



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 06:10 AM UTC

PDB ID : 3RNC / pdb_00003rnc
Title : Structure of the Toluene/o-Xylene Monooxygenase Hydroxylase T201S/I100A Double Mutant
Authors : Gucinski, G.; Song, W.J.; Lippard, S.J.; Sazinsky, M.H.
Deposited on : 2011-04-22
Resolution : 2.74 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

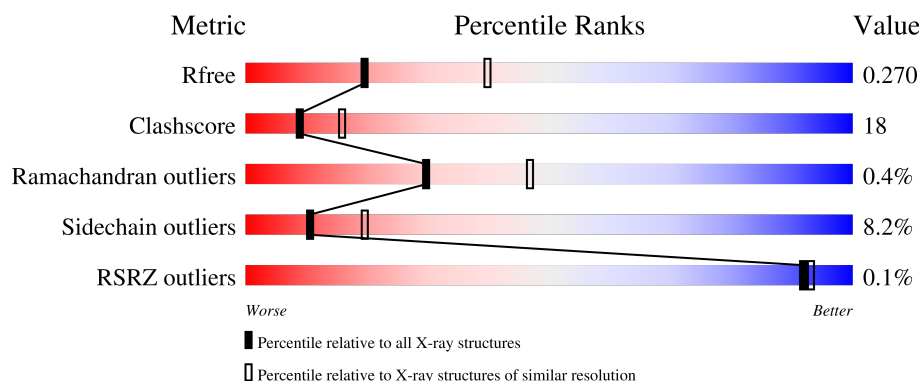
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

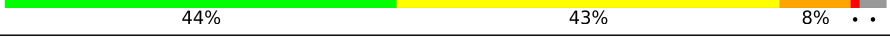
The reported resolution of this entry is 2.74 Å.

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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	
2	B	330	
3	C	86	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7380 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	0	0
			4014	2561	674	753	26			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ALA	ILE	engineered mutation	UNP Q6IV66
A	201	SER	THR	engineered mutation	UNP Q6IV66
A	445	LYS	GLU	engineered mutation	UNP Q6IV66

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	322	Total	C	N	O	S	0	0	0
			2641	1674	467	490	10			

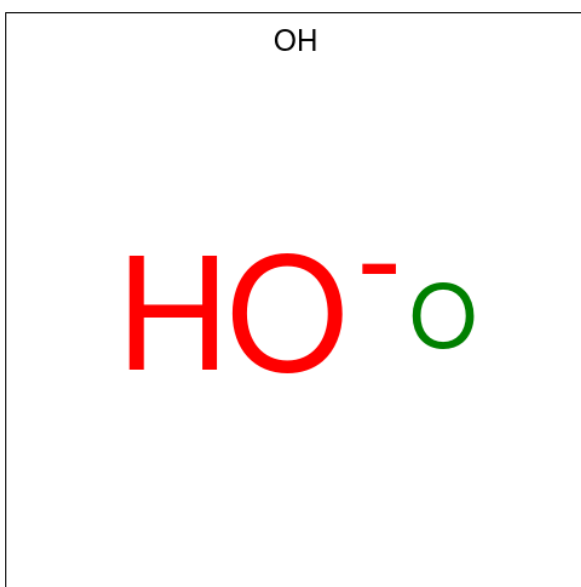
- Molecule 3 is a protein called Toluene o-xylene monooxygenase component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	83	Total	C	N	O	S	0	0	0
			676	425	120	126	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		

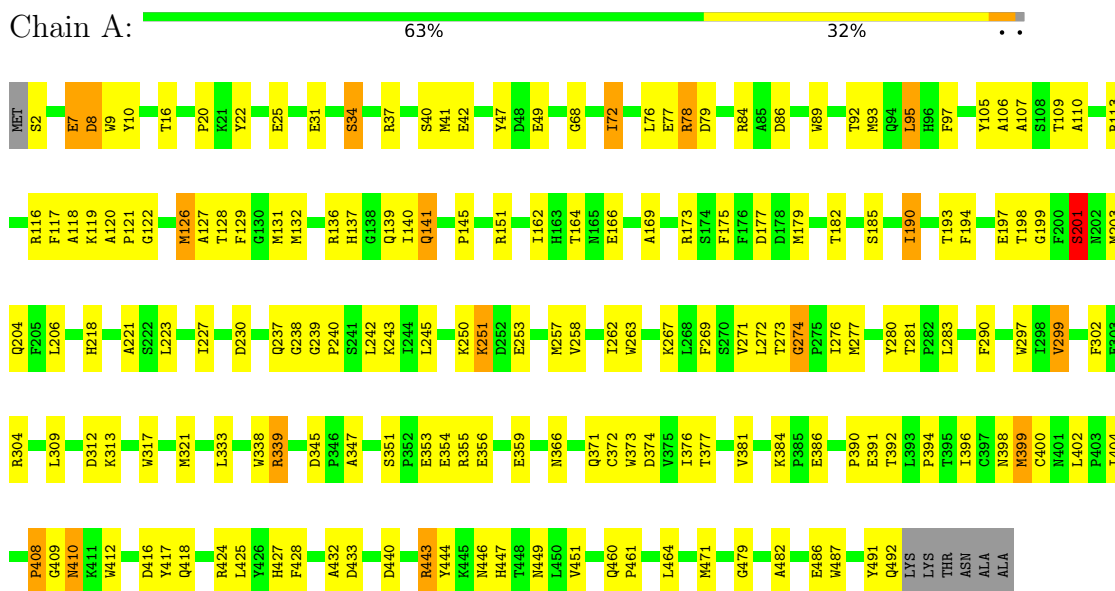
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	19	Total 19	O 19	0	0
7	B	20	Total 20	O 20	0	0
7	C	3	Total 3	O 3	0	0

