Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2023 – 07:21 PM EDT

PDB ID	:	1JNQ
Title	:	LIPOXYGENASE-3 (SOYBEAN) COMPLEX WITH EPIGALLOCATHECHIN (EGC)
Authors	:	Zhou, K.; Skrzypczak-Jankun, E.; Jankun, J.
Deposited on	:	2001-07-24
Resolution	:	2.10 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:

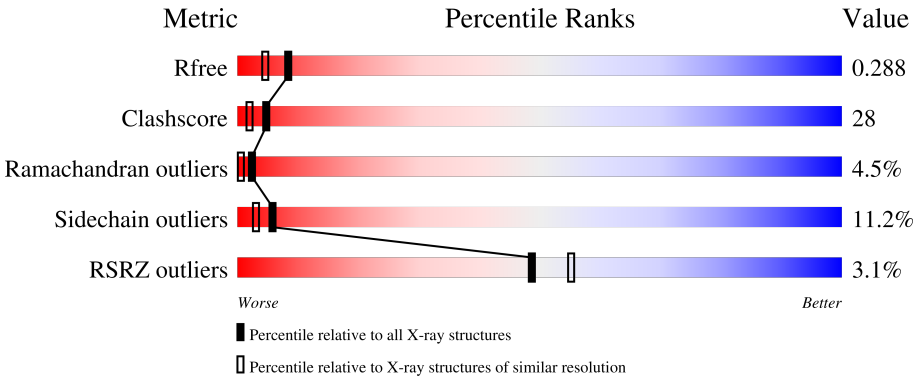
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	857	3%, 53%, 36%, 9%

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
3	EGT	A	871	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7313 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.

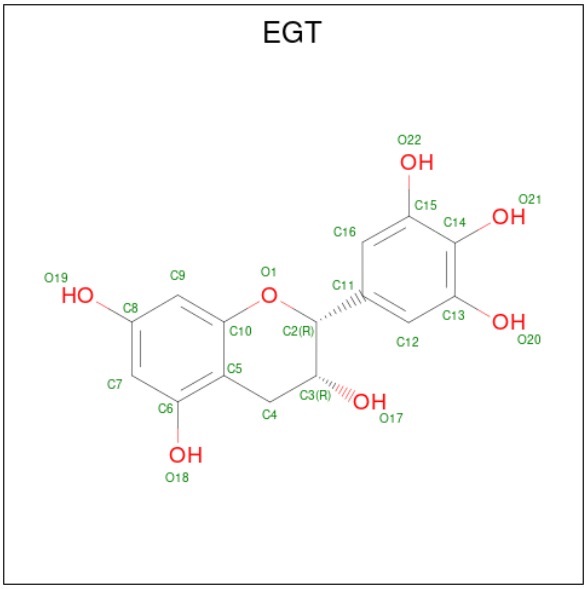
- Molecule 1 is a protein called lipoxygenase-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	849	Total	C	N	O	S	0	0	0
			6778	4329	1163	1268	18			

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		

- Molecule 3 is 2-(3,4,5-TRIHYDROXY-PHENYL)-CHROMAN-3,5,7-TRIOL (three-letter code: EGT) (formula: $C_{15}H_{14}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			22	15	7		

- Molecule 4 is water.

