Full wwPDB X-ray Structure Validation Report (i)

Aug 7, 2023 – 04:03 AM EDT

PDB ID	:	1KQ7
Title	:	E315Q Mutant Form of Fumarase C from E.coli
Authors	:	Weaver, T.M.; Estevez, M.; Skarda, J.; Spencer, J.
Deposited on	:	2002-01-04
Resolution	:	2.60 Å(reported)

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

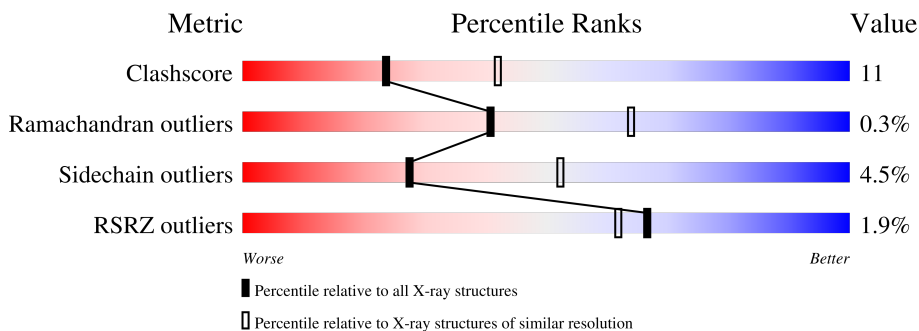|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.60 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	Percentile Ranks	Value
Clashscore		11
Ramachandran outliers		0.3%
Sidechain outliers		4.5%
RSRZ outliers		1.9%

Worse　　　　　　　　　　　　　　　　*Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	467	3% / 75% / 21% / · ·
1	B	467	75% / 21% / · ·

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	-
3	CIT	A	469	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CIT	B	468	-	X	X	X

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 6960 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 FUMARATE HYDRATASE CLASS II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	0	0
			3456	2158	618	657	23			
1	B	455	Total	C	N	O	S	0	0	0
			3451	2155	617	655	24			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	315	GLN	GLU	engineered mutation	UNP P05042
B	315	GLN	GLU	engineered mutation	UNP P05042

- Molecule 2 is D-MALATE (three-letter code: MLT) (formula: $C_4H_6O_5$).
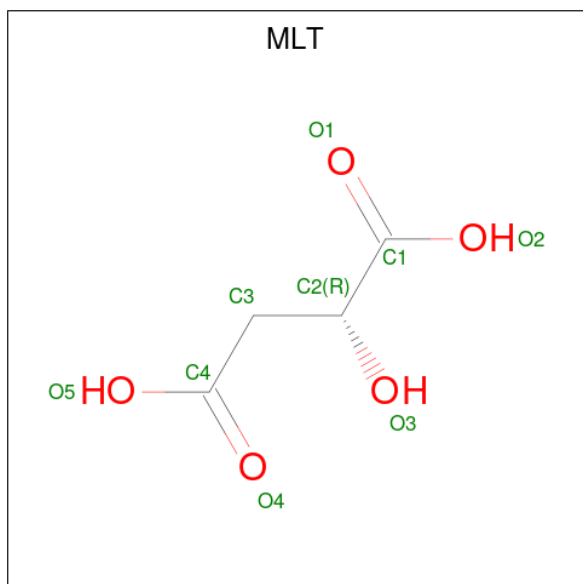
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	4	5		

