Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:19 PM GMT

PDB ID	:	1T0Q
Title	:	Structure of the Toluene/o-Xylene Monooxygenase Hydroxylase
Authors	:	Sazinsky, M.H.; Bard, J.; Di Donato, A.; Lippard, S.J.
Deposited on	:	2004-04-12
Resolution	:	2.15 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

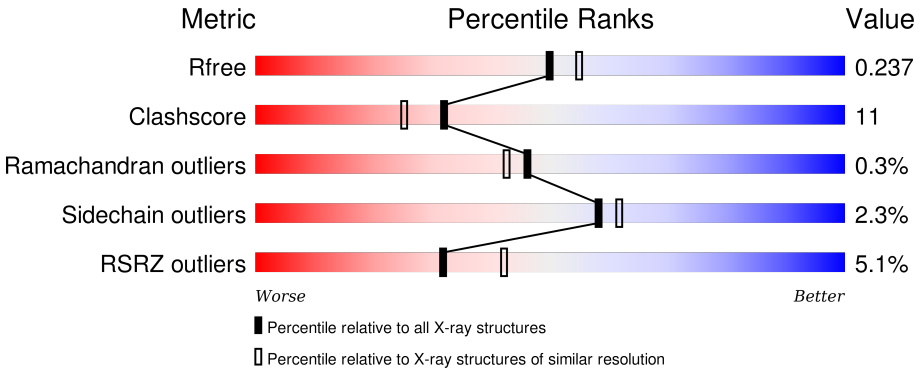
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.15 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}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	498	4% 73% 22%
2	B	330	6% 78% 18%
3	C	86	5% 60% 31% 5%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7590 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 oxygenase subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	0	0
			4018	2565	674	753	26			

- Molecule 2 is a protein called toluene, o-xylene monooxygenase oxygenase subunit.

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

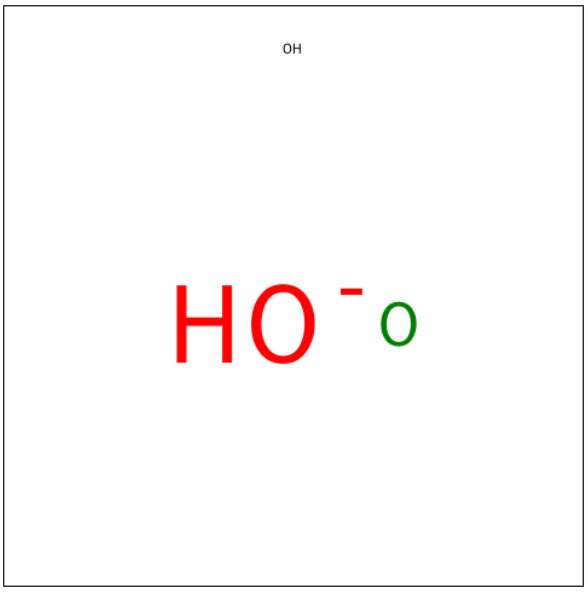
- Molecule 3 is a protein called touB.

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 (three-letter code: FE) (formula: Fe).

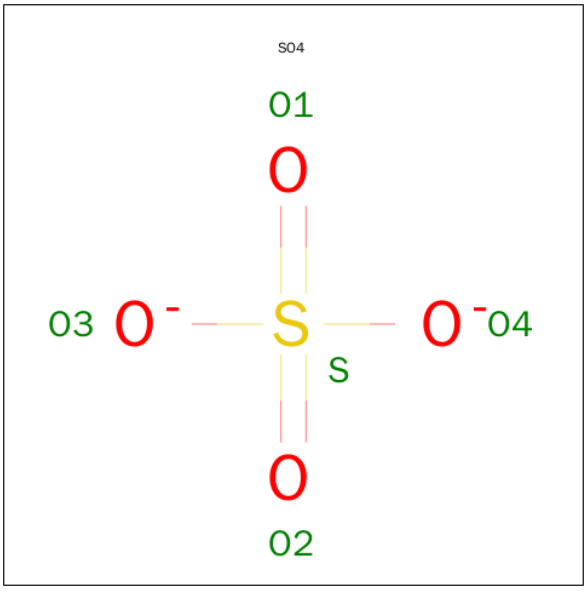
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Fe	0	0
			2	2		

