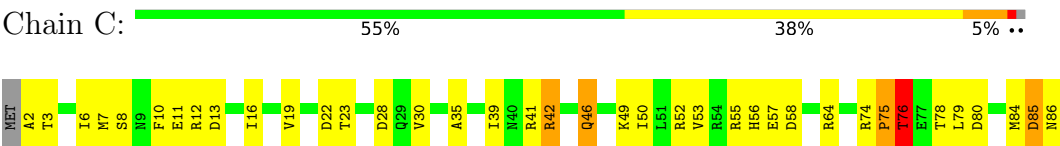
- Molecule 1: Toluene o-xylene monooxygenase component



- Molecule 2: Toluene o-xylene monooxygenase component



- Molecule 3: Toluene o-xylene monooxygenase component



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.29Å 183.29Å 68.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.02 – 2.40 38.02 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (38.02-2.40) 99.2 (38.02-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.90 (at 2.39Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.184 , 0.242 0.193 , 0.250	Depositor DCC
R_{free} test set	2592 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7520	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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: FE, EDO, SO4, OH

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	1.70	46/4148 (1.1%)	1.51	48/5637 (0.9%)
2	B	1.77	25/2730 (0.9%)	1.54	31/3711 (0.8%)
3	C	1.64	5/703 (0.7%)	1.54	7/952 (0.7%)
All	All	1.72	76/7581 (1.0%)	1.52	86/10300 (0.8%)

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	ALA	CA-CB	9.06	1.67	1.53
2	B	155	ALA	CA-CB	8.54	1.67	1.53
1	A	413	ASN	C-O	-8.08	1.17	1.24
2	B	74	ALA	CA-CB	7.36	1.66	1.53
1	A	451	VAL	CA-CB	7.27	1.62	1.54
2	B	162	HIS	CA-C	7.27	1.62	1.52
2	B	251	GLY	N-CA	7.26	1.54	1.45
1	A	60	SER	CA-C	7.20	1.61	1.52
1	A	402	LEU	CG-CD2	6.73	1.74	1.52
1	A	82	VAL	CA-CB	6.67	1.62	1.54
1	A	82	VAL	CA-C	6.65	1.60	1.52
1	A	75	ALA	CA-C	6.63	1.61	1.52
2	B	296	ALA	CA-CB	6.60	1.63	1.53
2	B	182	ASP	CB-CG	6.58	1.68	1.52
1	A	183	ARG	C-O	6.46	1.31	1.23
1	A	465	ALA	CA-CB	6.44	1.64	1.53
1	A	265	SER	C-O	6.38	1.31	1.24
1	A	392	THR	CA-CB	-6.36	1.45	1.53
1	A	73	LYS	N-CA	-6.29	1.38	1.46
1	A	198	THR	CA-CB	6.29	1.63	1.53
2	B	74	ALA	N-CA	6.26	1.54	1.46
1	A	169	ALA	CA-CB	6.23	1.63	1.53