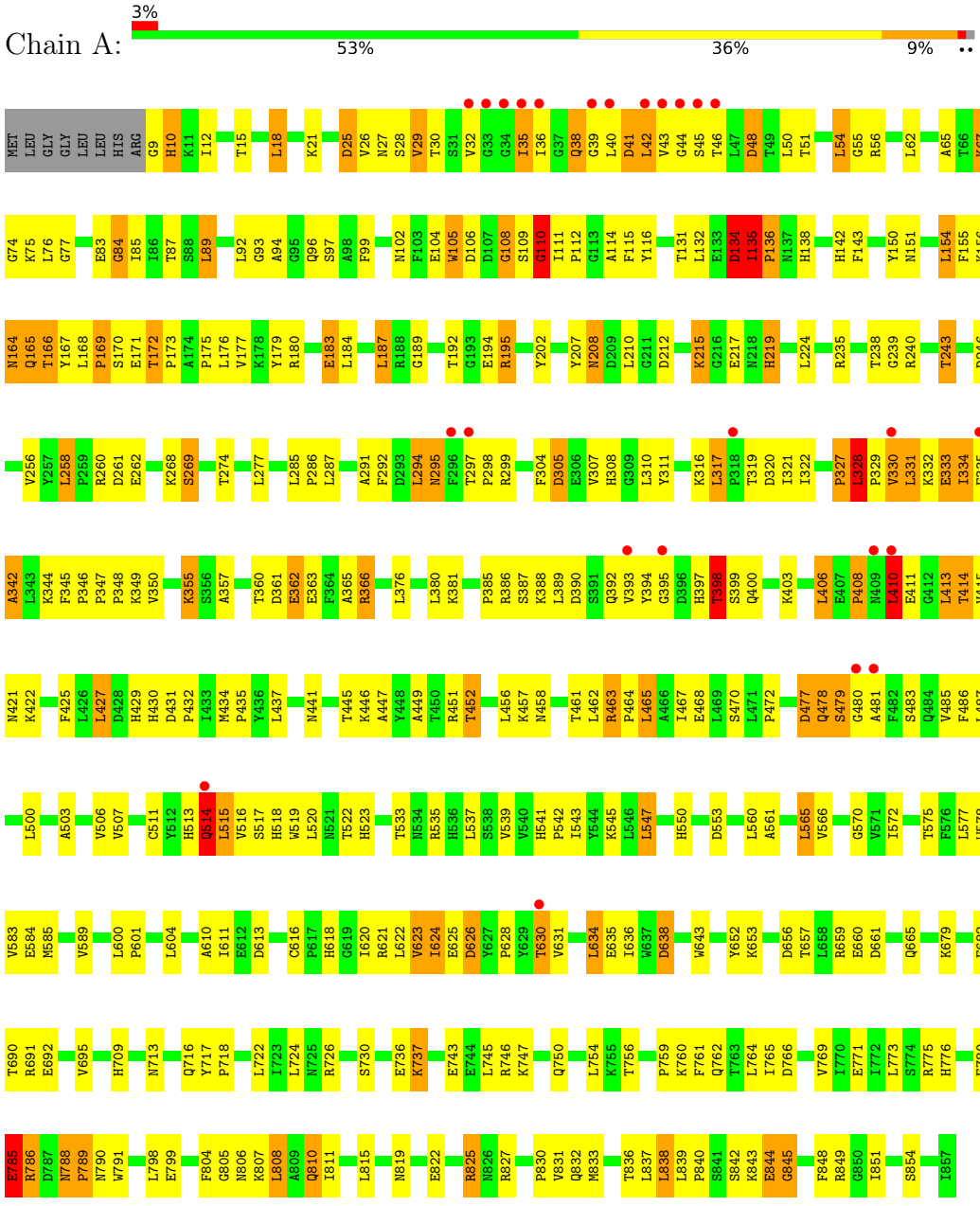
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	512	Total O 512 512	0	0

3 Residue-property plots (i)

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: lipoxygenase-3

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	112.73Å 137.27Å 61.88Å 90.00° 95.53° 90.00°	Depositor
Resolution (Å)	8.00 – 2.10 86.88 – 2.10	Depositor EDS
% Data completeness (in resolution range)	80.5 (8.00-2.10) 80.6 (86.88-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 2.10Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.199 , 0.295 0.198 , 0.288	Depositor DCC
R_{free} test set	5119 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å^2)	27.8	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 78.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7313	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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, 0.333 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: FE2, EGT

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	0.41	0/6950	0.73	8/9439 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	189	GLY	N-CA-C	6.08	128.31	113.10
1	A	623	VAL	N-CA-C	-5.71	95.58	111.00
1	A	134	ASP	N-CA-C	5.38	125.54	111.00
1	A	110	GLY	N-CA-C	5.32	126.40	113.10
1	A	108	GLY	N-CA-C	-5.28	99.91	113.10
1	A	845	GLY	N-CA-C	5.25	126.23	113.10
1	A	844	GLU	N-CA-C	5.14	124.88	111.00
1	A	89	LEU	CA-CB-CG	5.09	127.01	115.30

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	6778	0	6701	376	0
2	A	1	0	0	0	0
3	A	22	0	9	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	512	0	0	44	0
All	All	7313	0	6710	377	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 28.