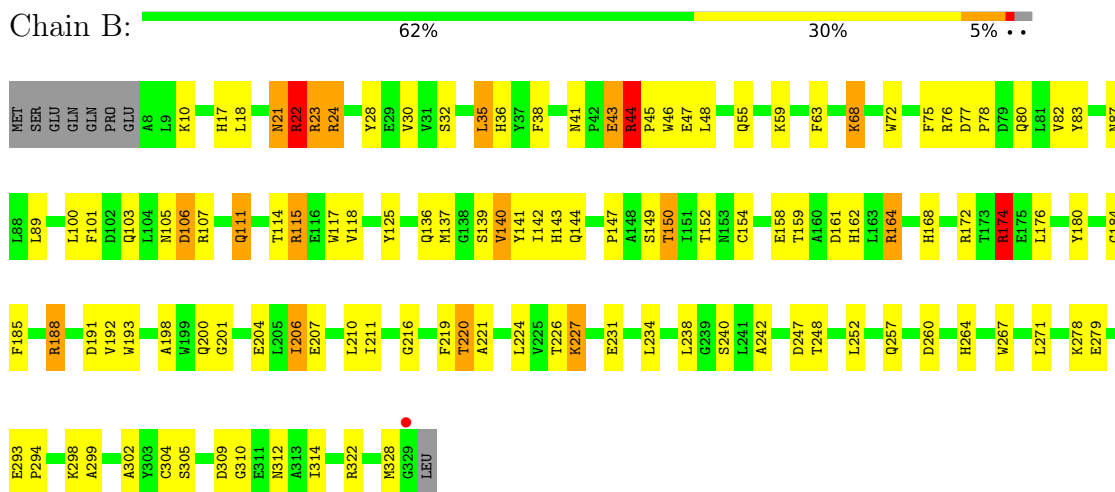
3 Residue-property plots

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

Chain C:

44%

43%

8%

••



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	182.57Å 182.57Å 67.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.64 – 2.74 45.64 – 2.74	Depositor EDS
% Data completeness (in resolution range)	93.2 (45.64-2.74) 93.1 (45.64-2.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.206 , 0.265 0.211 , 0.270	Depositor DCC
R_{free} test set	1600 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	58.7	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7380	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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: EDO, FE, 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	0.97	2/4138 (0.0%)	1.20	18/5623 (0.3%)
2	B	1.08	4/2713 (0.1%)	1.24	21/3688 (0.6%)
3	C	1.00	1/690 (0.1%)	1.25	5/934 (0.5%)
All	All	1.02	7/7541 (0.1%)	1.22	44/10245 (0.4%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	221	ALA	CA-CB	-6.61	1.43	1.53
1	A	396	ILE	CA-CB	6.50	1.62	1.54
3	C	53	VAL	CA-CB	5.88	1.61	1.54
1	A	106	ALA	CA-C	5.72	1.60	1.52
2	B	191	ASP	CA-C	-5.62	1.45	1.52
2	B	35	LEU	C-O	-5.17	1.18	1.24
2	B	150	THR	CA-CB	5.02	1.61	1.53