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).
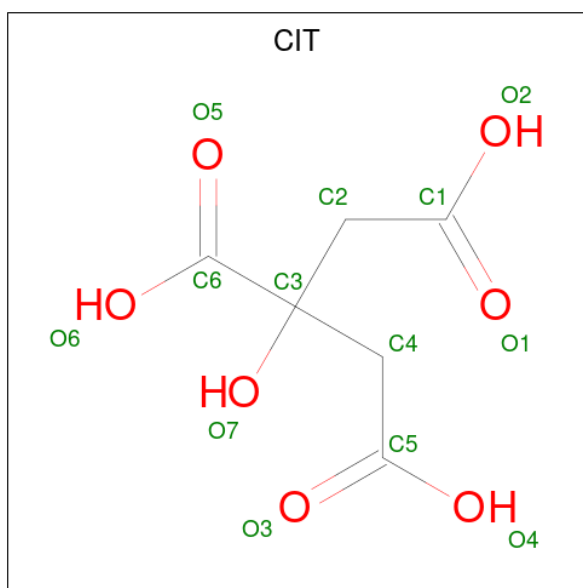
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total C O 13 6 7		0	0
3	B	1	Total C O 13 6 7		0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total O 8 8		0	0
4	B	10	Total O 10 10		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: FUMARATE HYDRATASE CLASS II

Chain A:

• Molecule 1: FUMARATE HYDRATASE CLASS II

Chain B:
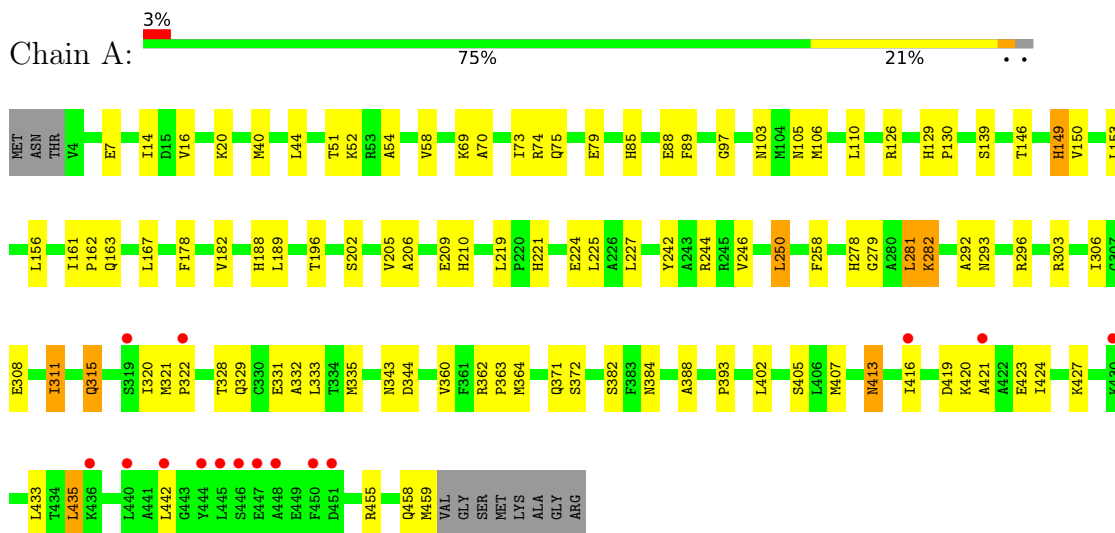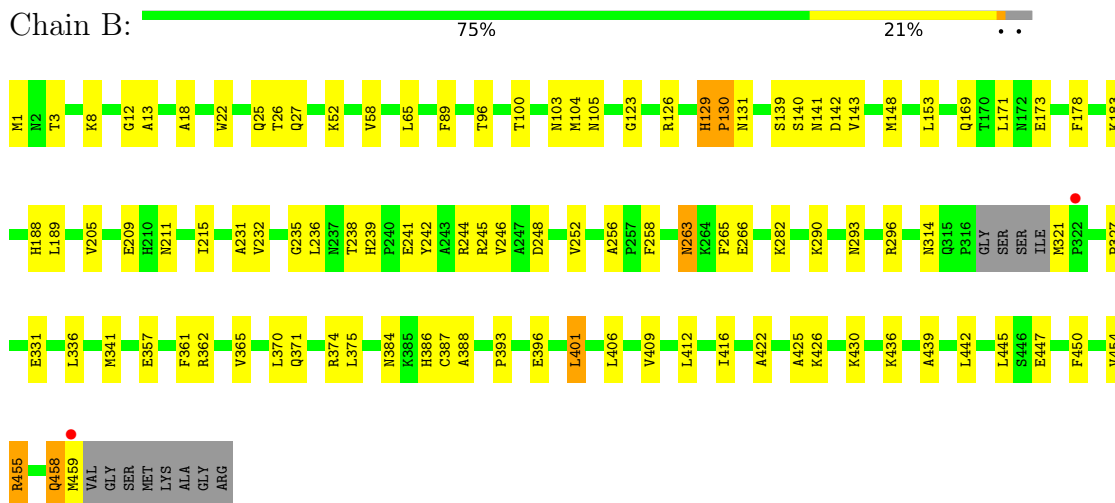
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	104.02Å　　220.00Å　　86.23Å 90.00°　　　90.00°　　　90.00°	Depositor
Resolution (Å)	8.00　–　2.60 47.02　–　2.58	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.60) 74.9 (47.02-2.58)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.18	Depositor
$< I/\sigma(I) >$ [1]	0.87 (at 2.58Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.179　,　　　0.251 0.191　,　(Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	16.2	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 30.9	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6960	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CIT, 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	0.28	0/3514	0.52	0/4760
1	B	0.30	0/3508	0.54	0/4751
All	All	0.29	0/7022	0.53	0/9511