All (377) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:HIS:HD1	3:A:871:EGT:C16	1.73	1.00
1:A:447:ALA:HB2	1:A:577:LEU:HD11	1.46	0.95
1:A:518:HIS:HD1	3:A:871:EGT:H16	1.29	0.95
1:A:393:VAL:HB	1:A:479:SER:HA	1.48	0.95
1:A:394:TYR:HA	1:A:397:HIS:HB3	1.51	0.92
1:A:135:ILE:HG23	1:A:136:PRO:HD3	1.53	0.91
1:A:518:HIS:ND1	3:A:871:EGT:H16	1.86	0.91
1:A:659:ARG:HD3	1:A:689:GLN:HG3	1.53	0.91
1:A:35:ILE:HD13	1:A:35:ILE:H	1.36	0.90
1:A:652:TYR:HD1	1:A:657:THR:HG22	1.36	0.89
1:A:74:GLY:H	1:A:179:TYR:HE2	1.19	0.85
1:A:77:GLY:HA3	1:A:105:TRP:HZ3	1.38	0.85
1:A:420:GLN:HG3	1:A:421:ASN:HD22	1.40	0.85
1:A:319:THR:HA	1:A:322:ILE:HG22	1.60	0.83
1:A:18:LEU:HD21	1:A:99:PHE:HE2	1.44	0.83
1:A:825:ARG:HE	1:A:825:ARG:HA	1.43	0.83
1:A:410:LEU:HD13	1:A:410:LEU:H	1.45	0.80
1:A:620:ILE:HD11	1:A:634:LEU:HD21	1.62	0.79
1:A:169:PRO:HD3	1:A:541:HIS:CE1	2.17	0.79
1:A:511:CYS:O	1:A:514:GLN:HB3	1.82	0.79
1:A:441:ASN:HD21	1:A:447:ALA:H	1.29	0.78
1:A:169:PRO:HD3	1:A:541:HIS:HE1	1.49	0.77
1:A:496:SER:HB3	1:A:745:LEU:HD22	1.66	0.77
1:A:171:GLU:HB2	1:A:177:VAL:HG22	1.66	0.77
1:A:336:ARG:HD3	1:A:344:LYS:HE3	1.68	0.76
1:A:171:GLU:HG2	1:A:180:ARG:HD3	1.67	0.76
1:A:357:ALA:O	1:A:360:THR:HG22	1.86	0.76
1:A:804:PHE:HD1	1:A:807:LYS:HE2	1.51	0.76
1:A:784:GLY:HA2	1:A:808:LEU:HD23	1.68	0.75
1:A:171:GLU:HA	1:A:180:ARG:NH1	2.02	0.75
1:A:154:LEU:H	1:A:154:LEU:HD23	1.50	0.74
1:A:334:ILE:HD12	1:A:334:ILE:H	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:785:GLU:HB3	1:A:805:GLY:HA3	1.69	0.74
1:A:565:LEU:HG	3:A:871:EGT:HC41	1.70	0.74
1:A:62:LEU:HD12	1:A:112:PRO:HB3	1.68	0.74
1:A:400:GLN:OE1	1:A:481:ALA:HB1	1.88	0.74
1:A:522:THR:HG21	1:A:709:HIS:CD2	2.23	0.74
1:A:215:LYS:HD2	1:A:219:HIS:CD2	2.22	0.73
1:A:441:ASN:ND2	1:A:447:ALA:H	1.85	0.73
1:A:360:THR:HG23	1:A:363:GLU:H	1.51	0.73
1:A:75:LYS:HB3	1:A:75:LYS:HZ3	1.52	0.73
1:A:585:MET:SD	4:A:1321:HOH:O	2.47	0.73
1:A:322:ILE:HD12	1:A:342:ALA:H	1.53	0.73
1:A:208:ASN:HD22	1:A:208:ASN:H	1.37	0.72
1:A:287:LEU:HB3	1:A:321:ILE:HG23	1.72	0.71
1:A:522:THR:HG21	1:A:709:HIS:HD2	1.56	0.71
1:A:362:GLU:O	1:A:366:ARG:HB2	1.91	0.70