2	B	146	ALA	CA-CB	6.20	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	25	PRO	C-O	-6.15	1.16	1.23
2	B	151	ILE	CA-C	6.08	1.60	1.52
2	B	306	ALA	C-O	-6.03	1.16	1.24
1	A	104	GLU	N-CA	5.98	1.53	1.46
1	A	315	TRP	C-O	-5.97	1.16	1.24
3	C	30	VAL	CA-CB	5.96	1.60	1.54
1	A	339	ARG	CA-C	5.90	1.60	1.52
1	A	111	GLU	N-CA	5.88	1.53	1.46
2	B	150	THR	CA-C	5.88	1.60	1.52
1	A	15	THR	CA-C	-5.87	1.47	1.53
1	A	372	CYS	C-O	5.80	1.30	1.24
2	B	139	SER	N-CA	5.80	1.53	1.46
1	A	160	LYS	C-O	-5.73	1.16	1.24
1	A	258	VAL	C-O	5.72	1.30	1.24
1	A	475	PRO	C-O	5.67	1.31	1.23
1	A	91	SER	N-CA	-5.67	1.39	1.46
1	A	256	GLN	CA-C	5.64	1.59	1.52
2	B	203	ARG	CD-NE	-5.63	1.38	1.46
2	B	30	VAL	N-CA	-5.61	1.39	1.46
2	B	316	GLU	N-CA	5.61	1.53	1.46
1	A	199	GLY	N-CA	5.60	1.52	1.45
2	B	48	LEU	C-O	5.60	1.30	1.24
1	A	55	TYR	C-O	-5.57	1.19	1.24
2	B	44	ARG	CB-CG	5.54	1.69	1.52
1	A	376	ILE	CA-CB	5.51	1.61	1.54
2	B	97	VAL	C-O	-5.45	1.17	1.24
1	A	288	GLN	CA-C	5.45	1.59	1.52
1	A	37	ARG	CA-C	5.42	1.60	1.53
2	B	185	PHE	CA-C	-5.40	1.46	1.52
2	B	167	THR	C-O	5.37	1.30	1.24
1	A	166	GLU	CA-C	5.33	1.59	1.52
1	A	114	MET	C-O	5.32	1.30	1.24
1	A	50	PRO	C-O	-5.28	1.17	1.24
2	B	290	ALA	C-O	-5.28	1.17	1.24
2	B	52	LEU	CG-CD2	5.27	1.70	1.52
1	A	433	ASP	N-CA	5.25	1.52	1.46
3	C	39	ILE	CA-CB	5.24	1.60	1.54
1	A	371	GLN	N-CA	5.23	1.52	1.46
1	A	242	LEU	CA-C	5.21	1.59	1.52
1	A	437	PHE	CE2-CZ	5.19	1.54	1.38
1	A	44	TRP	N-CA	5.14	1.52	1.46
3	C	19	VAL	CA-CB	-5.14	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	TYR	N-CA	5.14	1.52	1.46
3	C	53	VAL	CA-C	5.10	1.59	1.52
3	C	3	THR	C-O	-5.09	1.17	1.24
1	A	351	SER	CA-C	5.08	1.59	1.52
1	A	444	TYR	C-O	-5.08	1.17	1.24
1	A	427	HIS	CA-C	5.08	1.58	1.52
1	A	43	ALA	CA-CB	5.08	1.61	1.53
2	B	317	ALA	CA-CB	5.07	1.61	1.53
1	A	400	CYS	CA-C	5.02	1.59	1.52
1	A	135	ASN	C-O	5.00	1.29	1.24
2	B	323	TYR	C-O	5.00	1.30	1.24

