Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 07:29 PM GMT

PDB ID	:	1FUR
Title	:	FUMARASE MUTANT H188N WITH BOUND SUBSTRATE L-MALATE AT PUTATIVE ACTIVATOR SITE
Authors	:	Weaver, T.M.; Lees, M.; Banaszak, L.J.
Deposited on	:	1997-01-09
Resolution	:	1.95 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:

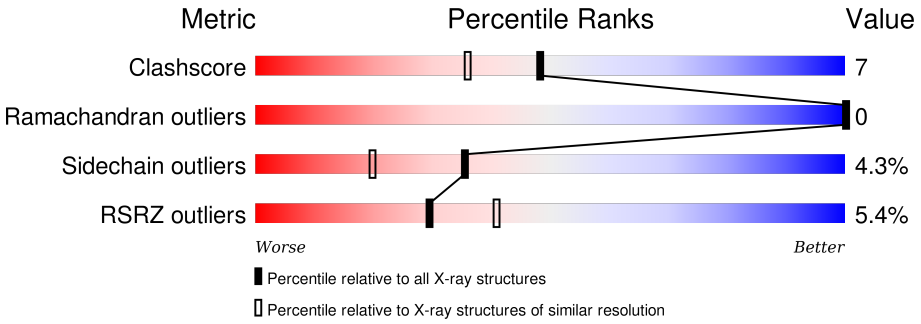
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.95 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	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	467	9% 78% 18%
1	B	467	% 84% 12%

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
2	MLT	A	468	X	-	X	-
2	MLT	B	468	X	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9695 atoms, of which 2368 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.

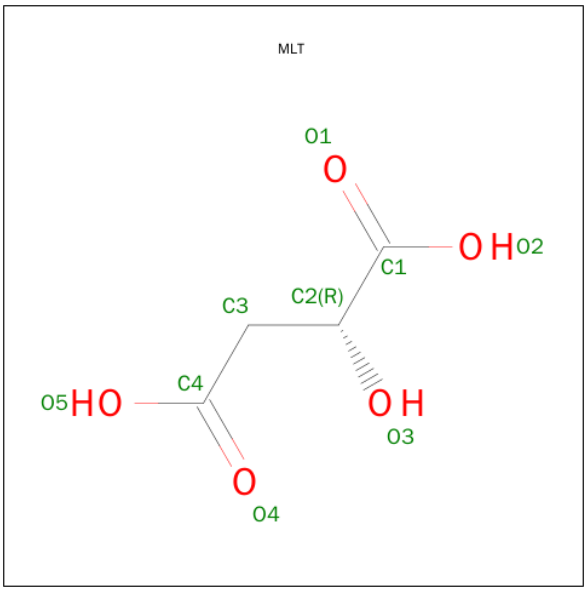
- Molecule 1 is a protein called FUMARASE C.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	456	Total	C	H	N	O	S	0	0	0
			4235	2156	781	616	659	23			
1	B	455	Total	C	H	N	O	S	0	0	0
			4236	2155	783	616	658	24			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	ASN	HIS	ENGINEERED	UNP P05042
B	188	ASN	HIS	ENGINEERED	UNP P05042

- Molecule 2 is MALATE ION (three-letter code: MLT) (formula: $C_4H_6O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	4	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			9	4	5		

- Molecule 3 is water.

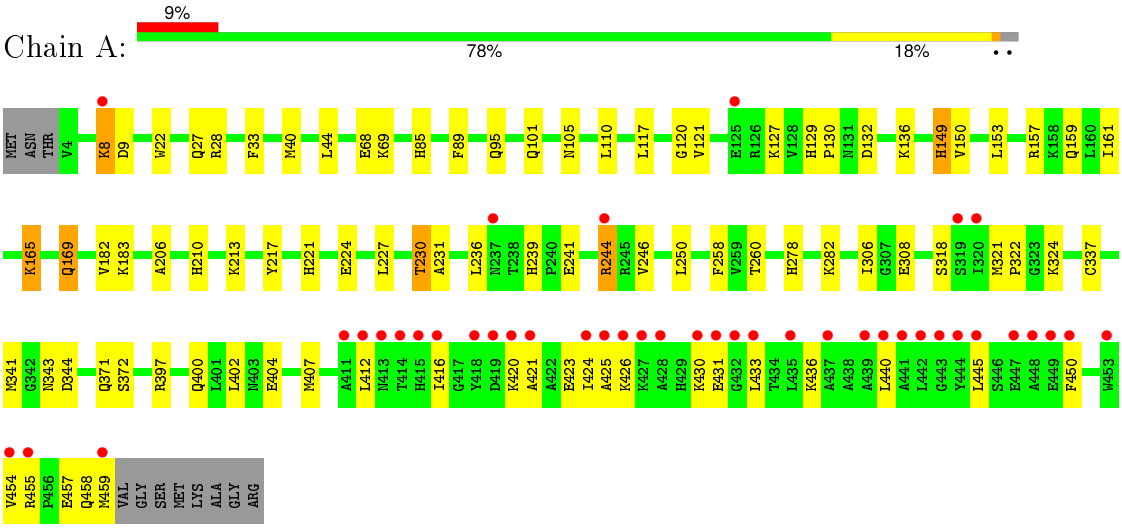
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	215	Total	H	O	0	0
			645	430	215		
3	B	187	Total	H	O	0	0
			561	374	187		