1:A:311:TYR:HA	1:A:345:PHE:O	1.91	0.70
1:A:759:PRO:HG2	1:A:762:GLN:HE21	1.55	0.69
1:A:851:ILE:HD12	4:A:1092:HOH:O	1.92	0.69
1:A:514:GLN:OE1	1:A:515:LEU:HB2	1.93	0.69
1:A:134:ASP:OD2	1:A:138:HIS:HB2	1.93	0.68
1:A:386:ARG:HG2	1:A:398:THR:HG22	1.75	0.68
1:A:18:LEU:HD21	1:A:99:PHE:CE2	2.28	0.68
1:A:168:LEU:HB3	1:A:169:PRO:HD2	1.76	0.68
1:A:585:MET:O	1:A:589:VAL:HG23	1.93	0.68
1:A:172:THR:HB	1:A:173:PRO:HD3	1.76	0.68
1:A:566:VAL:HG22	1:A:583:VAL:HG22	1.74	0.68
1:A:843:LYS:HG3	1:A:849:ARG:HH22	1.59	0.68
1:A:514:GLN:HG2	1:A:515:LEU:HD13	1.76	0.67
1:A:788:ASN:OD1	1:A:789:PRO:HD3	1.95	0.67
1:A:518:HIS:CE1	3:A:871:EGT:H16	2.30	0.66
1:A:496:SER:O	1:A:500:LEU:HD13	1.94	0.66
1:A:43:VAL:HG13	1:A:92:LEU:HD11	1.76	0.66
1:A:208:ASN:ND2	1:A:235:ARG:HH21	1.93	0.65
1:A:819:ASN:HD22	1:A:827:ARG:HE	1.45	0.65
1:A:385:PRO:HD2	1:A:399:SER:OG	1.97	0.65
1:A:819:ASN:ND2	1:A:827:ARG:HE	1.94	0.64
1:A:299:ARG:HD3	4:A:931:HOH:O	1.97	0.64
1:A:393:VAL:CB	1:A:479:SER:HA	2.23	0.64
1:A:291:ALA:HB2	1:A:321:ILE:CD1	2.28	0.64
1:A:208:ASN:HD21	1:A:235:ARG:NH2	1.95	0.64
1:A:626:ASP:HB3	4:A:999:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:SER:HB2	1:A:468:GLU:OE1	1.98	0.63
1:A:169:PRO:HG2	4:A:1336:HOH:O	1.98	0.63
1:A:656:ASP:O	1:A:660:GLU:HG2	1.99	0.63
1:A:50:LEU:HD11	1:A:97:SER:HB3	1.81	0.63
1:A:9:GLY:O	1:A:10:HIS:HB2	1.98	0.62
1:A:142:HIS:HB2	4:A:1278:HOH:O	1.99	0.62
1:A:836:THR:OG1	1:A:839:LEU:HD22	2.00	0.62
1:A:84:GLY:HA2	4:A:947:HOH:O	1.99	0.62
1:A:413:LEU:HA	4:A:1189:HOH:O	1.99	0.62
1:A:623:VAL:O	1:A:624:ILE:HG22	2.00	0.62
1:A:397:HIS:O	1:A:398:THR:HG23	2.00	0.61
1:A:386:ARG:HG2	1:A:398:THR:CG2	2.30	0.61
1:A:75:LYS:NZ	1:A:109:SER:HA	2.15	0.61
1:A:447:ALA:CB	1:A:577:LEU:HD11	2.25	0.61
1:A:39:GLY:O	1:A:40:LEU:HB2	1.99	0.61
1:A:616:CYS:HB3	4:A:1307:HOH:O	1.99	0.61
1:A:243:THR:HG22	1:A:246:ASP:O	2.01	0.60
1:A:150:TYR:HB2	1:A:155:PHE:HZ	1.65	0.60
1:A:75:LYS:HB3	1:A:75:LYS:NZ	2.17	0.60
1:A:106:ASP:O	1:A:109:SER:HB3	2.02	0.60
1:A:77:GLY:HA3	1:A:105:TRP:CZ3	2.30	0.59
1:A:166:THR:HG22	1:A:545:LYS:NZ	2.17	0.59
1:A:584:GLU:HG3	4:A:1117:HOH:O	2.01	0.59