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	3456	0	3475	74	0
1	B	3451	0	3469	70	0
2	A	9	0	3	4	0
3	A	13	0	2	1	0
3	B	13	0	8	16	0
4	A	8	0	0	0	0
4	B	10	0	0	0	0
All	All	6960	0	6957	155	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 11.

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PROTEIN DATA BANK

All (155) 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:B:468:CIT:C4	3:B:468:CIT:C5	2.17	1.22
3:B:468:CIT:C1	3:B:468:CIT:C2	2.20	1.19
3:B:468:CIT:C6	3:B:468:CIT:C3	2.22	1.18
3:B:468:CIT:C4	3:B:468:CIT:C3	2.22	1.17
3:B:468:CIT:C2	3:B:468:CIT:C3	2.23	1.16
3:B:468:CIT:C1	3:B:468:CIT:O1	1.97	1.12
3:B:468:CIT:C6	3:B:468:CIT:O5	1.98	1.12
3:B:468:CIT:C5	3:B:468:CIT:O4	1.99	1.11
3:B:468:CIT:C5	3:B:468:CIT:O3	1.98	1.11
3:B:468:CIT:C6	3:B:468:CIT:O6	1.99	1.10
3:B:468:CIT:C3	3:B:468:CIT:O7	2.01	1.08
3:B:468:CIT:C1	3:B:468:CIT:O2	2.01	1.07
1:A:343:ASN:HD21	1:A:371:GLN:HE21	1.10	0.93
1:B:22:TRP:HE1	1:B:27:GLN:HG2	1.38	0.89
1:B:439:ALA:HB1	1:B:445:LEU:HD21	1.60	0.84
1:B:293:ASN:HD21	1:B:296:ARG:HH21	1.34	0.76
1:A:424:ILE:HG22	1:A:442:LEU:HD12	1.71	0.73
1:A:343:ASN:HD21	1:A:371:GLN:NE2	1.86	0.71
1:A:427:LYS:HD2	1:A:442:LEU:HD11	1.75	0.69
1:B:293:ASN:HD22	1:B:296:ARG:HE	1.39	0.68
1:A:52:LYS:NZ	1:A:103:ASN:HD21	1.90	0.68
1:B:458:GLN:HE21	1:B:458:GLN:N	1.92	0.68
1:A:306:ILE:HG22	1:A:308:GLU:HG3	1.77	0.67
1:A:435:LEU:H	1:A:435:LEU:HD12	1.59	0.67
1:B:52:LYS:NZ	1:B:103:ASN:HD21	1.94	0.66
1:B:458:GLN:HE21	1:B:458:GLN:H	1.41	0.66
1:B:89:PHE:HA	1:B:105:ASN:HD21	1.62	0.65
1:A:129:HIS:ND1	2:A:468:MLT:H32	2.12	0.63
1:A:129:HIS:HB3	2:A:468:MLT:O2	1.99	0.63
1:A:163:GLN:HE21	1:A:163:GLN:HA	1.64	0.63
1:A:278:HIS:HA	1:A:281:LEU:HD23	1.81	0.63
1:B:235:GLY:O	1:B:238:THR:HG22	1.99	0.63
1:B:188:HIS:O	1:B:189:LEU:HB2	2.00	0.62
1:A:161:ILE:HB	1:A:162:PRO:HD3	1.81	0.61