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	227	LYS	CA-C-N	-11.78	106.33	119.28
2	B	227	LYS	C-N-CA	-11.78	106.33	119.28
1	A	49	GLU	CA-C-N	-11.29	108.24	119.64
1	A	49	GLU	C-N-CA	-11.29	108.24	119.64
1	A	190	ILE	CB-CA-C	-8.48	101.21	111.81
2	B	293	GLU	CA-C-N	-8.15	110.32	119.28
2	B	293	GLU	C-N-CA	-8.15	110.32	119.28
1	A	345	ASP	CA-C-N	-8.03	112.44	120.31
1	A	345	ASP	C-N-CA	-8.03	112.44	120.31
1	A	287	ASN	CB-CA-C	7.93	122.65	109.56
1	A	250	LYS	N-CA-C	7.80	122.85	112.25
1	A	407	THR	CA-C-N	7.73	129.51	119.84
1	A	407	THR	C-N-CA	7.73	129.51	119.84
2	B	196	ASP	CA-C-N	-7.56	110.96	119.28
2	B	196	ASP	C-N-CA	-7.56	110.96	119.28
1	A	198	THR	N-CA-C	-7.46	103.23	111.36
1	A	227	ILE	N-CA-C	-7.42	103.05	110.62
1	A	141	GLN	CA-CB-CG	-7.13	99.85	114.10
3	C	41	ARG	N-CA-C	-7.10	104.48	113.43
2	B	162	HIS	N-CA-C	-6.97	103.69	111.71
1	A	201	CYS	N-CA-C	6.89	118.79	111.28
1	A	170	ILE	N-CA-C	-6.87	103.51	111.00
1	A	438	GLN	N-CA-C	6.87	119.65	111.33
1	A	15	THR	N-CA-C	-6.75	99.53	109.11
1	A	142	LEU	N-CA-C	-6.60	104.87	113.12
2	B	251	GLY	N-CA-C	-6.60	104.85	112.50
2	B	194	GLU	N-CA-C	6.51	119.38	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	TRP	N-CA-C	6.40	118.79	111.11
2	B	87	ASN	N-CA-C	6.30	118.15	111.28
3	C	42	ARG	CG-CD-NE	-6.29	98.17	112.00
3	C	76	THR	N-CA-CB	-6.19	107.11	114.17
2	B	137	MET	N-CA-C	-6.05	104.76	111.36
1	A	158	ALA	N-CA-C	-6.03	104.78	111.71
1	A	179	MET	N-CA-C	5.93	118.70	111.82
2	B	234	LEU	CA-C-N	-5.93	110.95	121.81
2	B	234	LEU	C-N-CA	-5.93	110.95	121.81
2	B	313	ALA	N-CA-C	-5.90	104.93	111.36
1	A	153	ARG	NE-CZ-NH2	-5.87	113.92	119.20
2	B	146	ALA	N-CA-C	5.86	116.34	109.60
1	A	376	ILE	N-CA-C	-5.84	104.66	110.62
2	B	252	LEU	N-CA-C	5.82	117.70	111.36
2	B	291	LYS	N-CA-C	-5.80	104.92	112.23
2	B	103	GLN	CA-CB-CG	-5.75	102.60	114.10
1	A	248	ASN	O-C-N	-5.73	116.53	122.84
1	A	339	ARG	CA-C-N	-5.69	113.80	120.12
1	A	339	ARG	C-N-CA	-5.69	113.80	120.12
1	A	109	THR	N-CA-C	-5.66	104.72	111.69
1	A	224	ILE	CA-C-N	-5.66	111.71	121.66
1	A	224	ILE	C-N-CA	-5.66	111.71	121.66
1	A	77	GLU	N-CA-C	5.64	117.10	111.07
2	B	272	VAL	N-CA-C	-5.63	105.03	110.72
2	B	139	SER	N-CA-C	-5.63	106.25	113.23
3	C	75	PRO	CA-C-N	-5.58	116.57	126.45
3	C	75	PRO	C-N-CA	-5.58	116.57	126.45
2	B	80	GLN	CB-CA-C	-5.57	103.82	111.73
1	A	217	ASP	N-CA-C	5.54	118.20	108.56
1	A	257	MET	CG-SD-CE	-5.53	88.72	100.90
1	A	365	TRP	N-CA-C	5.53	117.75	111.11
1	A	253	GLU	N-CA-C	-5.51	105.28	111.28
2	B	108	GLY	N-CA-C	5.51	121.52	113.48
1	A	287	ASN	N-CA-C	-5.47	106.28	113.12
2	B	111	GLN	N-CA-C	5.44	117.97	111.71
2	B	230	VAL	CB-CA-C	-5.41	104.84	112.14
2	B	117	TRP	N-CA-C	5.35	116.80	111.07
3	C	46	GLN	CA-C-N	-5.33	115.39	120.83
3	C	46	GLN	C-N-CA	-5.33	115.39	120.83
1	A	248	ASN	CA-C-N	-5.33	109.30	121.19
1	A	248	ASN	C-N-CA	-5.33	109.30	121.19
2	B	224	LEU	CA-C-N	-5.33	117.69	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	224	LEU	C-N-CA	-5.33	117.69	123.08
1	A	131	MET	N-CA-C	-5.32	105.56	111.36
1	A	297	TRP	N-CA-C	5.31	119.91	113.38
1	A	173	ARG	NE-CZ-NH2	-5.28	114.45	119.20
2	B	283	GLU	CA-CB-CG	5.26	124.63	114.10
1	A	491	TYR	CA-C-N	5.22	131.09	121.70
1	A	491	TYR	C-N-CA	5.22	131.09	121.70
2	B	164	ARG	NE-CZ-NH1	-5.21	116.29	121.50
1	A	23	VAL	N-CA-C	-5.21	101.10	108.65
1	A	186	VAL	N-CA-C	-5.18	104.61	111.09
1	A	201	CYS	CA-CB-SG	-5.11	102.64	114.40
2	B	144	GLN	N-CA-C	-5.09	106.76	113.17
2	B	132	PHE	N-CA-C	-5.08	105.83	112.23
1	A	120	ALA	CA-C-N	5.06	125.09	119.32
1	A	120	ALA	C-N-CA	5.06	125.09	119.32
1	A	339	ARG	NE-CZ-NH2	5.05	123.74	119.20
1	A	339	ARG	NE-CZ-NH1	-5.04	116.47	121.50