1:A:831:VAL:HG13	1:A:833:MET:HB2	1.85	0.59
1:A:134:ASP:CG	1:A:135:ILE:H	2.04	0.59
1:A:269:SER:HB3	1:A:332:LYS:HE3	1.85	0.59
1:A:486:PHE:HB3	4:A:1305:HOH:O	2.03	0.59
1:A:581:TYR:HB2	1:A:585:MET:HE2	1.83	0.59
1:A:610:ALA:HB2	1:A:622:LEU:HD23	1.84	0.59
1:A:208:ASN:ND2	1:A:235:ARG:NH2	2.50	0.59
1:A:825:ARG:HB2	4:A:1395:HOH:O	2.03	0.59
1:A:394:TYR:HB3	1:A:481:ALA:HB2	1.85	0.59
1:A:541:HIS:HD2	1:A:543:ILE:H	1.49	0.59
1:A:479:SER:O	1:A:481:ALA:N	2.36	0.58
1:A:35:ILE:H	1:A:35:ILE:CD1	2.13	0.58
1:A:572:ILE:HG12	3:A:871:EGT:O17	2.04	0.58
1:A:690:THR:HG22	1:A:692:GLU:H	1.69	0.58
1:A:32:VAL:HG13	1:A:36:ILE:HG13	1.86	0.58
1:A:260:ARG:O	1:A:261:ASP:HB2	2.04	0.58
1:A:518:HIS:HD1	3:A:871:EGT:C15	2.16	0.58
1:A:636:ILE:HD12	1:A:838:LEU:HG	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:LYS:HE3	4:A:1326:HOH:O	2.04	0.58
1:A:565:LEU:O	1:A:572:ILE:HB	2.03	0.58
1:A:29:VAL:HG12	1:A:29:VAL:O	2.04	0.57
1:A:150:TYR:HB2	1:A:155:PHE:CZ	2.40	0.57
1:A:238:THR:HG21	4:A:985:HOH:O	2.04	0.57
1:A:51:THR:O	1:A:54:LEU:HB2	2.04	0.57
1:A:89:LEU:HD23	1:A:92:LEU:HD12	1.87	0.57
1:A:171:GLU:CG	1:A:180:ARG:HD3	2.35	0.57
1:A:169:PRO:HG3	1:A:661:ASP:CG	2.25	0.57
1:A:154:LEU:HD23	1:A:154:LEU:N	2.18	0.56
1:A:481:ALA:HA	4:A:1335:HOH:O	2.04	0.56
1:A:434:MET:HB3	1:A:435:PRO:HD3	1.87	0.56
1:A:785:GLU:CB	1:A:805:GLY:HA3	2.34	0.56
1:A:51:THR:HA	1:A:54:LEU:HD22	1.87	0.56
1:A:394:TYR:OH	1:A:434:MET:HG2	2.06	0.56
1:A:362:GLU:HG2	4:A:1257:HOH:O	2.05	0.56
1:A:746:ARG:HD3	4:A:1318:HOH:O	2.05	0.56
1:A:515:LEU:HA	1:A:519:TRP:HB3	1.88	0.55
1:A:32:VAL:HG11	1:A:268:LYS:HA	1.87	0.55
1:A:164:ASN:HB2	4:A:1374:HOH:O	2.05	0.55
1:A:169:PRO:O	1:A:171:GLU:HG3	2.07	0.55
1:A:171:GLU:OE2	1:A:177:VAL:HG13	2.06	0.55
1:A:341:GLN:HE21	1:A:341:GLN:N	2.04	0.55
1:A:50:LEU:CD1	1:A:97:SER:HB3	2.36	0.55
1:A:566:VAL:HG22	1:A:583:VAL:CG2	2.35	0.55
1:A:341:GLN:HE21	1:A:341:GLN:H	1.53	0.55
1:A:192:THR:O	1:A:195:ARG:NH2	2.40	0.54
1:A:533:THR:HG23	1:A:537:LEU:HD12	1.88	0.54
1:A:417:GLU:HA	1:A:420:GLN:HG2	1.90	0.54
1:A:93:GLY:H	1:A:96:GLN:NE2	2.06	0.54
1:A:322:ILE:HG12	1:A:322:ILE:O	2.09	0.53