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	22	ARG	CB-CA-C	-12.81	91.62	110.06
1	A	190	ILE	CB-CA-C	-10.38	98.47	111.87
1	A	190	ILE	N-CA-C	9.07	118.94	110.42
3	C	60	THR	CB-CA-C	-8.44	94.70	109.64
2	B	72	TRP	N-CA-C	-7.88	102.58	112.90
2	B	30	VAL	N-CA-C	7.44	117.56	110.42
1	A	339	ARG	CA-C-N	-7.43	112.02	120.04
1	A	339	ARG	C-N-CA	-7.43	112.02	120.04
1	A	86	ASP	CA-C-N	-7.30	112.19	119.56
1	A	86	ASP	C-N-CA	-7.30	112.19	119.56
2	B	164	ARG	N-CA-C	-7.22	103.35	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	ASP	N-CA-C	-7.18	103.49	112.90
2	B	38	PHE	N-CA-C	-6.79	104.47	112.89
2	B	180	TYR	CA-C-N	6.74	126.69	119.28
2	B	180	TYR	C-N-CA	6.74	126.69	119.28
1	A	239	GLY	CA-C-N	6.54	127.06	119.47
1	A	239	GLY	C-N-CA	6.54	127.06	119.47
3	C	60	THR	N-CA-C	6.39	118.55	110.24
3	C	41	ARG	N-CA-C	-6.34	104.25	112.68
1	A	250	LYS	N-CA-C	6.28	120.23	111.56
2	B	21	ASN	N-CA-C	-6.21	106.25	113.88
2	B	106	ASP	CA-C-N	5.97	130.16	120.60
2	B	106	ASP	C-N-CA	5.97	130.16	120.60
2	B	106	ASP	O-C-N	5.95	128.43	122.12
2	B	227	LYS	CA-C-N	-5.91	112.93	119.19
2	B	227	LYS	C-N-CA	-5.91	112.93	119.19
3	C	25	ASP	CB-CA-C	-5.85	100.37	109.61
2	B	174	ARG	CB-CA-C	-5.76	98.95	110.42
2	B	252	LEU	N-CA-C	5.74	117.62	111.36
1	A	274	GLY	CA-C-N	5.69	126.07	119.47
1	A	274	GLY	C-N-CA	5.69	126.07	119.47
1	A	16	THR	N-CA-C	5.67	121.46	113.02
3	C	48	GLU	N-CA-C	-5.66	105.58	112.88
1	A	122	GLY	N-CA-C	-5.55	105.77	112.49
1	A	8	ASP	N-CA-C	5.53	118.06	111.71
2	B	10	LYS	N-CA-C	5.52	116.65	109.64
1	A	201	SER	N-CA-C	5.44	116.89	111.07
2	B	101	PHE	N-CA-C	-5.42	105.06	110.97
1	A	299	VAL	N-CA-C	5.32	115.42	110.42
2	B	210	LEU	N-CA-C	5.19	119.09	112.34
2	B	211	ILE	N-CA-C	5.14	117.11	111.77
1	A	151	ARG	N-CA-C	5.06	116.88	111.36
2	B	44	ARG	CA-C-N	5.05	124.54	119.19
2	B	44	ARG	C-N-CA	5.05	124.54	119.19

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	4014	0	3763	133	0
2	B	2641	0	2537	111	0
3	C	676	0	667	53	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	4	0	5	0	0
7	A	19	0	0	0	0
7	B	20	0	0	2	0
7	C	3	0	0	0	0
All	All	7380	0	6972	264	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 18.