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	4021	0	3770	94	0
2	B	2658	0	2554	69	0
3	C	689	0	678	30	0
4	A	2	0	0	0	0
5	A	1	0	0	1	0
6	A	4	0	6	0	0
7	B	5	0	0	0	0
8	A	73	0	0	1	0
8	B	62	0	0	0	0
8	C	5	0	0	0	0
All	All	7520	0	7008	174	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 12.

All (174) 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:402:LEU:CD2	1:A:402:LEU:CG	1.74	1.59
2:B:219:PHE:O	2:B:223:ASN:HB2	1.53	1.06
1:A:445:GLU:HG2	1:A:446:ASN:H	1.16	1.06
1:A:445:GLU:HG2	1:A:446:ASN:N	1.70	1.05
1:A:427:HIS:HE1	3:C:76:THR:HG23	1.22	1.04
1:A:445:GLU:CG	1:A:446:ASN:N	2.27	0.96
2:B:305:SER:HB3	2:B:314:ILE:HD11	1.52	0.90
2:B:126:THR:HB	2:B:189:GLU:CG	2.01	0.90
2:B:168:HIS:HD2	2:B:257:GLN:HE21	1.20	0.89
2:B:126:THR:OG1	2:B:127:PRO:HD3	1.72	0.88
1:A:139:GLN:HE22	2:B:83:TYR:H	1.19	0.88
1:A:372:CYS:O	1:A:376:ILE:HD13	1.75	0.85
1:A:474:GLU:O	1:A:477:VAL:HG22	1.76	0.84
1:A:427:HIS:CE1	3:C:76:THR:HG23	2.12	0.83
2:B:126:THR:HB	2:B:189:GLU:HG3	1.62	0.80
2:B:327:MET:HA	2:B:327:MET:CE	2.11	0.80
1:A:8:ASP:O	2:B:174:ARG:HD2	1.85	0.77
1:A:416:ASP:OD2	1:A:427:HIS:HD2	1.67	0.77
2:B:327:MET:HA	2:B:327:MET:HE2	1.66	0.77
1:A:76:LEU:CD1	1:A:218:HIS:HB2	2.14	0.76
2:B:168:HIS:CD2	2:B:257:GLN:HE21	2.05	0.75
1:A:445:GLU:HG2	2:B:49:ASP:OD1	1.85	0.75
3:C:2:ALA:HA	3:C:23:THR:OG1	1.86	0.73
1:A:2:SER:N	2:B:105:ASN:HD22	1.85	0.73
1:A:9:TRP:HB3	2:B:174:ARG:HG3	1.71	0.72
2:B:219:PHE:O	2:B:223:ASN:CB	2.37	0.70
2:B:162:HIS:HE1	2:B:227:LYS:NZ	1.91	0.69
2:B:126:THR:HG21	2:B:189:GLU:OE1	1.93	0.68
3:C:52:ARG:HH11	3:C:52:ARG:HG3	1.59	0.67
3:C:55:ARG:HD2	3:C:58:ASP:OD1	1.94	0.67
1:A:9:TRP:CB	2:B:174:ARG:HG3	2.24	0.67
2:B:162:HIS:HE1	2:B:227:LYS:HZ2	1.42	0.67
1:A:203:MET:HG3	1:A:297:TRP:HB3	1.78	0.66
3:C:56:HIS:HD2	3:C:80:ASP:OD1	1.79	0.65
1:A:367:ASP:HB3	1:A:410:ASN:ND2	2.12	0.65
3:C:75:PRO:O	3:C:76:THR:CB	2.45	0.65
3:C:75:PRO:O	3:C:76:THR:HB	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:LEU:CD2	1:A:402:LEU:CD1	2.70	0.64