1:A:393:VAL:HB	1:A:479:SER:CA	2.28	0.53
1:A:691:ARG:O	1:A:695:VAL:HG23	2.07	0.53
1:A:773:LEU:HD11	3:A:871:EGT:O18	2.07	0.53
1:A:317:LEU:HD23	1:A:321:ILE:HB	1.90	0.53
1:A:785:GLU:O	1:A:785:GLU:HG2	2.07	0.53
1:A:790:ASN:HB2	4:A:1004:HOH:O	2.09	0.53
1:A:838:LEU:HD12	1:A:851:ILE:HD11	1.91	0.53
1:A:408:PRO:HD2	1:A:410:LEU:HD11	1.89	0.53
1:A:38:GLN:HG3	1:A:39:GLY:H	1.74	0.53
1:A:457:LYS:HD3	1:A:461:THR:OG1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LYS:HD2	4:A:1157:HOH:O	2.08	0.53
1:A:21:LYS:HE2	4:A:1090:HOH:O	2.09	0.52
1:A:240:ARG:HH21	1:A:256:VAL:HA	1.74	0.52
1:A:506:VAL:HG11	1:A:726:ARG:HA	1.92	0.52
1:A:171:GLU:CB	1:A:180:ARG:HD3	2.40	0.52
1:A:652:TYR:CD1	1:A:657:THR:HG22	2.29	0.52
1:A:785:GLU:HB3	1:A:805:GLY:CA	2.39	0.52
1:A:116:TYR:HH	1:A:179:TYR:HE1	1.55	0.52
1:A:331:LEU:HG	1:A:335:PHE:CE2	2.44	0.52
1:A:15:THR:CG2	1:A:131:THR:HB	2.40	0.52
1:A:317:LEU:O	1:A:341:GLN:HA	2.10	0.52
1:A:420:GLN:HG3	1:A:421:ASN:ND2	2.17	0.52
1:A:747:LYS:HE2	1:A:747:LYS:HA	1.91	0.52
1:A:406:LEU:HG	1:A:465:LEU:HD23	1.91	0.52
1:A:415:VAL:HB	4:A:1161:HOH:O	2.10	0.51
1:A:780:GLU:HG2	4:A:1007:HOH:O	2.10	0.51
1:A:479:SER:C	1:A:481:ALA:H	2.14	0.51
1:A:810:GLN:HG3	4:A:1110:HOH:O	2.10	0.51
1:A:507:VAL:HG12	1:A:577:LEU:HD22	1.93	0.51
1:A:305:ASP:HA	4:A:1250:HOH:O	2.11	0.51
1:A:427:LEU:HB3	1:A:452:THR:HG23	1.93	0.51
1:A:806:ASN:HB2	4:A:1206:HOH:O	2.10	0.51
1:A:381:LYS:NZ	1:A:422:LYS:HG2	2.26	0.51
1:A:791:TRP:CD1	1:A:791:TRP:N	2.78	0.50
1:A:575:THR:HG21	1:A:766:ASP:HB2	1.93	0.50
1:A:68:ALA:HB2	1:A:175:PRO:HG3	1.93	0.50
1:A:348:PRO:HB2	1:A:350:VAL:HG12	1.93	0.50
1:A:238:THR:HG23	1:A:250:GLU:OE2	2.12	0.50
1:A:208:ASN:HD22	1:A:208:ASN:N	2.03	0.50
1:A:25:ASP:O	1:A:29:VAL:HG23	2.12	0.50
1:A:679:LYS:HB3	1:A:682:GLU:HG3	1.94	0.50
1:A:110:GLY:HA2	4:A:1389:HOH:O	2.11	0.50
1:A:773:LEU:HD21	3:A:871:EGT:C6	2.42	0.50
1:A:765:ILE:HG21	4:A:1155:HOH:O	2.11	0.49
1:A:168:LEU:CB	1:A:169:PRO:HD2	2.40	0.49
1:A:316:LYS:HB2	4:A:1223:HOH:O	2.11	0.49
1:A:687:LYS:O	1:A:689:GLN:N	2.45	0.49
1:A:769:VAL:O	1:A:773:LEU:HD13	2.13	0.49
1:A:736:GLU:HG2	1:A:737:LYS:H	1.77	0.49