All (264) 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)
2:B:22:ARG:HH11	2:B:22:ARG:CG	1.58	1.10
1:A:9:TRP:HB3	2:B:174:ARG:HG3	1.32	1.09
1:A:116:ARG:HB2	2:B:140:VAL:CG1	1.84	1.07
2:B:22:ARG:HG2	2:B:22:ARG:NH1	1.42	0.98
2:B:111:GLN:HE21	2:B:111:GLN:N	1.64	0.96
2:B:111:GLN:HE21	2:B:111:GLN:H	1.11	0.93
1:A:37:ARG:NH2	1:A:257:MET:HE1	1.84	0.93
2:B:309:ASP:OD1	2:B:312:ASN:HB3	1.69	0.92
1:A:416:ASP:OD2	1:A:427:HIS:HD2	1.54	0.90
2:B:23:ARG:NH1	2:B:23:ARG:CB	2.36	0.89
1:A:34:SER:HB3	1:A:117:PHE:O	1.72	0.89
3:C:28:ASP:OD1	3:C:64:ARG:HB3	1.72	0.89
1:A:427:HIS:HE1	3:C:76:THR:HG23	1.36	0.88
2:B:23:ARG:CZ	2:B:23:ARG:HB2	2.02	0.85
1:A:139:GLN:HE22	2:B:83:TYR:H	1.24	0.85
2:B:111:GLN:H	2:B:111:GLN:NE2	1.73	0.85
2:B:23:ARG:HH11	2:B:23:ARG:CG	1.90	0.85
3:C:11:GLU:HG2	3:C:12:ARG:HG3	1.57	0.85
2:B:21:ASN:O	2:B:22:ARG:HB2	1.79	0.83
1:A:427:HIS:CE1	3:C:76:THR:HG23	2.14	0.82
1:A:418:GLN:HE22	3:C:78:THR:H	1.26	0.80
2:B:139:SER:OG	2:B:162:HIS:HD2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LEU:O	1:A:276:ILE:HD12	1.86	0.76
2:B:23:ARG:HH11	2:B:23:ARG:HG2	1.49	0.76
1:A:9:TRP:HB3	2:B:174:ARG:CG	2.13	0.76
2:B:77:ASP:HB2	2:B:154:CYS:SG	2.25	0.76
3:C:26:THR:HG22	3:C:29:GLN:H	1.49	0.75
2:B:43:GLU:CD	2:B:43:GLU:H	1.95	0.74
1:A:425:LEU:HD23	3:C:76:THR:HG22	1.70	0.74
1:A:118:ALA:HB2	1:A:185:SER:OG	1.88	0.73
2:B:227:LYS:NZ	2:B:264:HIS:ND1	2.35	0.73
2:B:206:ILE:HD13	2:B:226:THR:HG21	1.70	0.73
3:C:75:PRO:O	3:C:76:THR:HB	1.88	0.73
2:B:45:PRO:HD2	2:B:55:GLN:OE1	1.88	0.72
1:A:372:CYS:O	1:A:376:ILE:HG12	1.89	0.72
1:A:487:TRP:CD1	1:A:487:TRP:H	2.04	0.72
2:B:21:ASN:O	2:B:22:ARG:CB	2.36	0.72
2:B:23:ARG:CB	2:B:23:ARG:CZ	2.67	0.71
2:B:201:GLY:HA3	2:B:299:ALA:HA	1.72	0.70
1:A:8:ASP:O	2:B:174:ARG:HD2	1.91	0.70
2:B:137:MET:O	2:B:140:VAL:HG12	1.91	0.70
1:A:116:ARG:HG2	2:B:141:TYR:HB2	1.74	0.70
1:A:37:ARG:HH21	1:A:257:MET:HE1	1.58	0.69
2:B:23:ARG:O	2:B:24:ARG:C	2.31	0.69
2:B:75:PHE:O	2:B:76:ARG:NH2	2.25	0.69
3:C:61:LEU:HD12	3:C:62:PHE:H	1.57	0.69
1:A:2:SER:N	2:B:105:ASN:HD22	1.91	0.69
3:C:60:THR:CG2	3:C:61:LEU:N	2.47	0.68
1:A:267:LYS:NZ	1:A:433:ASP:OD2	2.26	0.68
1:A:116:ARG:HB2	2:B:140:VAL:HG13	1.74	0.68
2:B:161:ASP:O	2:B:164:ARG:HB3	1.93	0.68
2:B:136:GLN:O	2:B:140:VAL:HB	1.95	0.67
2:B:304:CYS:HB2	2:B:314:ILE:HG12	1.77	0.67
1:A:78:ARG:HH11	1:A:78:ARG:HB3	1.61	0.66
3:C:26:THR:HG21	3:C:28:ASP:HB2	1.78	0.65
1:A:443:ARG:HG2	1:A:444:TYR:CE1	2.32	0.65
2:B:22:ARG:CG	2:B:22:ARG:NH1	2.30	0.64
2:B:23:ARG:NH1	2:B:23:ARG:HB3	2.13	0.64
3:C:26:THR:CG2	3:C:28:ASP:HB2	2.27	0.64
3:C:26:THR:HG23	3:C:64:ARG:O	1.97	0.63
3:C:61:LEU:HD12	3:C:62:PHE:N	2.13	0.62
1:A:398:ASN:HD22	1:A:427:HIS:H	1.46	0.62
1:A:9:TRP:CB	2:B:174:ARG:HG3	2.19	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ASP:OD2	1:A:427:HIS:CD2	2.45	0.62
1:A:427:HIS:HE1	3:C:76:THR:CG2	2.10	0.62
1:A:204:GLN:HB2	1:A:269:PHE:HZ	1.64	0.62
2:B:158:GLU:HG3	2:B:264:HIS:CG	2.35	0.62
2:B:293:GLU:HB3	2:B:294:PRO:HD3	1.81	0.61
1:A:164:THR:O	1:A:173:ARG:NH1	2.30	0.61
3:C:54:ARG:O	3:C:54:ARG:HG3	1.99	0.61
2:B:305:SER:HB3	2:B:314:ILE:HD11	1.81	0.61
1:A:190:ILE:HD12	1:A:242:LEU:HG	1.81	0.60
1:A:417:TYR:O	1:A:428:PHE:HB2	2.01	0.60
3:C:10:PHE:CE1	3:C:81:ILE:HG21	2.36	0.60
3:C:75:PRO:O	3:C:76:THR:CB	2.49	0.60
1:A:137:HIS:CD2	1:A:227:ILE:HG23	2.37	0.60
2:B:158:GLU:HG3	2:B:264:HIS:CD2	2.37	0.60
3:C:56:HIS:HD2	3:C:80:ASP:OD1	1.85	0.59
3:C:60:THR:HG22	3:C:61:LEU:N	2.07	0.59
2:B:23:ARG:CB	2:B:23:ARG:HH11	2.08	0.59
3:C:30:VAL:HG12	3:C:31:ALA:N	2.16	0.59
1:A:391:GLU:HA	1:A:464:LEU:HD11	1.85	0.58
1:A:299:VAL:HG11	1:A:321:MET:HE1	1.84	0.58
1:A:116:ARG:HB2	2:B:140:VAL:HG12	1.81	0.58
1:A:218:HIS:HA	1:A:221:ALA:HB3	1.85	0.58
1:A:377:THR:O	1:A:381:VAL:HG23	2.03	0.58
2:B:59:LYS:HA	2:B:63:PHE:HD2	1.69	0.57
1:A:274:GLY:HA2	1:A:290:PHE:CD1	2.40	0.57
2:B:142:ILE:O	2:B:143:HIS:C	2.47	0.57