1:B:293:ASN:ND2	1:B:296:ARG:HH21	1.98	0.61
1:A:182:VAL:HG12	1:A:196:THR:HG22	1.83	0.61
1:B:239:HIS:HD2	1:B:241:GLU:H	1.49	0.61
1:A:311:ILE:H	1:A:311:ILE:HD13	1.66	0.60
1:B:293:ASN:ND2	1:B:296:ARG:HE	1.99	0.59
3:B:468:CIT:C4	3:B:468:CIT:C6	2.81	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ASN:HD21	1:B:296:ARG:NH2	2.01	0.58
1:B:178:PHE:CZ	1:B:393:PRO:HD3	2.39	0.57
1:B:384:ASN:HA	1:B:388:ALA:HB3	1.86	0.57
1:A:413:ASN:HD22	1:A:413:ASN:N	2.03	0.56
1:A:40:MET:SD	1:A:44:LEU:HD23	2.45	0.56
1:A:202:SER:HA	1:A:205:VAL:HG12	1.88	0.56
1:A:106:MET:O	1:A:110:LEU:HB2	2.06	0.55
1:A:292:ALA:O	1:A:296:ARG:HG3	2.06	0.55
3:B:468:CIT:C6	3:B:468:CIT:H41	2.36	0.55
1:A:150:VAL:HA	1:A:258:PHE:CZ	2.42	0.55
1:A:139:SER:HB2	3:A:469:CIT:O2	2.07	0.55
1:A:405:SER:O	1:A:435:LEU:HD11	2.07	0.55
1:B:8:LYS:HB3	1:B:13:ALA:HA	1.87	0.55
1:B:450:PHE:CE1	1:B:454:VAL:HG11	2.42	0.54
1:A:293:ASN:HA	1:A:296:ARG:HD3	1.88	0.54
1:A:7:GLU:HG3	1:A:16:VAL:HG11	1.88	0.53
1:B:241:GLU:O	1:B:245:ARG:HG3	2.09	0.53
1:B:450:PHE:O	1:B:454:VAL:HG12	2.09	0.53
1:A:278:HIS:HE1	1:A:372:SER:OG	1.92	0.53
1:B:139:SER:O	1:B:143:VAL:HG23	2.09	0.52
1:A:206:ALA:O	1:A:210:HIS:HD2	1.93	0.52
1:B:263:ASN:HD22	1:B:266:GLU:H	1.57	0.51
1:A:89:PHE:HA	1:A:105:ASN:HD21	1.75	0.51
1:B:371:GLN:O	1:B:375:LEU:HG	2.11	0.51
1:B:426:LYS:O	1:B:430:LYS:HD3	2.11	0.51
1:A:75:GLN:O	1:A:79:GLU:HG3	2.11	0.50
1:A:146:THR:HG23	1:A:225:LEU:HD22	1.93	0.50
1:B:256:ALA:HB3	1:B:258:PHE:CE2	2.47	0.50
1:A:70:ALA:O	1:A:74:ARG:HG3	2.11	0.49
1:A:416:ILE:HG13	1:A:420:LYS:HD2	1.93	0.49
1:B:458:GLN:N	1:B:458:GLN:NE2	2.60	0.49
1:B:239:HIS:HB3	1:B:242:TYR:HB2	1.95	0.49
1:B:123:GLY:O	1:B:126:ARG:HG3	2.12	0.48
1:A:156:LEU:O	1:A:161:ILE:HG12	2.13	0.48
1:A:384:ASN:HA	1:A:388:ALA:HB3	1.95	0.48
1:B:139:SER:HB3	1:B:142:ASP:OD1	2.13	0.48