- Molecule 5 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



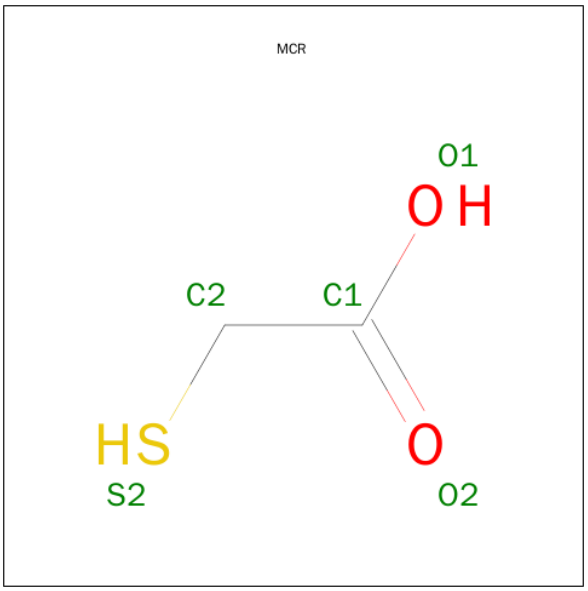
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 1 1	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 7 is SULFANYLACETIC ACID (three-letter code: MCR) (formula: $C_2H_4O_2S$).



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

- Molecule 8 is water.

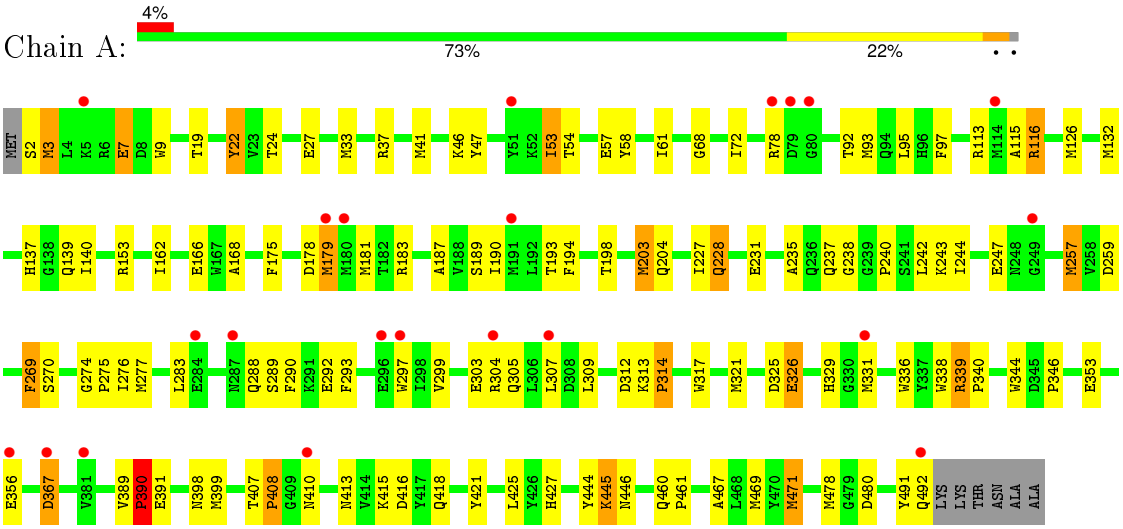
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	114	Total O 114 114	0	0
8	B	118	Total O 118 118	0	0
8	C	10	Total O 10 10	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