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.

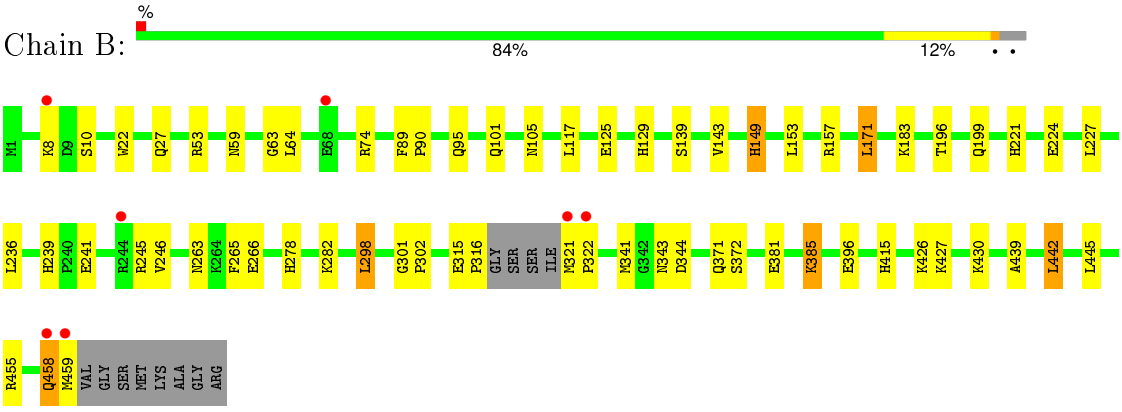
- Molecule 1: FUMARASE C

Chain A:



- Molecule 1: FUMARASE C

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	104.03Å 219.32Å 86.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.95 14.50 – 1.82	Depositor EDS
% Data completeness (in resolution range)	87.6 (8.00-1.95) 80.3 (14.50-1.82)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	0.25 (at 1.82Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.170 , 0.209 0.172 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	15.3	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 58.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 79307 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9695	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 5.51% 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: MLT

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	0.33	0/3511	0.58	0/4756
1	B	0.34	0/3509	0.58	0/4752
All	All	0.33	0/7020	0.58	0/9508

There are no bond length outliers.

There are no bond angle outliers.

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	3454	781	3472	61	1
1	B	3453	783	3472	43	1
2	A	9	0	3	4	0
2	B	9	0	3	2	0
3	A	215	430	0	7	1
3	B	187	374	0	5	1
All	All	7327	2368	6950	101	2

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 7.