2:B:35:LEU:HB2	2:B:149:SER:HB2	1.85	0.57
1:A:97:PHE:CE1	1:A:145:PRO:HD3	2.39	0.57
1:A:400:CYS:O	1:A:402:LEU:HG	2.05	0.57
1:A:410:ASN:ND2	1:A:410:ASN:H	1.99	0.57
1:A:116:ARG:HB2	2:B:140:VAL:HG11	1.77	0.56
1:A:179:MET:HE2	1:A:179:MET:HA	1.88	0.56
2:B:149:SER:HB3	7:B:349:HOH:O	2.04	0.56
1:A:446:ASN:C	1:A:446:ASN:OD1	2.48	0.56
1:A:347:ALA:HA	1:A:482:ALA:HB3	1.88	0.56
1:A:372:CYS:HB3	3:C:42:ARG:HG2	1.88	0.56
2:B:22:ARG:HH11	2:B:22:ARG:HG2	0.63	0.55
2:B:293:GLU:HB3	2:B:294:PRO:CD	2.36	0.55
1:A:128:THR:OG1	2:B:136:GLN:NE2	2.39	0.55
1:A:25:GLU:OE2	1:A:119:LYS:HE2	2.07	0.55
1:A:162:ILE:O	1:A:173:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:GLN:HG3	2:B:159:THR:HG23	1.87	0.55
1:A:95:LEU:HD11	1:A:272:LEU:HD22	1.89	0.55
2:B:140:VAL:CG1	2:B:141:TYR:N	2.70	0.55
3:C:26:THR:HG23	3:C:27:MET:N	2.20	0.55
1:A:345:ASP:O	1:A:482:ALA:HB2	2.07	0.54
2:B:35:LEU:HB2	2:B:149:SER:CB	2.37	0.54
3:C:63:PRO:HD2	3:C:66:MET:HE3	1.89	0.54
1:A:49:GLU:HG3	1:A:126:MET:CG	2.37	0.54
1:A:460:GLN:HA	1:A:461:PRO:C	2.33	0.53
1:A:223:LEU:O	1:A:227:ILE:HG12	2.08	0.53
1:A:353:GLU:CD	1:A:353:GLU:H	2.15	0.53
3:C:26:THR:HG22	3:C:29:GLN:N	2.21	0.53
1:A:199:GLY:HA3	1:A:302:PHE:CZ	2.44	0.53
2:B:17:HIS:CE1	2:B:18:LEU:HG	2.44	0.53
2:B:46:TRP:O	2:B:48:LEU:N	2.42	0.53
2:B:140:VAL:O	2:B:143:HIS:HB3	2.09	0.53
2:B:201:GLY:CA	2:B:299:ALA:HA	2.37	0.53
3:C:46:GLN:O	3:C:49:LYS:HB2	2.09	0.53
2:B:257:GLN:O	2:B:260:ASP:HB2	2.09	0.52
1:A:190:ILE:O	1:A:194:PHE:HB3	2.10	0.52
2:B:227:LYS:HE3	2:B:231:GLU:OE2	2.09	0.52
2:B:115:ARG:HD2	2:B:115:ARG:O	2.10	0.52
2:B:117:TRP:CH2	2:B:242:ALA:HA	2.45	0.52
3:C:76:THR:HG23	3:C:76:THR:O	2.10	0.52
1:A:139:GLN:HE22	2:B:83:TYR:N	2.01	0.52
3:C:27:MET:HG3	3:C:62:PHE:HB3	1.92	0.52
2:B:174:ARG:HA	2:B:174:ARG:NE	2.24	0.52
1:A:253:GLU:O	1:A:257:MET:HG3	2.10	0.51
1:A:68:GLY:O	1:A:72:ILE:HD12	2.10	0.51
2:B:139:SER:OG	2:B:162:HIS:CD2	2.53	0.51
2:B:168:HIS:HD2	2:B:257:GLN:HE21	1.59	0.51
1:A:47:TYR:CE1	1:A:240:PRO:HB2	2.46	0.51
1:A:107:ALA:O	1:A:110:ALA:HB3	2.11	0.51
1:A:338:TRP:CD1	1:A:390:PRO:HG3	2.46	0.51
1:A:49:GLU:HG3	1:A:126:MET:HG2	1.93	0.51
1:A:371:GLN:O	1:A:374:ASP:HB2	2.11	0.51
1:A:105:TYR:HE2	2:B:36:HIS:CD2	2.29	0.50
2:B:47:GLU:C	2:B:48:LEU:HG	2.36	0.50
3:C:60:THR:HG23	3:C:61:LEU:N	2.26	0.50
2:B:193:TRP:O	2:B:200:GLN:NE2	2.45	0.50
1:A:418:GLN:NE2	3:C:78:THR:H	2.04	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:TYR:O	1:A:492:GLN:HB2	2.11	0.50
1:A:339:ARG:HG2	1:A:339:ARG:HH21	1.78	0.49
1:A:351:SER:OG	1:A:354:GLU:HG3	2.12	0.49
3:C:55:ARG:HA	3:C:79:LEU:HD23	1.94	0.49
2:B:309:ASP:OD1	2:B:309:ASP:O	2.31	0.49
1:A:9:TRP:O	1:A:10:TYR:C	2.55	0.49
1:A:443:ARG:HG2	1:A:444:TYR:CZ	2.47	0.49
1:A:31:GLU:OE1	1:A:31:GLU:HA	2.13	0.49
1:A:182:THR:HG22	2:B:46:TRP:CD1	2.48	0.48
2:B:125:TYR:HB2	2:B:238:LEU:HD21	1.95	0.48
3:C:50:ILE:HD13	3:C:64:ARG:NH1	2.28	0.48
1:A:194:PHE:O	1:A:198:THR:HB	2.13	0.48
1:A:20:PRO:HA	2:B:207:GLU:OE2	2.13	0.48
1:A:258:VAL:O	1:A:262:ILE:HG13	2.12	0.48
1:A:203:MET:HG2	1:A:297:TRP:HB3	1.96	0.48
3:C:35:ALA:O	3:C:36:TYR:C	2.57	0.48
2:B:159:THR:O	2:B:162:HIS:HB2	2.14	0.48
3:C:74:ARG:O	3:C:75:PRO:C	2.57	0.47
1:A:40:SER:O	1:A:41:MET:C	2.57	0.47
1:A:416:ASP:H	3:C:56:HIS:CE1	2.32	0.47
2:B:143:HIS:C	2:B:143:HIS:CD2	2.93	0.47
1:A:317:TRP:O	1:A:321:MET:HG2	2.15	0.47
2:B:28:TYR:CD2	2:B:80:GLN:HG2	2.49	0.47
1:A:2:SER:HB2	2:B:105:ASN:ND2	2.29	0.47
1:A:136:ARG:O	1:A:140:ILE:HG22	2.15	0.47
2:B:184:GLY:O	2:B:185:PHE:C	2.58	0.47
1:A:120:ALA:HA	1:A:121:PRO:HD3	1.84	0.46
1:A:129:PHE:HA	1:A:132:MET:HB2	1.97	0.46
1:A:78:ARG:HH11	1:A:78:ARG:CB	2.28	0.46
1:A:128:THR:O	1:A:131:MET:HB3	2.15	0.46
2:B:143:HIS:CG	2:B:152:THR:HG23	2.50	0.46
3:C:76:THR:CG2	3:C:76:THR:O	2.63	0.46
2:B:75:PHE:HD2	2:B:150:THR:OG1	1.98	0.46
2:B:219:PHE:CZ	2:B:271:LEU:HD23	2.51	0.46
1:A:89:TRP:CD1	1:A:93:MET:HE2	2.49	0.46