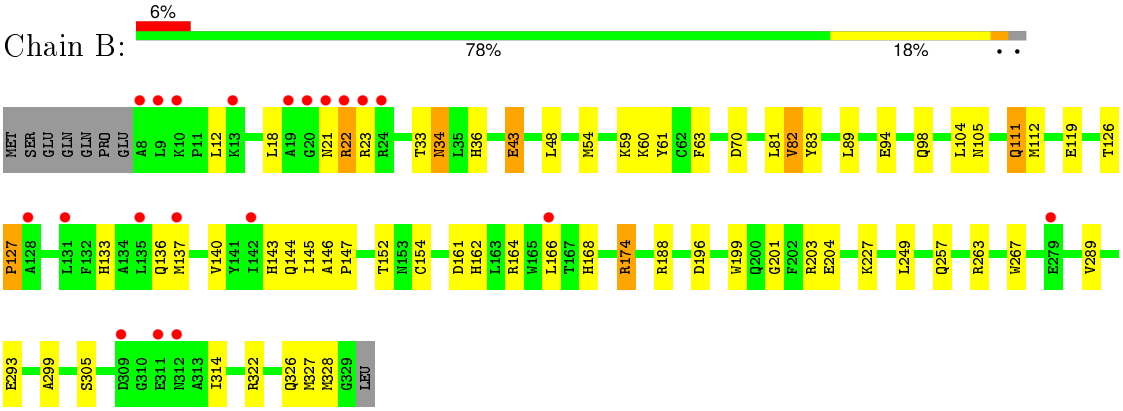
- Molecule 1: toluene, o-xylene monooxygenase oxygenase subunit

Chain A:



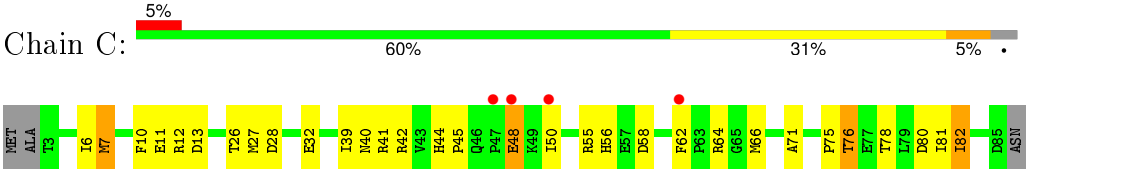
- Molecule 2: toluene, o-xylene monooxygenase oxygenase subunit

Chain B:



- Molecule 3: touB

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	182.81Å 182.81Å 68.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.92 – 2.15 29.92 – 2.15	Depositor EDS
% Data completeness (in resolution range)	95.9 (29.92-2.15) 97.1 (29.92-2.15)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	0.03	Depositor
$< I/\sigma(I) >$ [1]	4.01 (at 2.16Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.199 , 0.225 0.209 , 0.237	Depositor DCC
R_{free} test set	3395 reflections (5.21%)	DCC
Wilson B-factor (Å^2)	33.1	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 51.9	EDS
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	2 of 135163 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7590	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MCR, FE, 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	0.64	18/4142 (0.4%)	0.77	14/5629 (0.2%)
2	B	0.59	8/2713 (0.3%)	0.75	10/3688 (0.3%)
3	C	0.58	2/690 (0.3%)	0.63	0/934
All	All	0.62	28/7545 (0.4%)	0.75	24/10251 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	119	GLU	CD-OE2	7.43	1.33	1.25
1	A	132	MET	CG-SD	7.01	1.99	1.81
1	A	469	MET	CG-SD	6.00	1.96	1.81
3	C	27	MET	CG-SD	5.98	1.96	1.81
2	B	327	MET	CG-SD	5.87	1.96	1.81
3	C	7	MET	CG-SD	5.82	1.96	1.81
1	A	179	MET	CG-SD	5.75	1.96	1.81
2	B	328	MET	CG-SD	5.72	1.96	1.81
2	B	137	MET	CG-SD	5.68	1.96	1.81
2	B	54	MET	CG-SD	5.63	1.95	1.81
1	A	331	MET	CG-SD	5.48	1.95	1.81
2	B	147	PRO	N-CD	5.46	1.55	1.47
1	A	33	MET	CG-SD	5.45	1.95	1.81
1	A	390	PRO	N-CD	5.41	1.55	1.47
1	A	471	MET	CG-SD	5.41	1.95	1.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	112	MET	CG-SD	5.36	1.95	1.81
1	A	126	MET	CG-SD	5.34	1.95	1.81
1	A	478	MET	CG-SD	5.32	1.95	1.81
1	A	314	PRO	N-CD	5.26	1.55	1.47
1	A	3	MET	CG-SD	5.25	1.94	1.81
1	A	257	MET	CG-SD	5.24	1.94	1.81
1	A	399	MET	CG-SD	5.24	1.94	1.81
1	A	181	MET	CG-SD	5.24	1.94	1.81
1	A	41	MET	CG-SD	5.17	1.94	1.81
1	A	203	MET	CG-SD	5.16	1.94	1.81
1	A	277	MET	CG-SD	5.06	1.94	1.81
2	B	126	THR	C-N	5.03	1.43	1.34
1	A	339	ARG	C-N	5.03	1.43	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	22	TYR	CB-CG-CD2	-14.54	112.28	121.00
1	A	339	ARG	C-N-CD	9.56	148.48	128.40
2	B	126	THR	C-N-CD	9.13	147.58	128.40
1	A	313	LYS	C-N-CD	9.08	147.47	128.40
1	A	389	VAL	C-N-CD	8.38	145.99	128.40
1	A	444	TYR	CB-CG-CD1	-8.29	116.02	121.00
1	A	22	TYR	CB-CG-CD1	8.05	125.83	121.00
2	B	146	ALA	C-N-CD	8.01	145.22	128.40
2	B	70	ASP	CB-CG-OD2	7.98	125.48	118.30
2	B	34	ASN	O-C-N	-6.59	112.15	122.70
2	B	82	VAL	CA-CB-CG1	6.56	120.73	110.90
1	A	312	ASP	CB-CG-OD1	6.41	124.06	118.30
2	B	147	PRO	CA-N-CD	-6.08	102.98	111.50
1	A	390	PRO	CA-N-CD	-5.90	103.24	111.50
1	A	314	PRO	CA-N-CD	-5.89	103.25	111.50
2	B	127	PRO	CA-N-CD	-5.83	103.34	111.50
1	A	444	TYR	CB-CG-CD2	5.73	124.44	121.00
1	A	340	PRO	CA-N-CD	-5.72	103.49	111.50
1	A	367	ASP	CB-CG-OD1	5.25	123.03	118.30
2	B	196	ASP	CB-CG-OD2	5.24	123.02	118.30
2	B	146	ALA	CA-C-N	-5.20	102.54	117.10
1	A	446	ASN	O-C-N	-5.19	114.39	122.70
1	A	389	VAL	CA-C-N	-5.16	102.65	117.10
2	B	34	ASN	CA-C-O	5.13	130.87	120.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	ARG	Mainchain

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	4018	0	3773	95	0
2	B	2641	0	2537	47	0
3	C	676	0	667	32	1
4	A	2	0	0	0	0
5	A	1	0	0	1	0
6	B	5	0	0	0	0
7	A	5	0	3	0	0
8	A	114	0	0	5	0
8	B	118	0	0	1	0
8	C	10	0	0	0	0
All	All	7590	0	6980	152	1

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 11.