All (101) 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:B:89:PHE:HA	1:B:105:ASN:HD21	1.52	0.74
1:A:343:ASN:HD21	1:A:371:GLN:HE21	1.34	0.73
1:B:263:ASN:HD22	1:B:266:GLU:H	1.38	0.71
1:B:439:ALA:HB1	1:B:445:LEU:HD21	1.70	0.71
1:A:407:MET:SD	1:B:321:MET:HG2	2.30	0.71
1:A:431:GLU:HB3	1:A:433:LEU:HD13	1.73	0.69
1:A:230:THR:HG23	1:A:231:ALA:H	1.58	0.68
1:A:230:THR:CG2	1:A:231:ALA:H	2.07	0.67
1:A:423:GLU:HA	1:A:426:LYS:HD2	1.76	0.67
1:A:85:HIS:HD2	3:A:535:HOH:O	1.80	0.65
1:A:455:ARG:HH11	1:A:458:GLN:HE22	1.44	0.64
1:B:426:LYS:O	1:B:430:LYS:HD3	1.97	0.64
1:B:343:ASN:HD21	1:B:371:GLN:HE21	1.45	0.63
1:B:125:GLU:HG2	3:B:575:HOH:O	1.97	0.62
1:B:415:HIS:HD2	3:B:557:HOH:O	1.82	0.62
1:B:415:HIS:HE1	3:B:556:HOH:O	1.82	0.61
1:B:196:THR:H	1:B:199:GLN:HE21	1.50	0.60
1:A:445:LEU:HD13	1:A:450:PHE:HB2	1.83	0.60
1:A:230:THR:HG21	1:A:236:LEU:O	2.02	0.60
1:A:244:ARG:NH1	1:A:260:THR:H	2.00	0.59
1:A:95:GLN:HB2	1:A:101:GLN:OE1	2.04	0.58
1:A:230:THR:HG22	3:A:486:HOH:O	2.02	0.57
1:B:427:LYS:HE2	1:B:442:LEU:HD13	1.85	0.57
1:A:244:ARG:HH12	1:A:260:THR:H	1.53	0.57
1:A:230:THR:CG2	1:A:231:ALA:N	2.68	0.56
1:B:139:SER:O	1:B:143:VAL:HG23	2.05	0.56
1:B:22:TRP:HE1	1:B:27:GLN:NE2	2.03	0.56
1:A:89:PHE:HA	1:A:105:ASN:HD21	1.71	0.56
1:B:439:ALA:HB1	1:B:445:LEU:CD2	2.36	0.56
1:A:149:HIS:HD2	1:A:224:GLU:O	1.90	0.54
1:A:343:ASN:HD21	1:A:371:GLN:NE2	2.05	0.54
1:B:263:ASN:HD21	1:B:265:PHE:HB2	1.72	0.54
1:B:196:THR:H	1:B:199:GLN:NE2	2.06	0.54
1:B:95:GLN:HB2	1:B:101:GLN:NE2	2.23	0.54
1:B:227:LEU:HD23	1:B:246:VAL:HG21	1.90	0.54
1:B:278:HIS:HE1	1:B:372:SER:OG	1.91	0.54
1:A:9:ASP:HB2	3:A:604:HOH:O	2.07	0.53
1:A:129:HIS:HD2	2:A:468:MLT:O4	1.92	0.53
1:B:59:ASN:HD22	1:B:64:LEU:HD12	1.72	0.53
1:A:455:ARG:NH1	1:A:458:GLN:HE22	2.08	0.52
1:A:412:LEU:O	1:A:416:ILE:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:TRP:HE1	1:A:27:GLN:NE2	2.08	0.52
1:A:33:PHE:HE2	1:A:101:GLN:HE22	1.52	0.51
1:B:455:ARG:O	1:B:458:GLN:HG3	2.11	0.50
1:B:22:TRP:HE1	1:B:27:GLN:HE21	1.58	0.50
1:A:400:GLN:O	1:A:404:GLU:HB2	2.11	0.50
1:A:182:VAL:HG21	1:A:457:GLU:HA	1.92	0.50
1:A:22:TRP:HE1	1:A:27:GLN:HE21	1.60	0.49
1:A:318:SER:HB2	1:A:321:MET:HB2	1.93	0.49
1:A:306:ILE:HG22	1:A:308:GLU:HG3	1.93	0.49