1:A:54:ALA:O	1:A:58:VAL:HG23	2.13	0.48
1:A:407:MET:SD	1:B:321:MET:HB3	2.54	0.48
1:A:292:ALA:HB2	1:A:333:LEU:HD23	1.95	0.47
1:B:455:ARG:HB3	1:B:458:GLN:HE22	1.80	0.47
1:A:329:GLN:NE2	1:A:382:SER:OG	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:THR:HG21	1:B:100:THR:HB	1.95	0.47
1:B:412:LEU:O	1:B:416:ILE:HG12	2.14	0.47
1:B:140:SER:N	3:B:468:CIT:O2	2.48	0.47
1:A:182:VAL:HA	1:A:196:THR:HA	1.96	0.47
1:A:85:HIS:HB3	1:A:88:GLU:HG3	1.97	0.47
1:A:188:HIS:O	1:A:189:LEU:HB2	2.15	0.47
1:B:370:LEU:O	1:B:374:ARG:HG3	2.15	0.47
1:B:8:LYS:CB	1:B:13:ALA:HA	2.45	0.47
1:A:52:LYS:HZ1	1:A:103:ASN:HD21	1.60	0.47
1:A:315:GLN:NE2	1:A:328:THR:HG21	2.29	0.46
1:A:40:MET:SD	1:A:44:LEU:CD2	3.04	0.46
1:A:130:PRO:HG2	2:A:468:MLT:O1	2.14	0.46
1:B:248:ASP:O	1:B:252:VAL:HG23	2.15	0.46
1:A:303:ARG:CZ	1:B:406:LEU:HD11	2.45	0.46
1:B:52:LYS:HZ3	1:B:103:ASN:HD21	1.64	0.46
1:A:421:ALA:O	1:A:424:ILE:HG12	2.14	0.46
1:B:169:GLN:O	1:B:173:GLU:HG3	2.15	0.46
1:A:163:GLN:HA	1:A:163:GLN:NE2	2.30	0.46
1:A:202:SER:HA	1:A:205:VAL:CG1	2.46	0.45
1:A:244:ARG:HH11	1:A:244:ARG:HG3	1.81	0.45
1:B:314:ASN:HD21	1:B:386:HIS:HB3	1.82	0.45
1:B:409:VAL:HG21	1:B:425:ALA:HB2	1.97	0.45
1:A:279:GLY:O	1:A:282:LYS:HG3	2.17	0.45
1:A:278:HIS:HD2	1:A:344:ASP:OD1	1.98	0.45
1:B:22:TRP:NE1	1:B:27:GLN:HG2	2.20	0.45
1:B:263:ASN:ND2	1:B:266:GLU:H	2.14	0.45
1:A:205:VAL:O	1:A:209:GLU:HG3	2.16	0.45
1:B:205:VAL:O	1:B:209:GLU:HG3	2.16	0.45
1:B:232:VAL:HB	1:B:357:GLU:HG2	1.99	0.45
1:A:242:TYR:O	1:A:246:VAL:HG22	2.17	0.45
1:A:58:VAL:HG21	1:A:246:VAL:HA	1.98	0.45
1:A:455:ARG:HD2	1:A:458:GLN:OE1	2.17	0.45
1:B:8:LYS:HB2	1:B:12:GLY:O	2.17	0.45
1:A:97:GLY:HA3	1:A:360:VAL:HB	1.99	0.44
1:A:69:LYS:O	1:A:73:ILE:HG13	2.17	0.44
1:B:239:HIS:CD2	1:B:241:GLU:H	2.33	0.44
1:B:361:PHE:O	1:B:365:VAL:HG23	2.17	0.44
1:A:51:THR:HG23	1:A:227:LEU:HD11	2.00	0.44