All (152) 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)
3:C:75:PRO:O	3:C:76:THR:HG22	1.75	0.86
3:C:13:ASP:OD1	3:C:42:ARG:HD2	1.78	0.84
1:A:190:ILE:HD12	1:A:242:LEU:HG	1.61	0.83
1:A:9:TRP:HB3	2:B:174:ARG:HG3	1.61	0.82
1:A:139:GLN:HE22	2:B:83:TYR:H	1.26	0.81
1:A:53:ILE:HD13	1:A:54:THR:N	1.99	0.78
1:A:398:ASN:HD22	1:A:427:HIS:H	1.31	0.76
1:A:2:SER:N	2:B:105:ASN:HD22	1.84	0.75
1:A:367:ASP:HB3	1:A:410:ASN:HD22	1.53	0.73
1:A:92:THR:HG23	1:A:276:ILE:HD13	1.69	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:TYR:O	1:A:492:GLN:HB2	1.90	0.72
1:A:304:ARG:HH21	1:A:307:LEU:HD23	1.55	0.71
1:A:427:HIS:HE1	3:C:76:THR:HG23	1.53	0.71
1:A:113:ARG:HH11	2:B:144:GLN:HE21	1.39	0.71
2:B:18:LEU:O	2:B:21:ASN:HB2	1.90	0.71
3:C:11:GLU:HG2	3:C:12:ARG:HG3	1.74	0.70
2:B:168:HIS:HD2	2:B:257:GLN:HE21	1.38	0.69
1:A:289:SER:OG	1:A:292:GLU:HG3	1.92	0.69
1:A:314:PRO:HD2	1:A:317:TRP:CE3	2.28	0.69
1:A:153:ARG:CZ	2:B:12:LEU:HD21	2.24	0.68
3:C:56:HIS:HD2	3:C:80:ASP:OD1	1.77	0.68
1:A:353:GLU:O	1:A:356:GLU:HG2	1.94	0.67
1:A:427:HIS:CE1	3:C:76:THR:HG23	2.29	0.67
2:B:111:GLN:H	2:B:111:GLN:NE2	1.92	0.67
1:A:7:GLU:H	1:A:7:GLU:CD	1.97	0.66
1:A:304:ARG:NH2	1:A:307:LEU:HD23	2.09	0.66
2:B:21:ASN:O	2:B:22:ARG:HB3	1.96	0.66
1:A:317:TRP:O	1:A:321:MET:HG2	1.96	0.65
2:B:111:GLN:H	2:B:111:GLN:HE21	1.45	0.65
3:C:62:PHE:HB3	3:C:66:MET:HE2	1.77	0.65
1:A:416:ASP:OD2	1:A:427:HIS:HD2	1.79	0.64
1:A:427:HIS:HE1	3:C:76:THR:CG2	2.10	0.64
1:A:57:GLU:O	1:A:61:ILE:HD13	1.99	0.63
1:A:189:SER:O	1:A:193:THR:HB	2.01	0.61
1:A:338:TRP:CD1	1:A:390:PRO:HG3	2.36	0.60
1:A:326:GLU:HG2	1:A:407:THR:OG1	2.03	0.59
1:A:203:MET:HG2	1:A:297:TRP:HB3	1.84	0.59
1:A:140:ILE:HG21	1:A:227:ILE:HD11	1.83	0.59
3:C:28:ASP:OD2	3:C:64:ARG:HB3	2.03	0.59
2:B:168:HIS:CD2	2:B:257:GLN:HE21	2.19	0.58
1:A:19:THR:O	2:B:203:ARG:NH2	2.36	0.58
3:C:55:ARG:HD2	3:C:58:ASP:OD1	2.04	0.58
1:A:53:ILE:HD13	1:A:54:THR:H	1.69	0.57
1:A:416:ASP:H	3:C:56:HIS:CE1	2.21	0.57
1:A:137:HIS:CD2	1:A:227:ILE:HD12	2.40	0.57
2:B:59:LYS:HA	2:B:63:PHE:HD2	1.70	0.57
1:A:9:TRP:CB	2:B:174:ARG:HG3	2.34	0.57
2:B:12:LEU:N	2:B:12:LEU:HD22	2.20	0.56
1:A:398:ASN:ND2	1:A:427:HIS:H	2.01	0.56
1:A:190:ILE:HD12	1:A:242:LEU:CG	2.34	0.56