1:A:398:ASN:OD1	1:A:449:ASN:ND2	2.49	0.46
3:C:54:ARG:HG2	3:C:80:ASP:HB2	1.96	0.46
1:A:197:GLU:HA	1:A:201:SER:HB2	1.97	0.46
1:A:136:ARG:HD2	2:B:83:TYR:CE1	2.51	0.45
1:A:491:TYR:O	1:A:492:GLN:CB	2.65	0.45
2:B:198:ALA:HA	2:B:302:ALA:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:GLU:OE1	1:A:366:ASN:HB2	2.16	0.45
3:C:52:ARG:HG3	3:C:52:ARG:HH11	1.80	0.45
1:A:408:PRO:HB2	1:A:409:GLY:H	1.63	0.45
2:B:68:LYS:O	2:B:278:LYS:HD3	2.17	0.45
1:A:169:ALA:O	1:A:173:ARG:HG3	2.16	0.45
1:A:399:MET:HE2	1:A:399:MET:HA	1.98	0.45
2:B:114:THR:O	2:B:118:VAL:HG23	2.17	0.45
3:C:26:THR:HB	3:C:29:GLN:OE1	2.17	0.45
2:B:188:ARG:HB3	7:B:344:HOH:O	2.16	0.45
3:C:30:VAL:HG11	3:C:53:VAL:HG11	1.98	0.45
1:A:76:LEU:O	1:A:77:GLU:C	2.59	0.44
1:A:193:THR:HA	1:A:197:GLU:OE1	2.17	0.44
1:A:424:ARG:NH2	1:A:447:HIS:O	2.34	0.44
3:C:80:ASP:C	3:C:81:ILE:HD12	2.43	0.44
1:A:116:ARG:CB	2:B:140:VAL:CG1	2.76	0.44
2:B:206:ILE:HD12	2:B:206:ILE:HA	1.83	0.44
1:A:136:ARG:NH1	1:A:230:ASP:OD2	2.47	0.44
1:A:443:ARG:HG2	1:A:444:TYR:CD1	2.53	0.44
1:A:313:LYS:HD2	1:A:317:TRP:CD1	2.52	0.44
1:A:274:GLY:HA2	1:A:290:PHE:CG	2.53	0.44
1:A:399:MET:HE3	1:A:399:MET:HB2	1.84	0.44
2:B:242:ALA:HB1	2:B:247:ASP:HB3	1.99	0.44
2:B:111:GLN:N	2:B:111:GLN:NE2	2.42	0.43
2:B:32:SER:O	2:B:149:SER:OG	2.29	0.43
3:C:10:PHE:CE1	3:C:81:ILE:CG2	3.01	0.43
3:C:73:LEU:HD22	3:C:79:LEU:HD21	2.01	0.43
2:B:82:VAL:O	2:B:83:TYR:C	2.60	0.43
1:A:110:ALA:O	1:A:113:ARG:HB3	2.19	0.43
1:A:194:PHE:HB2	1:A:238:GLY:HA3	2.01	0.43
3:C:52:ARG:NH2	3:C:63:PRO:HA	2.34	0.43
1:A:105:TYR:CD2	2:B:35:LEU:HB3	2.54	0.43
1:A:166:GLU:HA	1:A:471:MET:HB3	2.00	0.43
1:A:345:ASP:HB3	1:A:482:ALA:HA	2.00	0.43
1:A:339:ARG:O	1:A:479:GLY:HA3	2.18	0.43
2:B:77:ASP:HA	2:B:78:PRO:HD2	1.86	0.43
2:B:227:LYS:HE3	2:B:227:LYS:HB3	1.85	0.43
2:B:304:CYS:O	2:B:310:GLY:HA2	2.18	0.43
1:A:394:PRO:HA	3:C:17:GLN:HA	2.00	0.42
3:C:74:ARG:O	3:C:77:GLU:HB2	2.19	0.42
2:B:100:LEU:HD23	2:B:100:LEU:HA	1.74	0.42
2:B:158:GLU:OE1	2:B:267:TRP:HZ2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:220:THR:HG23	2:B:224:LEU:HD12	2.01	0.42
1:A:127:ALA:HB2	1:A:237:GLN:HE22	1.84	0.42
1:A:203:MET:CG	1:A:297:TRP:HB3	2.49	0.42
1:A:251:LYS:NZ	1:A:251:LYS:HB3	2.34	0.42
1:A:408:PRO:HA	1:A:412:TRP:HD1	1.84	0.42
2:B:44:ARG:O	2:B:44:ARG:HG2	2.18	0.42
2:B:192:VAL:O	2:B:193:TRP:C	2.62	0.42
3:C:27:MET:N	3:C:66:MET:O	2.49	0.42
1:A:109:THR:HG23	2:B:144:GLN:HB2	2.00	0.42
1:A:245:LEU:HD23	1:A:245:LEU:HA	1.91	0.42
2:B:87:ASN:HD22	2:B:87:ASN:HA	1.57	0.42
1:A:92:THR:HG23	1:A:276:ILE:HD13	2.02	0.42
1:A:263:TRP:CE2	1:A:432:ALA:HB3	2.55	0.42
3:C:52:ARG:HH21	3:C:63:PRO:HA	1.84	0.42
3:C:30:VAL:HG12	3:C:53:VAL:HG21	2.02	0.41
1:A:392:THR:OG1	3:C:18:LEU:O	2.33	0.41
3:C:30:VAL:CG1	3:C:31:ALA:N	2.84	0.41
1:A:440:ASP:HB3	1:A:444:TYR:CE1	2.55	0.41
1:A:47:TYR:CB	1:A:120:ALA:HB1	2.51	0.41
1:A:427:HIS:CE1	3:C:76:THR:O	2.73	0.41
2:B:216:GLY:O	2:B:220:THR:OG1	2.37	0.41
2:B:293:GLU:O	2:B:294:PRO:C	2.63	0.41
1:A:7:GLU:CD	1:A:7:GLU:H	2.27	0.41
2:B:219:PHE:CE2	2:B:224:LEU:HD11	2.55	0.41
1:A:22:TYR:CG	2:B:204:GLU:HG3	2.56	0.41
1:A:218:HIS:HA	1:A:221:ALA:CB	2.49	0.41
1:A:333:LEU:HD13	1:A:373:TRP:CE2	2.56	0.41
2:B:174:ARG:HA	2:B:174:ARG:CZ	2.51	0.41
1:A:137:HIS:O	1:A:141:GLN:HB2	2.20	0.41
1:A:277:MET:HE2	1:A:277:MET:HB3	1.88	0.41
2:B:176:LEU:HD23	2:B:176:LEU:HA	1.89	0.41
2:B:41:ASN:HB2	2:B:44:ARG:O	2.21	0.40
1:A:355:ARG:NH2	1:A:366:ASN:OD1	2.38	0.40
3:C:40:ASN:HD21	3:C:45:PRO:HG3	1.86	0.40
1:A:164:THR:O	1:A:173:ARG:NH2	2.52	0.40
1:A:175:PHE:O	1:A:179:MET:HG2	2.21	0.40
2:B:103:GLN:O	2:B:106:ASP:HB2	2.21	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	489/498 (98%)	446 (91%)	41 (8%)	2 (0%)	30	47
2	B	320/330 (97%)	296 (92%)	22 (7%)	2 (1%)	21	36
3	C	81/86 (94%)	71 (88%)	10 (12%)	0	100	100
All	All	890/914 (97%)	813 (91%)	73 (8%)	4 (0%)	30	47