1:A:398:ASN:HD22	1:A:427:HIS:H	1.45	0.64
2:B:21:ASN:O	2:B:22:ARG:HB2	1.98	0.63
2:B:59:LYS:HA	2:B:63:PHE:HD2	1.64	0.62
1:A:314:PRO:HD2	1:A:317:TRP:CE3	2.34	0.62
1:A:92:THR:HG23	1:A:276:ILE:HD13	1.80	0.62
1:A:474:GLU:H	1:A:477:VAL:CG2	2.13	0.62
1:A:402:LEU:CD2	1:A:402:LEU:CB	2.75	0.61
2:B:204:GLU:OE1	2:B:298:LYS:NZ	2.33	0.61
2:B:126:THR:HB	2:B:189:GLU:HG2	1.79	0.61
1:A:95:LEU:HD12	1:A:95:LEU:C	2.27	0.60
2:B:21:ASN:O	2:B:22:ARG:CB	2.50	0.59
2:B:126:THR:CB	2:B:127:PRO:HD3	2.33	0.59
2:B:143:HIS:CG	2:B:152:THR:HG23	2.37	0.59
3:C:75:PRO:O	3:C:76:THR:HG22	2.02	0.58
1:A:405:ALA:O	1:A:406:HIS:HB2	2.01	0.58
1:A:218:HIS:O	1:A:219:THR:C	2.46	0.58
1:A:243:LYS:O	1:A:247:GLU:HG3	2.05	0.57
1:A:317:TRP:O	1:A:321:MET:HG2	2.05	0.57
2:B:219:PHE:HE1	2:B:223:ASN:HD22	1.50	0.56
1:A:425:LEU:HD23	3:C:76:THR:HG22	1.87	0.56
3:C:11:GLU:HG2	3:C:12:ARG:HG3	1.88	0.56
1:A:139:GLN:NE2	2:B:83:TYR:H	1.97	0.56
2:B:33:THR:HB	2:B:34:ASN:HD22	1.71	0.56
1:A:97:PHE:CD2	1:A:145:PRO:HB3	2.40	0.55
1:A:231:GLU:OE1	5:A:501:OH:O	2.25	0.55
2:B:94:GLU:O	2:B:98:GLN:HG2	2.07	0.55
1:A:427:HIS:HE1	3:C:76:THR:CG2	2.08	0.55
1:A:95:LEU:HD11	1:A:272:LEU:HD22	1.87	0.55
1:A:413:ASN:OD1	1:A:415:LYS:HE2	2.08	0.54
2:B:126:THR:CG2	2:B:189:GLU:OE1	2.55	0.54
2:B:219:PHE:CE1	2:B:223:ASN:ND2	2.76	0.54
1:A:460:GLN:HA	1:A:461:PRO:C	2.33	0.53
1:A:190:ILE:HD12	1:A:242:LEU:CD2	2.38	0.53
1:A:444:TYR:O	1:A:445:GLU:C	2.53	0.52
3:C:52:ARG:HG3	3:C:52:ARG:NH1	2.23	0.52
1:A:485:TYR:O	1:A:488:VAL:HB	2.09	0.52
1:A:416:ASP:H	3:C:56:HIS:CE1	2.28	0.52
2:B:125:TYR:O	2:B:126:THR:C	2.50	0.52
2:B:161:ASP:O	2:B:164:ARG:HB3	2.11	0.51
2:B:305:SER:CB	2:B:314:ILE:HD11	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ARG:HH11	2:B:144:GLN:HE21	1.58	0.51
1:A:220:PHE:CE2	1:A:224:ILE:HG13	2.46	0.51
1:A:193:THR:HA	1:A:197:GLU:OE1	2.11	0.50
1:A:449:ASN:O	1:A:452:ASP:HB2	2.11	0.50