1:A:413:ASN:OD1	1:A:415:LYS:HE2	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:MET:HE3	1:A:97:PHE:HE2	1.70	0.55
3:C:26:THR:HG22	3:C:64:ARG:O	2.07	0.55
1:A:243:LYS:O	1:A:247:GLU:HG2	2.07	0.54
1:A:305:GLN:O	1:A:309:LEU:HD13	2.08	0.54
1:A:68:GLY:O	1:A:72:ILE:HG12	2.07	0.54
1:A:418:GLN:HE22	3:C:78:THR:H	1.55	0.53
1:A:24:THR:OG1	1:A:27:GLU:HG3	2.08	0.53
2:B:162:HIS:HE1	2:B:227:LYS:HZ2	1.55	0.53
1:A:187:ALA:HB2	1:A:257:MET:HE1	1.91	0.53
1:A:425:LEU:HD23	3:C:76:THR:CG2	2.39	0.52
1:A:47:TYR:CE1	1:A:240:PRO:HB2	2.44	0.52
8:A:585:HOH:O	2:B:82:VAL:HG13	2.10	0.52
3:C:82:ILE:HD13	3:C:82:ILE:H	1.75	0.52
1:A:240:PRO:O	1:A:244:ILE:HG12	2.10	0.51
2:B:322:ARG:O	2:B:326:GLN:HG3	2.10	0.51
1:A:336:TRP:CH2	1:A:339:ARG:NH2	2.80	0.50
3:C:39:ILE:O	3:C:40:ASN:HB2	2.12	0.50
1:A:193:THR:HG21	1:A:237:GLN:HB2	1.94	0.49
2:B:305:SER:HB3	2:B:314:ILE:HD11	1.95	0.49
1:A:46:LYS:HD2	8:A:603:HOH:O	2.11	0.49
1:A:491:TYR:O	1:A:492:GLN:CB	2.60	0.49
1:A:336:TRP:O	1:A:339:ARG:HB3	2.13	0.49
1:A:274:GLY:HA2	1:A:290:PHE:CD1	2.48	0.49
2:B:143:HIS:CD2	2:B:143:HIS:C	2.86	0.49
1:A:460:GLN:HA	1:A:461:PRO:C	2.34	0.48
1:A:288:GLN:NE2	1:A:293:PHE:HA	2.28	0.48
3:C:75:PRO:O	3:C:76:THR:CG2	2.53	0.48
1:A:425:LEU:HD23	3:C:76:THR:HG22	1.96	0.48
2:B:33:THR:HB	2:B:34:ASN:HD22	1.78	0.48
1:A:421:TYR:HE2	1:A:445:LYS:HE2	1.78	0.48
1:A:37:ARG:NH2	1:A:257:MET:HE1	2.28	0.48
2:B:201:GLY:HA3	2:B:299:ALA:HA	1.95	0.48
2:B:81:LEU:HD11	2:B:263:ARG:HD3	1.96	0.48
1:A:166:GLU:OE1	1:A:168:ALA:HB3	2.13	0.48
1:A:53:ILE:HD13	1:A:54:THR:O	2.15	0.47
1:A:231:GLU:OE2	5:A:501:OH:O	2.32	0.47
2:B:127:PRO:HG2	2:B:199:TRP:CZ2	2.49	0.47
1:A:353:GLU:CD	1:A:353:GLU:H	2.18	0.47
1:A:193:THR:CG2	1:A:238:GLY:H	2.28	0.47
2:B:249:LEU:HD23	2:B:249:LEU:C	2.35	0.47
1:A:193:THR:HG22	1:A:238:GLY:H	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ARG:HH11	1:A:78:ARG:HB3	1.80	0.46
1:A:95:LEU:HD13	1:A:344:TRP:CZ3	2.50	0.46
1:A:95:LEU:HD23	1:A:276:ILE:HD11	1.97	0.46
1:A:194:PHE:O	1:A:198:THR:HB	2.16	0.46
1:A:193:THR:HG23	1:A:235:ALA:C	2.36	0.46
1:A:113:ARG:HH11	2:B:144:GLN:NE2	2.09	0.45
1:A:204:GLN:HB2	1:A:269:PHE:HZ	1.80	0.45
2:B:23:ARG:HH11	2:B:23:ARG:HG3	1.81	0.45