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	408	PRO
1	A	386	GLU
2	B	172	ARG
2	B	174	ARG

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	416/421 (99%)	386 (93%)	30 (7%)	13	24
2	B	274/282 (97%)	251 (92%)	23 (8%)	10	18
3	C	77/79 (98%)	67 (87%)	10 (13%)	4	7
All	All	767/782 (98%)	704 (92%)	63 (8%)	10	19

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	34	SER
1	A	42	GLU
1	A	72	ILE
1	A	78	ARG
1	A	79	ASP
1	A	84	ARG
1	A	95	LEU
1	A	126	MET
1	A	141	GLN
1	A	201	SER
1	A	206	LEU
1	A	243	LYS
1	A	251	LYS
1	A	271	VAL
1	A	273	THR
1	A	280	TYR
1	A	281	THR
1	A	283	LEU
1	A	304	ARG
1	A	309	LEU
1	A	312	ASP
1	A	356	GLU
1	A	384	LYS
1	A	399	MET
1	A	404	ILE
1	A	410	ASN
1	A	443	ARG
1	A	451	VAL
1	A	486	GLU
2	B	22	ARG
2	B	23	ARG
2	B	24	ARG
2	B	43	GLU
2	B	44	ARG
2	B	68	LYS
2	B	89	LEU
2	B	107	ARG
2	B	111	GLN
2	B	115	ARG
2	B	140	VAL
2	B	147	PRO
2	B	174	ARG