3:C:85:ASP:O	3:C:86:ASN:CB	2.59	0.50
2:B:127:PRO:HA	2:B:189:GLU:HB3	1.93	0.50
3:C:2:ALA:O	3:C:23:THR:N	2.42	0.50
2:B:107:ARG:O	2:B:107:ARG:HG3	2.12	0.50
3:C:2:ALA:O	3:C:22:ASP:HA	2.12	0.49
1:A:445:GLU:CG	2:B:49:ASP:OD1	2.60	0.49
3:C:75:PRO:O	3:C:76:THR:CG2	2.60	0.49
2:B:77:ASP:HB2	2:B:154:CYS:SG	2.53	0.49
2:B:232:GLU:OE2	2:B:258:LYS:NZ	2.46	0.49
3:C:50:ILE:N	3:C:84:MET:O	2.26	0.48
3:C:28:ASP:OD1	3:C:64:ARG:HB3	2.13	0.48
3:C:13:ASP:OD1	3:C:42:ARG:HD2	2.13	0.48
1:A:218:HIS:O	1:A:221:ALA:N	2.47	0.48
1:A:391:GLU:HA	1:A:464:LEU:HD11	1.94	0.48
1:A:80:GLY:O	1:A:81:PHE:C	2.56	0.48
2:B:223:ASN:ND2	2:B:268:SER:OG	2.47	0.48
1:A:135:ASN:O	1:A:139:GLN:HG3	2.13	0.47
1:A:351:SER:O	1:A:355:ARG:HG3	2.14	0.47
1:A:341:THR:HA	1:A:473:LEU:HD13	1.95	0.47
1:A:76:LEU:CD1	1:A:218:HIS:CB	2.90	0.47
1:A:293:PHE:CD2	1:A:293:PHE:C	2.93	0.47
2:B:304:CYS:HB2	2:B:314:ILE:HG12	1.97	0.47
3:C:6:ILE:HD13	3:C:79:LEU:HD12	1.96	0.47
1:A:396:ILE:CG2	1:A:401:ASN:HA	2.45	0.46
1:A:166:GLU:HA	1:A:471:MET:HB3	1.98	0.46
1:A:169:ALA:O	1:A:173:ARG:HG3	2.15	0.46
1:A:332:HIS:HE1	1:A:347:ALA:O	1.99	0.46
2:B:133:HIS:O	2:B:136:GLN:HB3	2.15	0.46
2:B:312:ASN:O	2:B:316:GLU:HG3	2.16	0.46
1:A:76:LEU:HD11	1:A:218:HIS:HB2	1.95	0.46
1:A:76:LEU:HD11	1:A:218:HIS:CB	2.46	0.45
2:B:117:TRP:CZ2	2:B:242:ALA:HA	2.52	0.45
1:A:486:GLU:C	1:A:488:VAL:H	2.24	0.45
2:B:117:TRP:CE3	2:B:245:GLU:HG3	2.52	0.45
2:B:305:SER:HB3	2:B:314:ILE:CD1	2.35	0.45
2:B:126:THR:HG1	2:B:127:PRO:HD3	1.79	0.45
1:A:6:ARG:HD2	1:A:54:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:GLU:HG3	1:A:446:ASN:N	2.24	0.44
3:C:7:MET:HG2	3:C:76:THR:O	2.16	0.44
1:A:104:GLU:O	1:A:134:GLU:HB3	2.18	0.44
3:C:10:PHE:CE1	3:C:35:ALA:HA	2.52	0.44
1:A:47:TYR:CE1	1:A:240:PRO:HB2	2.52	0.44
1:A:371:GLN:H	1:A:371:GLN:HG2	1.64	0.44
2:B:154:CYS:HB3	2:B:267:TRP:CE2	2.52	0.44
1:A:10:TYR:CZ	1:A:52:LYS:HB3	2.53	0.44
1:A:190:ILE:O	1:A:194:PHE:HB3	2.17	0.43
2:B:318:LYS:O	2:B:322:ARG:HG3	2.18	0.43