1:A:325:ASP:O	1:A:329:HIS:HD2	2.00	0.45
1:A:299:VAL:O	1:A:303:GLU:HG3	2.17	0.45
1:A:190:ILE:CD1	1:A:242:LEU:HG	2.40	0.44
2:B:23:ARG:HG3	2:B:23:ARG:NH1	2.31	0.44
8:A:584:HOH:O	2:B:36:HIS:HD2	2.00	0.44
1:A:53:ILE:HD11	1:A:58:TYR:N	2.32	0.44
3:C:66:MET:HE3	3:C:71:ALA:HB2	2.00	0.44
1:A:22:TYR:CD2	2:B:204:GLU:HA	2.53	0.44
3:C:11:GLU:O	3:C:12:ARG:HB2	2.18	0.44
1:A:162:ILE:O	1:A:162:ILE:HG22	2.18	0.44
1:A:259:ASP:OD1	1:A:314:PRO:HG3	2.18	0.43
2:B:133:HIS:O	2:B:136:GLN:HB3	2.18	0.43
1:A:344:TRP:O	1:A:346:PRO:HD3	2.18	0.43
1:A:467:ALA:O	1:A:471:MET:HG3	2.18	0.43
1:A:113:ARG:HD3	2:B:144:GLN:NE2	2.34	0.43
3:C:10:PHE:CE1	3:C:81:ILE:HG21	2.54	0.43
1:A:116:ARG:HB2	2:B:140:VAL:HG13	1.99	0.43
1:A:116:ARG:HB2	2:B:140:VAL:CG1	2.49	0.43
3:C:26:THR:CG2	3:C:64:ARG:O	2.66	0.42
2:B:43:GLU:H	2:B:43:GLU:CD	2.21	0.42
2:B:36:HIS:HE1	2:B:152:THR:OG1	2.01	0.42
1:A:247:GLU:HG3	8:A:536:HOH:O	2.20	0.42
1:A:339:ARG:HD2	1:A:480:ASP:HA	2.00	0.42
1:A:270:SER:O	1:A:275:PRO:HD3	2.20	0.42
3:C:6:ILE:HD12	3:C:6:ILE:C	2.40	0.42
1:A:193:THR:CG2	1:A:235:ALA:O	2.68	0.42
1:A:175:PHE:CE1	1:A:179:MET:HG3	2.55	0.42
3:C:7:MET:HG2	3:C:76:THR:O	2.20	0.42
2:B:104:LEU:HD23	2:B:104:LEU:HA	1.86	0.42
1:A:78:ARG:NH1	1:A:78:ARG:HB3	2.35	0.42
2:B:289:VAL:O	2:B:293:GLU:HB2	2.20	0.42
3:C:48:GLU:OE1	3:C:48:GLU:C	2.58	0.41
1:A:190:ILE:HD12	1:A:242:LEU:CD2	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ILE:CD1	1:A:54:THR:O	2.68	0.41
3:C:44:HIS:HA	3:C:45:PRO:HD3	1.88	0.41
3:C:50:ILE:HD13	3:C:64:ARG:NH1	2.36	0.41
3:C:62:PHE:CG	3:C:66:MET:HE2	2.56	0.41
2:B:60:LYS:HE3	2:B:61:TYR:CE1	2.55	0.41
3:C:56:HIS:CD2	3:C:80:ASP:OD1	2.66	0.41
2:B:145:ILE:HG13	2:B:145:ILE:O	2.21	0.41
1:A:115:ALA:HB3	2:B:140:VAL:HG21	2.02	0.40
2:B:154:CYS:HB3	2:B:267:TRP:CE2	2.56	0.40
2:B:161:ASP:O	2:B:164:ARG:HB3	2.21	0.40
1:A:391:GLU:OE2	3:C:41:ARG:NH2	2.54	0.40
3:C:62:PHE:CB	3:C:66:MET:HE2	2.49	0.40
2:B:98:GLN:HG2	8:B:435:HOH:O	2.21	0.40
1:A:178:ASP:HA	2:B:48:LEU:HD11	2.03	0.40
1:A:183:ARG:HB3	1:A:187:ALA:HB3	2.03	0.40
3:C:39:ILE:HG23	3:C:45:PRO:HG3	2.04	0.40
2:B:94:GLU:O	2:B:98:GLN:HG3	2.21	0.40
1:A:228:GLN:HG2	8:A:616:HOH:O	2.20	0.40
2:B:162:HIS:HE1	2:B:227:LYS:NZ	2.19	0.40