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Mol	Chain	Res	Type
2	B	188	ARG
2	B	206	ILE
2	B	220	THR
2	B	234	LEU
2	B	240	SER
2	B	248	THR
2	B	279	GLU
2	B	298	LYS
2	B	322	ARG
2	B	328	MET
3	C	3	THR
3	C	26	THR
3	C	30	VAL
3	C	43	VAL
3	C	50	ILE
3	C	54	ARG
3	C	60	THR
3	C	66	MET
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	139	GLN
1	A	141	GLN
1	A	237	GLN
1	A	248	ASN
1	A	322	GLN
1	A	379	ASN
1	A	418	GLN
1	A	427	HIS
2	B	34	ASN
2	B	36	HIS
2	B	87	ASN
2	B	105	ASN
2	B	111	GLN
2	B	136	GLN
2	B	153	ASN
2	B	162	HIS
2	B	168	HIS
2	B	223	ASN

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Mol	Chain	Res	Type
2	B	257	GLN
2	B	326	GLN
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 4 ligands modelled in this entry, 2 are monoatomic and 1 is modelled with single atom - leaving 1 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	0.79	0	2,2,2	0.24	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	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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%)	-0.00	0 100 100	44, 64, 79, 91	0
2	B	322/330 (97%)	-0.04	1 (0%) 90 91	42, 58, 80, 97	0
3	C	83/86 (96%)	0.47	0 100 100	65, 74, 86, 92	0
All	All	896/914 (98%)	0.03	1 (0%) 92 93	42, 63, 81, 97	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	329	GLY	2.8

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
6	EDO	A	502	4/4	0.95	0.11	66,66,67,67	0
5	OH	A	501	1/1	0.99	0.03	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FE	A	499	1/1	1.00	0.02	68,68,68,68	0
4	FE	A	500	1/1	1.00	0.03	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.