1:B:58:VAL:HG21	1:B:246:VAL:HA	1.98	0.44
1:B:436:LYS:HD2	1:B:447:GLU:HG3	1.99	0.44
1:A:7:GLU:CG	1:A:16:VAL:HG11	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:HB3	1:B:3:THR:HG22	1.99	0.43
1:A:20:LYS:HD3	1:A:20:LYS:HA	1.86	0.43
1:B:129:HIS:HA	1:B:130:PRO:HD3	1.82	0.43
1:A:149:HIS:HD2	1:A:224:GLU:O	2.01	0.43
1:B:25:GLN:NE2	1:B:104:MET:HG3	2.34	0.43
1:B:26:THR:OG1	1:B:105:ASN:HA	2.19	0.43
1:A:315:GLN:CD	1:A:315:GLN:H	2.22	0.43
1:A:153:LEU:HD12	1:A:219:LEU:HD22	2.01	0.43
1:B:89:PHE:HD1	1:B:105:ASN:ND2	2.18	0.42
1:A:306:ILE:CG2	1:A:308:GLU:HG3	2.47	0.42
1:B:336:LEU:HD13	1:B:375:LEU:HB3	2.00	0.42
1:B:263:ASN:HD21	1:B:265:PHE:HB2	1.85	0.42
1:A:320:ILE:HG13	1:B:422:ALA:HA	2.01	0.42
1:B:3:THR:HG23	1:B:18:ALA:HB3	2.01	0.42
1:B:52:LYS:NZ	1:B:103:ASN:ND2	2.66	0.42
1:B:148:MET:SD	1:B:362:ARG:HB3	2.60	0.42
1:B:100:THR:HA	1:B:140:SER:HB2	2.02	0.41
1:B:439:ALA:HB1	1:B:445:LEU:CD2	2.41	0.41
1:A:250:LEU:HD13	1:A:250:LEU:HA	1.88	0.41
1:A:419:ASP:O	1:A:423:GLU:HB2	2.19	0.41
1:B:327:PRO:O	1:B:331:GLU:HG3	2.20	0.41
1:B:454:VAL:O	1:B:454:VAL:HG13	2.21	0.41
1:A:343:ASN:ND2	1:A:371:GLN:HE21	1.94	0.41
1:B:401:LEU:HD12	1:B:401:LEU:HA	1.89	0.41
1:A:178:PHE:CZ	1:A:393:PRO:HD3	2.56	0.41
1:A:321:MET:N	1:A:322:PRO:HD3	2.36	0.41
1:B:211:ASN:O	1:B:215:ILE:HG13	2.20	0.41
1:B:141:ASN:ND2	3:B:468:CIT:O3	2.54	0.41
1:A:126:ARG:HD2	2:A:468:MLT:O4	2.21	0.40
1:A:331:GLU:O	1:A:335:MET:HG3	2.21	0.40
1:A:332:ALA:HA	1:A:335:MET:HE2	2.02	0.40
1:A:362:ARG:HB2	1:A:363:PRO:HD3	2.03	0.40
1:B:8:LYS:HB2	1:B:8:LYS:HE3	1.92	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	454/467 (97%)	432 (95%)	22 (5%)	0	100	100
1	B	451/467 (97%)	423 (94%)	25 (6%)	3 (1%)	22	43
All	All	905/934 (97%)	855 (94%)	47 (5%)	3 (0%)	41	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	231	ALA
1	B	387	CYS
1	B	130	PRO