1:A:40:MET:SD	1:A:44:LEU:HD23	2.51	0.49
1:A:121:VAL:HG12	3:A:582:HOH:O	2.12	0.49
1:B:149:HIS:HD2	1:B:224:GLU:O	1.94	0.49
1:B:278:HIS:HD2	1:B:344:ASP:OD1	1.96	0.49
1:B:241:GLU:O	1:B:245:ARG:HG3	2.13	0.49
1:A:421:ALA:O	1:A:424:ILE:HG12	2.13	0.48
1:A:169:GLN:NE2	3:A:570:HOH:O	2.46	0.48
1:A:129:HIS:CD2	2:A:468:MLT:H32	2.49	0.48
1:B:239:HIS:HD2	1:B:241:GLU:H	1.61	0.48
1:A:161:ILE:HG22	1:A:165:LYS:HE2	1.96	0.47
1:A:454:VAL:O	1:A:454:VAL:HG13	2.15	0.47
1:A:8:LYS:HB2	1:A:8:LYS:NZ	2.29	0.47
1:B:63:GLY:HA2	3:B:567:HOH:O	2.14	0.47
1:A:278:HIS:HD2	1:A:344:ASP:OD1	1.97	0.46
1:A:239:HIS:CD2	1:A:241:GLU:H	2.34	0.46
1:B:427:LYS:HE2	1:B:442:LEU:CD1	2.45	0.46
1:B:53:ARG:HG3	1:B:74:ARG:HG3	1.98	0.45
1:A:149:HIS:HE1	3:A:500:HOH:O	1.99	0.45
1:A:450:PHE:O	1:A:454:VAL:HG12	2.17	0.45
1:B:149:HIS:HE1	3:B:488:HOH:O	2.00	0.45
1:A:425:ALA:HB1	1:B:322:PRO:HG2	1.99	0.45
1:A:206:ALA:O	1:A:210:HIS:HD2	2.00	0.45
1:A:132:ASP:O	1:A:136:LYS:HE3	2.17	0.44
1:A:210:HIS:CE1	3:A:588:HOH:O	2.71	0.44
1:A:227:LEU:HD13	1:A:246:VAL:HG21	1.99	0.44
1:A:420:LYS:HD3	1:A:420:LYS:HA	1.80	0.44
1:A:436:LYS:O	1:A:440:LEU:HG	2.18	0.43
1:B:239:HIS:CD2	1:B:241:GLU:H	2.36	0.43
1:A:120:GLY:CA	1:A:127:LYS:HE2	2.49	0.43
1:A:68:GLU:HG3	1:A:69:LYS:N	2.32	0.43
1:A:213:LYS:HG2	1:A:217:TYR:CE2	2.54	0.43
1:B:263:ASN:ND2	1:B:266:GLU:H	2.11	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:CYS:O	1:A:341:MET:HG2	2.19	0.42
1:A:321:MET:CE	1:A:324:LYS:HD3	2.50	0.42
1:A:244:ARG:HD3	1:A:244:ARG:HA	1.72	0.42
1:A:130:PRO:HG2	2:A:468:MLT:O1	2.18	0.42
1:B:315:GLU:HB3	1:B:316:PRO:HD2	2.01	0.42
1:A:322:PRO:HG3	1:B:426:LYS:HA	2.02	0.42
1:A:120:GLY:HA2	1:A:127:LYS:HE2	2.01	0.42
1:B:171:LEU:HA	1:B:171:LEU:HD12	1.92	0.41
1:A:278:HIS:HE1	1:A:372:SER:OG	2.03	0.41
1:A:150:VAL:HA	1:A:258:PHE:CZ	2.55	0.41
1:B:301:GLY:HA3	1:B:302:PRO:HA	1.91	0.41
1:A:153:LEU:HG	1:A:157:ARG:HD3	2.02	0.41
1:B:381:GLU:HG2	1:B:385:LYS:HE2	2.02	0.41
1:A:129:HIS:CD2	2:A:468:MLT:O4	2.73	0.40
1:B:298:LEU:HD12	1:B:298:LEU:HA	1.92	0.40
1:B:8:LYS:HE3	1:B:8:LYS:HB2	1.76	0.40
1:B:153:LEU:HG	1:B:157:ARG:HD3	2.04	0.40
1:B:129:HIS:CG	2:B:468:MLT:H32	2.56	0.40
1:B:129:HIS:HB3	2:B:468:MLT:O2	2.21	0.40