1:A:618:HIS:HD2	1:A:638:ASP:OD2	1.96	0.49
1:A:389:LEU:HD13	1:A:394:TYR:OH	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:SER:HB3	1:A:395:GLY:HA2	1.95	0.49
1:A:397:HIS:HE1	1:A:400:GLN:HG3	1.77	0.48
1:A:736:GLU:HG2	1:A:737:LYS:N	2.28	0.48
1:A:782:TYR:HB2	1:A:786:ARG:HH11	1.78	0.48
1:A:414:THR:HG23	1:A:417:GLU:OE1	2.14	0.48
1:A:624:ILE:HG23	1:A:624:ILE:O	2.13	0.48
1:A:687:LYS:O	1:A:689:GLN:HB2	2.13	0.48
1:A:26:VAL:HG13	1:A:27:ASN:N	2.27	0.48
1:A:410:LEU:HD23	1:A:411:GLU:H	1.77	0.48
1:A:516:VAL:HA	1:A:520:LEU:HB3	1.95	0.48
1:A:840:PRO:HG3	4:A:1092:HOH:O	2.12	0.48
1:A:514:GLN:HG2	1:A:515:LEU:N	2.27	0.48
1:A:298:PRO:O	1:A:760:LYS:HD3	2.14	0.47
1:A:403:LYS:HD2	4:A:1161:HOH:O	2.14	0.47
1:A:503:ALA:O	1:A:507:VAL:HG23	2.14	0.47
1:A:411:GLU:HB2	1:A:458:ASN:HD21	1.78	0.47
1:A:470:SER:OG	1:A:483:SER:HB3	2.14	0.47
1:A:425:PHE:HE1	1:A:456:LEU:HB2	1.79	0.47
1:A:653:LYS:HG3	4:A:953:HOH:O	2.14	0.47
1:A:775:ARG:HD2	4:A:1357:HOH:O	2.13	0.47
1:A:171:GLU:HG2	1:A:180:ARG:CD	2.42	0.47
1:A:431:ASP:HB2	1:A:432:PRO:HD3	1.97	0.47
1:A:477:ASP:O	1:A:479:SER:N	2.47	0.47
1:A:73:LYS:HE3	4:A:1043:HOH:O	2.15	0.47
1:A:50:LEU:HD11	1:A:97:SER:CB	2.43	0.47
1:A:172:THR:CB	1:A:173:PRO:HD3	2.44	0.47
1:A:212:ASP:OD2	1:A:215:LYS:HB2	2.15	0.47
1:A:215:LYS:HD2	1:A:219:HIS:NE2	2.29	0.47
1:A:277:LEU:HB2	1:A:560:LEU:HD21	1.97	0.47
1:A:304:PHE:H	1:A:750:GLN:NE2	2.12	0.47
1:A:776:HIS:HB2	1:A:844:GLU:O	2.14	0.47
1:A:804:PHE:HD1	1:A:807:LYS:CE	2.25	0.47
1:A:804:PHE:HA	1:A:807:LYS:HE2	1.96	0.47
1:A:12:ILE:O	1:A:102:ASN:HA	2.14	0.47
1:A:171:GLU:HB3	1:A:180:ARG:HD3	1.96	0.47
1:A:155:PHE:C	1:A:157:SER:H	2.19	0.47
1:A:394:TYR:HE1	1:A:430:HIS:HE2	1.60	0.47
1:A:410:LEU:CD2	1:A:411:GLU:H	2.28	0.47
1:A:643:TRP:HD1	4:A:1170:HOH:O	1.98	0.47
1:A:36:ILE:HG22	1:A:36:ILE:O	2.15	0.47
1:A:135:ILE:CG2	1:A:136:PRO:HD3	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:776:HIS:O	1:A:844:GLU:O	2.32	0.47
1:A:43:VAL:C	1:A:45:SER:H	2.17	0.46
1:A:111:ILE:HG12	1:A:138:HIS:CE1	2.50	0.46
1:A:32:VAL:HG12	1:A:32:VAL:O	2.15	0.46
1:A:487:LEU:N	1:A:487:LEU:HD22	2.30	0.46