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	368/376 (98%)	353 (96%)	15 (4%)	30	56
1	B	367/376 (98%)	349 (95%)	18 (5%)	25	48
All	All	735/752 (98%)	702 (96%)	33 (4%)	27	52

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ILE
1	A	149	HIS
1	A	167	LEU

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Mol	Chain	Res	Type
1	A	221	HIS
1	A	250	LEU
1	A	281	LEU
1	A	282	LYS
1	A	311	ILE
1	A	315	GLN
1	A	364	MET
1	A	402	LEU
1	A	413	ASN
1	A	433	LEU
1	A	435	LEU
1	A	459	MET
1	B	65	LEU
1	B	129	HIS
1	B	131	ASN
1	B	153	LEU
1	B	171	LEU
1	B	183	LYS
1	B	236	LEU
1	B	244	ARG
1	B	263	ASN
1	B	282	LYS
1	B	290	LYS
1	B	341	MET
1	B	396	GLU
1	B	401	LEU
1	B	442	LEU
1	B	455	ARG
1	B	458	GLN
1	B	459	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	59	ASN
1	A	103	ASN
1	A	105	ASN
1	A	107	ASN
1	A	131	ASN
1	A	149	HIS
1	A	163	GLN

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Mol	Chain	Res	Type
1	A	210	HIS
1	A	239	HIS
1	A	278	HIS
1	A	315	GLN
1	A	329	GLN
1	A	339	GLN
1	A	368	ASN
1	A	371	GLN
1	A	400	GLN
1	A	413	ASN
1	B	25	GLN
1	B	59	ASN
1	B	101	GLN
1	B	103	ASN
1	B	105	ASN
1	B	112	ASN
1	B	149	HIS
1	B	163	GLN
1	B	169	GLN
1	B	172	ASN
1	B	239	HIS
1	B	263	ASN
1	B	278	HIS
1	B	293	ASN
1	B	314	ASN
1	B	339	GLN
1	B	343	ASN
1	B	368	ASN
1	B	371	GLN
1	B	384	ASN
1	B	394	ASN
1	B	403	ASN
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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 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	-	8,8,8	1.16	0	10,10,10	3.82	4 (40%)
3	CIT	B	468	-	12,12,12	35.67	12 (100%)	17,17,17	5.98	13 (76%)
3	CIT	A	469	-	12,12,12	4.52	5 (41%)	17,17,17	6.06	10 (58%)

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	3/8/8/8	-
3	CIT	B	468	-	-	7/16/16/16	-
3	CIT	A	469	-	-	9/16/16/16	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	468	CIT	C3-C6	66.42	2.22	1.53
3	B	468	CIT	C2-C3	56.02	2.23	1.53
3	B	468	CIT	C4-C3	54.87	2.22	1.53
3	B	468	CIT	O7-C3	30.26	2.01	1.43
3	B	468	CIT	O5-C6	23.76	1.98	1.22
3	B	468	CIT	O3-C5	23.14	1.98	1.22
3	B	468	CIT	C2-C1	22.74	2.20	1.50
3	B	468	CIT	O1-C1	22.67	1.97	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	468	CIT	C4-C5	21.56	2.17	1.50
3	B	468	CIT	O2-C1	20.90	2.01	1.30
3	B	468	CIT	O4-C5	20.29	1.99	1.30
3	B	468	CIT	O6-C6	18.58	1.99	1.30
3	A	469	CIT	C2-C3	12.56	1.69	1.53
3	A	469	CIT	C4-C5	-7.26	1.28	1.50
3	A	469	CIT	O7-C3	-3.34	1.36	1.43
3	A	469	CIT	C3-C6	2.89	1.56	1.53
3	A	469	CIT	O4-C5	-2.44	1.22	1.30