All (2) 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)
1:A:183:LYS:HZ2	3:B:477:HOH:H1[3_756]	1.21	0.39
1:B:183:LYS:HZ2	3:A:473:HOH:H2[3_756]	1.31	0.29

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	454/467 (97%)	441 (97%)	13 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	451/467 (97%)	439 (97%)	12 (3%)	0	100 100
All	All	905/934 (97%)	880 (97%)	25 (3%)	0	100 100

There are no Ramachandran outliers to report.

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	368/376 (98%)	351 (95%)	17 (5%)	33 17
1	B	368/376 (98%)	353 (96%)	15 (4%)	37 22
All	All	736/752 (98%)	704 (96%)	32 (4%)	35 20

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	28	ARG
1	A	110	LEU
1	A	117	LEU
1	A	149	HIS
1	A	159	GLN
1	A	165	LYS
1	A	169	GLN
1	A	221	HIS
1	A	230	THR
1	A	244	ARG
1	A	250	LEU
1	A	282	LYS
1	A	397	ARG
1	A	402	LEU
1	A	430	LYS
1	A	459	MET
1	B	10	SER

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Mol	Chain	Res	Type
1	B	90	PRO
1	B	117	LEU
1	B	149	HIS
1	B	171	LEU
1	B	221	HIS
1	B	236	LEU
1	B	282	LYS
1	B	298	LEU
1	B	341	MET
1	B	385	LYS
1	B	396	GLU
1	B	442	LEU
1	B	458	GLN
1	B	459	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	85	HIS
1	A	105	ASN
1	A	129	HIS
1	A	149	HIS
1	A	163	GLN
1	A	169	GLN
1	A	190	GLN
1	A	210	HIS
1	A	239	HIS
1	A	278	HIS
1	A	329	GLN
1	A	339	GLN
1	A	368	ASN
1	A	371	GLN
1	A	384	ASN
1	A	399	ASN
1	A	413	ASN
1	A	458	GLN
1	B	25	GLN
1	B	27	GLN
1	B	59	ASN
1	B	101	GLN
1	B	105	ASN

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Mol	Chain	Res	Type
1	B	149	HIS
1	B	163	GLN
1	B	199	GLN
1	B	239	HIS
1	B	263	ASN
1	B	278	HIS
1	B	314	ASN
1	B	329	GLN
1	B	339	GLN
1	B	368	ASN
1	B	371	GLN
1	B	399	ASN
1	B	415	HIS
1	B	429	HIS
1	B	458	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 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	$\#\|Z\|>2$
2	MLT	A	468	-	1,8,8	0.78	0	2,10,10	3.17	2 (100%)
2	MLT	B	468	-	1,8,8	0.83	0	2,10,10	3.00	2 (100%)

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
2	MLT	A	468	-	1/1/3/3	0/2/8/8	0/0/0/0
2	MLT	B	468	-	1/1/3/3	0/2/8/8	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	468	MLT	O3-C2-C1	-2.58	103.53	111.44
2	A	468	MLT	O3-C2-C1	-2.57	103.55	111.44
2	B	468	MLT	C3-C2-C1	3.36	116.01	111.19
2	A	468	MLT	C3-C2-C1	3.67	116.45	111.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	468	MLT	C2
2	B	468	MLT	C2

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	468	MLT	4	0
2	B	468	MLT	2	0

5.7 Other polymers (i)

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	456/467 (97%)	0.18	42 (9%) 11 18	4, 16, 78, 92	0
1	B	455/467 (97%)	-0.17	7 (1%) 76 84	4, 15, 38, 83	0
All	All	911/934 (97%)	0.00	49 (5%) 29 41	4, 15, 65, 92	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	442	LEU	6.7
1	A	424	ILE	6.5
1	A	453	TRP	6.4
1	A	418	TYR	6.2
1	A	412	LEU	5.9
1	B	459	MET	5.5
1	A	414	THR	5.4
1	A	415	HIS	5.1
1	A	416	ILE	5.0
1	A	441	ALA	4.8
1	B	322	PRO	4.5
1	B	321	MET	4.4
1	B	458	GLN	4.1
1	A	425	ALA	4.1
1	A	419	ASP	4.1
1	A	420	LYS	4.0
1	A	433	LEU	3.8
1	A	450	PHE	3.8
1	A	439	ALA	3.8
1	A	448	ALA	3.7
1	A	426	LYS	3.7
1	A	444	TYR	3.5
1	A	455	ARG	3.5
1	A	445	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	319	SER	3.0
1	A	459	MET	3.0
1	A	430	LYS	2.9
1	A	431	GLU	2.8
1	A	447	GLU	2.8
1	A	413	ASN	2.7
1	A	435	LEU	2.7
1	A	449	GLU	2.5
1	A	427	LYS	2.5
1	A	125	GLU	2.5
1	A	437	ALA	2.5
1	A	428	ALA	2.4
1	A	244	ARG	2.4
1	A	432	GLY	2.4
1	A	421	ALA	2.4
1	A	443	GLY	2.3
1	B	68	GLU	2.3
1	A	320	ILE	2.2
1	A	454	VAL	2.2
1	A	237	ASN	2.1
1	A	411	ALA	2.1
1	A	440	LEU	2.1
1	B	8	LYS	2.0
1	B	244	ARG	2.0
1	A	8	LYS	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
2	MLT	B	468	9/9	0.79	0.22	2.29	38,42,43,49	0
2	MLT	A	468	9/9	0.88	0.16	0.04	34,38,41,42	0

6.5 Other polymers (i)

There are no such residues in this entry.