2:B:126:THR:CB	2:B:127:PRO:CD	2.97	0.43
2:B:184:GLY:O	2:B:185:PHE:C	2.58	0.43
2:B:276:LEU:HD22	2:B:282:ARG:HB2	2.01	0.43
3:C:74:ARG:O	3:C:75:PRO:C	2.60	0.43
1:A:367:ASP:HB3	1:A:410:ASN:HD21	1.82	0.43
1:A:178:ASP:HA	2:B:48:LEU:HD11	2.01	0.43
2:B:295:LEU:HD23	2:B:295:LEU:HA	1.80	0.43
1:A:404:ILE:HG12	1:A:429:GLY:HA2	2.01	0.42
1:A:416:ASP:H	3:C:56:HIS:HE1	1.67	0.42
1:A:474:GLU:H	1:A:477:VAL:HG22	1.83	0.42
1:A:398:ASN:ND2	1:A:427:HIS:H	2.15	0.42
2:B:304:CYS:O	2:B:310:GLY:HA2	2.19	0.42
1:A:109:THR:HG23	2:B:144:GLN:HB2	2.01	0.42
1:A:232:SER:HA	1:A:235:ALA:HB3	2.02	0.42
1:A:78:ARG:HD3	1:A:78:ARG:HA	1.94	0.42
1:A:199:GLY:HA3	1:A:302:PHE:CZ	2.55	0.42
1:A:399:MET:HE2	1:A:399:MET:HB2	1.93	0.42
1:A:309:LEU:HD13	1:A:309:LEU:HA	1.85	0.42
1:A:396:ILE:HG12	1:A:451:VAL:HG23	2.02	0.42
1:A:418:GLN:HE22	3:C:78:THR:H	1.68	0.42
1:A:393:LEU:N	1:A:393:LEU:HD23	2.34	0.41
2:B:312:ASN:ND2	2:B:316:GLU:OE1	2.52	0.41
1:A:338:TRP:CD1	1:A:390:PRO:HG3	2.55	0.41
2:B:111:GLN:OE1	2:B:111:GLN:N	2.46	0.41
2:B:117:TRP:CH2	2:B:242:ALA:HA	2.55	0.41
3:C:13:ASP:OD2	3:C:42:ARG:NH1	2.52	0.41
1:A:274:GLY:HA2	1:A:290:PHE:CG	2.56	0.41
3:C:46:GLN:O	3:C:49:LYS:HB2	2.21	0.41
1:A:73:LYS:NZ	8:A:569:HOH:O	2.49	0.41
1:A:114:MET:HA	1:A:185:SER:OG	2.20	0.41
1:A:224:ILE:HD13	1:A:224:ILE:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ILE:CG2	1:A:227:ILE:HD11	2.51	0.41
2:B:220:THR:HG21	2:B:288:TRP:HB3	2.02	0.41
3:C:8:SER:O	3:C:16:ILE:HA	2.21	0.41
2:B:88:LEU:HD23	2:B:88:LEU:HA	1.98	0.41
2:B:125:TYR:HB2	2:B:238:LEU:HD21	2.03	0.41
1:A:396:ILE:HG22	1:A:401:ASN:HA	2.03	0.40
2:B:298:LYS:HE2	2:B:298:LYS:HB3	1.90	0.40
1:A:474:GLU:H	1:A:477:VAL:HG21	1.86	0.40
1:A:484:ASP:O	1:A:485:TYR:HB2	2.22	0.40
1:A:136:ARG:HB2	2:B:83:TYR:CD1	2.56	0.40
2:B:139:SER:OG	2:B:162:HIS:HD2	2.05	0.40
2:B:196:ASP:O	2:B:197:PRO:C	2.58	0.40
1:A:76:LEU:HD13	1:A:218:HIS:HB2	2.01	0.40
2:B:249:LEU:HD23	2:B:249:LEU:C	2.47	0.40