All (1) 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)
3:C:32:GLU:OE1	3:C:32:GLU:OE1[6_555]	1.87	0.33

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	489/498 (98%)	472 (96%)	15 (3%)	2 (0%)	39 34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	320/330 (97%)	313 (98%)	6 (2%)	1 (0%)	46 42
3	C	81/86 (94%)	76 (94%)	5 (6%)	0	100 100
All	All	890/914 (97%)	861 (97%)	26 (3%)	3 (0%)	46 42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	22	ARG
1	A	408	PRO
1	A	445	LYS

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	417/422 (99%)	408 (98%)	9 (2%)	60 63
2	B	274/282 (97%)	268 (98%)	6 (2%)	60 63
3	C	77/79 (98%)	74 (96%)	3 (4%)	39 36
All	All	768/783 (98%)	750 (98%)	18 (2%)	58 62

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	MET
1	A	7	GLU
1	A	53	ILE
1	A	228	GLN
1	A	269	PHE
1	A	283	LEU
1	A	326	GLU
1	A	390	PRO
1	A	408	PRO
2	B	43	GLU
2	B	89	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	111	GLN
2	B	166	LEU
2	B	174	ARG
2	B	188	ARG
3	C	48	GLU
3	C	76	THR
3	C	82	ILE

Some 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	228	GLN
1	A	248	ASN
1	A	287	ASN
1	A	288	GLN
1	A	322	GLN
1	A	379	ASN
1	A	398	ASN
1	A	418	GLN
1	A	427	HIS
2	B	17	HIS
2	B	34	ASN
2	B	36	HIS
2	B	73	ASN
2	B	80	GLN
2	B	87	ASN
2	B	111	GLN
2	B	144	GLN
2	B	153	ASN
2	B	162	HIS
2	B	168	HIS
3	C	56	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is modelled with single atom and 2 are monoatomic - 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	$\#\|Z\| > 2$
7	MCR	A	502	4	1,4,4	0.45	0	0,4,4	0.00	-
6	SO4	B	331	-	4,4,4	0.25	0	6,6,6	0.10	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
7	MCR	A	502	4	-	0/0/2/2	0/0/0/0
6	SO4	B	331	-	-	0/0/0/0	0/0/0/0

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.22	22 (4%) 37 48	23, 38, 56, 69	0
2	B	322/330 (97%)	0.17	20 (6%) 24 33	14, 32, 52, 82	0
3	C	83/86 (96%)	0.51	4 (4%) 34 45	35, 48, 63, 72	0
All	All	896/914 (98%)	0.23	46 (5%) 32 42	14, 37, 57, 82	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	21	ASN	4.7
1	A	51	TYR	4.7
1	A	249	GLY	4.7
2	B	22	ARG	4.3
3	C	48	GLU	4.3
2	B	23	ARG	4.2
1	A	78	ARG	4.1
2	B	20	GLY	4.1
2	B	8	ALA	4.1
1	A	287	ASN	4.0
3	C	47	PRO	3.7
1	A	304	ARG	3.4
2	B	24	ARG	3.4
1	A	356	GLU	3.2
1	A	297	TRP	3.2
2	B	10	LYS	3.2
1	A	367	ASP	3.1
1	A	331	MET	3.1
2	B	137	MET	3.0
2	B	311	GLU	2.9
1	A	284	GLU	2.9
1	A	296	GLU	2.9
1	A	307	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	135	LEU	2.8
1	A	492	GLN	2.7
1	A	180	MET	2.7
2	B	279	GLU	2.7
2	B	166	LEU	2.6
2	B	13	LYS	2.6
2	B	312	ASN	2.6
1	A	79	ASP	2.6
2	B	131	LEU	2.5
1	A	114	MET	2.4
2	B	9	LEU	2.4
3	C	62	PHE	2.4
2	B	309	ASP	2.3
1	A	5	LYS	2.3
1	A	80	GLY	2.3
2	B	19	ALA	2.3
1	A	381	VAL	2.2
2	B	128	ALA	2.2
3	C	50	ILE	2.2
1	A	191	MET	2.1
2	B	142	ILE	2.1
1	A	410	ASN	2.1
1	A	179	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
7	MCR	A	502	5/5	0.87	0.20	1.78	55,56,61,61	0
5	OH	A	501	1/1	0.99	0.12	0.20	26,26,26,26	0
4	FE	A	500	1/1	1.00	0.09	-1.79	29,29,29,29	0
4	FE	A	499	1/1	0.99	0.09	-2.08	34,34,34,34	0
6	SO4	B	331	5/5	0.94	0.29	-	85,86,87,87	0

6.5 Other polymers (i)

There are no such residues in this entry.