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	468	CIT	C4-C3-C6	-14.65	78.62	110.11
3	A	469	CIT	C3-C4-C5	14.06	147.86	113.81
3	A	469	CIT	C3-C2-C1	13.17	145.71	113.81
3	A	469	CIT	C4-C3-C6	-11.19	86.05	110.11
2	A	468	MLT	O3-C2-C3	10.67	136.23	110.05
3	B	468	CIT	C3-C4-C5	10.02	138.09	113.81
3	B	468	CIT	O7-C3-C2	9.94	132.66	109.40
3	B	468	CIT	O6-C6-C3	7.64	126.31	113.05
3	A	469	CIT	O7-C3-C2	6.92	125.60	109.40
3	B	468	CIT	C3-C2-C1	5.22	126.46	113.81
3	B	468	CIT	O7-C3-C6	5.08	116.00	108.86
3	A	469	CIT	O6-C6-C3	4.96	121.66	113.05
3	B	468	CIT	C4-C3-C2	-4.69	96.93	109.16
3	B	468	CIT	C2-C3-C6	-3.90	101.72	110.11
3	A	469	CIT	O7-C3-C6	3.79	114.18	108.86
3	B	468	CIT	O7-C3-C4	3.23	116.96	109.40
2	A	468	MLT	C3-C2-C1	3.19	117.87	110.33
3	A	469	CIT	C4-C3-C2	-3.09	101.10	109.16
3	B	468	CIT	O6-C6-O5	-3.07	114.04	123.82
3	B	468	CIT	O4-C5-O3	2.98	130.72	123.30
3	A	469	CIT	O7-C3-C4	2.92	116.22	109.40
2	A	468	MLT	O2-C1-C2	2.69	118.64	112.72
3	A	469	CIT	O4-C5-O3	2.54	129.64	123.30
3	A	469	CIT	O6-C6-O5	-2.52	115.80	123.82
2	A	468	MLT	C2-C3-C4	2.40	118.07	112.13
3	B	468	CIT	O1-C1-C2	-2.33	116.14	122.94
3	B	468	CIT	O4-C5-C4	-2.31	106.94	114.35

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	468	MLT	C2

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	468	MLT	O1-C1-C2-O3
2	A	468	MLT	O2-C1-C2-O3
2	A	468	MLT	O3-C2-C3-C4
3	A	469	CIT	C1-C2-C3-O7
3	A	469	CIT	C1-C2-C3-C4
3	A	469	CIT	C1-C2-C3-C6
3	A	469	CIT	O7-C3-C4-C5
3	A	469	CIT	C6-C3-C4-C5
3	A	469	CIT	C2-C3-C6-O5
3	A	469	CIT	C2-C3-C6-O6
3	B	468	CIT	O7-C3-C4-C5
3	B	468	CIT	C6-C3-C4-C5
3	A	469	CIT	C2-C3-C4-C5
3	B	468	CIT	C1-C2-C3-C4
3	B	468	CIT	C2-C3-C4-C5
3	B	468	CIT	C2-C3-C6-O5
3	B	468	CIT	C2-C3-C6-O6
3	B	468	CIT	C1-C2-C3-O7
3	A	469	CIT	C4-C3-C6-O5

There are no ring outliers.

3 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	468	MLT	4	0
3	B	468	CIT	16	0
3	A	469	CIT	1	0

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, 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(Å²)	Q<0.9
1	A	456/467 (97%)	-0.19	15 (3%)	46	39	2, 9, 68, 82	0
1	B	455/467 (97%)	-0.52	2 (0%)	92	91	2, 8, 29, 70	0
All	All	911/934 (97%)	-0.35	17 (1%)	66	62	2, 8, 57, 82	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	322	PRO	3.7
1	A	447	GLU	3.6
1	A	450	PHE	3.5
1	A	440	LEU	3.3
1	A	448	ALA	3.3
1	B	322	PRO	3.1
1	A	442	LEU	3.1
1	A	421	ALA	2.8
1	A	451	ASP	2.6
1	A	416	ILE	2.5
1	A	436	LYS	2.5
1	A	445	LEU	2.4
1	A	446	SER	2.2
1	A	319	SER	2.2
1	A	430	LYS	2.1
1	B	459	MET	2.1
1	A	444	TYR	2.0

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

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

6.3   Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4   Ligands ⓘ

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
3	CIT	B	468	13/13	0.61	0.59	55,64,69,70	0
2	MLT	A	468	9/9	0.79	0.27	39,42,45,46	0
3	CIT	A	469	13/13	0.83	0.27	54,58,60,61	0

6.5   Other polymers ⓘ

There are no such residues in this entry.