There are no symmetry-related clashes.

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	490/498 (98%)	451 (92%)	37 (8%)	2 (0%)	30	43
2	B	322/330 (98%)	310 (96%)	9 (3%)	3 (1%)	14	22
3	C	83/86 (96%)	74 (89%)	9 (11%)	0	100	100
All	All	895/914 (98%)	835 (93%)	55 (6%)	5 (1%)	21	32

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	445	GLU
1	A	406	HIS
2	B	22	ARG

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Mol	Chain	Res	Type
2	B	126	THR
2	B	20	GLY

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	417/422 (99%)	396 (95%)	21 (5%)	22	38
2	B	276/282 (98%)	255 (92%)	21 (8%)	12	21
3	C	78/79 (99%)	75 (96%)	3 (4%)	29	49
All	All	771/783 (98%)	726 (94%)	45 (6%)	18	32

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	21	LYS
1	A	95	LEU
1	A	100	ILE
1	A	174	SER
1	A	203	MET
1	A	206	LEU
1	A	225	SER
1	A	250	LYS
1	A	251	LYS
1	A	283	LEU
1	A	287	ASN
1	A	296	GLU
1	A	309	LEU
1	A	371	GLN
1	A	376	ILE
1	A	393	LEU
1	A	397	CYS
1	A	410	ASN
1	A	456	LYS

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Mol	Chain	Res	Type
1	A	469	MET
2	B	13	LYS
2	B	22	ARG
2	B	24	ARG
2	B	41	ASN
2	B	43	GLU
2	B	80	GLN
2	B	89	LEU
2	B	107	ARG
2	B	113	LEU
2	B	115	ARG
2	B	126	THR
2	B	140	VAL
2	B	174	ARG
2	B	187	LYS
2	B	206	ILE
2	B	244	SER
2	B	248	THR
2	B	279	GLU
2	B	283	GLU
2	B	309	ASP
2	B	327	MET
3	C	57	GLU
3	C	76	THR
3	C	85	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	A	135	ASN
1	A	139	GLN
1	A	237	GLN
1	A	305	GLN
1	A	322	GLN
1	A	371	GLN
1	A	398	ASN
1	A	418	GLN
1	A	427	HIS
2	B	34	ASN
2	B	80	GLN
2	B	98	GLN

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Mol	Chain	Res	Type
2	B	144	GLN
2	B	153	ASN
2	B	162	HIS
2	B	168	HIS
2	B	223	ASN
2	B	237	GLN
2	B	312	ASN
3	C	40	ASN
3	C	56	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic and 1 is modelled with single atom - leaving 2 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	502	4	3,3,3	0.96	0	2,2,2	0.48	0
7	SO4	B	331	-	4,4,4	0.19	0	6,6,6	0.69	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	502	4	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	502	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	491/498 (98%)	-0.25	3 (0%) 85 83	37, 54, 69, 85	1 (0%)
2	B	324/330 (98%)	-0.31	4 (1%) 76 73	38, 51, 71, 95	1 (0%)
3	C	85/86 (98%)	0.00	0 100 100	52, 61, 72, 84	0
All	All	900/914 (98%)	-0.25	7 (0%) 82 80	37, 54, 71, 95	2 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	223	ASN	6.9
1	A	218	HIS	6.9
1	A	445	GLU	4.4
2	B	126	THR	3.8
2	B	40	ASP	3.7
2	B	70	ASP	2.6
1	A	477	VAL	2.6

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 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(Å ²)	Q<0.9
7	SO4	B	331	5/5	0.86	0.07	93,96,97,98	0
6	EDO	A	502	4/4	0.93	0.20	57,60,64,66	0
5	OH	A	501	1/1	0.97	0.09	43,43,43,43	0
4	FE	A	500	1/1	1.00	0.03	52,52,52,52	0
4	FE	A	499	1/1	1.00	0.02	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.