1:A:89:LEU:HB2	1:A:92:LEU:HB2	1.98	0.46
1:A:518:HIS:O	1:A:522:THR:HB	2.15	0.46
1:A:636:ILE:HD11	1:A:838:LEU:O	2.15	0.46
1:A:349:LYS:HE3	4:A:1089:HOH:O	2.16	0.46
1:A:759:PRO:HG2	1:A:762:GLN:NE2	2.26	0.46
1:A:65:ALA:HA	1:A:176:LEU:CD2	2.45	0.46
1:A:194:GLU:HA	1:A:239:GLY:HA3	1.98	0.46
1:A:332:LYS:HD2	4:A:1160:HOH:O	2.16	0.46
1:A:836:THR:HG23	1:A:848:PHE:O	2.15	0.46
1:A:45:SER:CB	1:A:87:THR:HA	2.45	0.46
1:A:807:LYS:O	1:A:811:ILE:HG13	2.16	0.46
1:A:522:THR:HG22	1:A:523:HIS:N	2.29	0.45
1:A:308:HIS:C	1:A:310:LEU:H	2.19	0.45
1:A:329:PRO:C	1:A:331:LEU:H	2.20	0.45
1:A:518:HIS:CE1	3:A:871:EGT:C9	3.00	0.45
1:A:782:TYR:HB2	1:A:786:ARG:NH1	2.32	0.45
1:A:151:ASN:HB3	1:A:154:LEU:HD21	1.98	0.45
1:A:578:TRP:HB3	1:A:585:MET:CE	2.47	0.45
1:A:690:THR:HG22	1:A:692:GLU:N	2.32	0.45
1:A:43:VAL:HG22	1:A:92:LEU:HD22	1.99	0.45
1:A:111:ILE:N	1:A:111:ILE:HD12	2.32	0.45
1:A:169:PRO:C	1:A:171:GLU:N	2.68	0.44
1:A:341:GLN:O	1:A:342:ALA:HB2	2.16	0.44
1:A:393:VAL:CG1	1:A:479:SER:HA	2.47	0.44
1:A:165:GLN:HG3	1:A:167:TYR:OH	2.17	0.44
1:A:116:TYR:OH	1:A:179:TYR:HE1	2.00	0.44
1:A:843:LYS:HG3	1:A:849:ARG:NH2	2.29	0.44
1:A:136:PRO:HA	4:A:1358:HOH:O	2.16	0.44
1:A:804:PHE:CD1	1:A:807:LYS:HE2	2.41	0.44
1:A:75:LYS:HZ1	1:A:109:SER:HA	1.80	0.44
1:A:747:LYS:HE2	1:A:747:LYS:CA	2.48	0.44
3:A:871:EGT:H16	3:A:871:EGT:C10	2.47	0.44
1:A:41:ASP:HA	1:A:94:ALA:HA	2.00	0.44
1:A:543:ILE:HG22	1:A:547:LEU:HD22	1.99	0.44
1:A:604:LEU:HD21	1:A:630:THR:HG23	1.99	0.44
1:A:307:VAL:O	1:A:310:LEU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:THR:HB	1:A:467:ILE:HG12	2.00	0.44
1:A:600:LEU:HB3	1:A:601:PRO:HD3	1.99	0.44
1:A:335:PHE:HB2	4:A:1300:HOH:O	2.18	0.43
1:A:38:GLN:CG	1:A:39:GLY:H	2.31	0.43
1:A:45:SER:HB3	1:A:87:THR:HG22	2.00	0.43
1:A:298:PRO:HD2	1:A:760:LYS:NZ	2.33	0.43
1:A:514:GLN:CG	1:A:515:LEU:HD13	2.46	0.43
1:A:514:GLN:HG3	3:A:871:EGT:O20	2.18	0.43
1:A:44:GLY:C	1:A:46:THR:H	2.19	0.43
1:A:376:LEU:HD21	1:A:429:HIS:CE1	2.53	0.43
1:A:463:ARG:HH11	1:A:463:ARG:HB3	1.84	0.43
1:A:784:GLY:O	1:A:786:ARG:N	2.52	0.43
1:A:394:TYR:HD2	1:A:479:SER:O	2.01	0.43
1:A:541:HIS:CD2	1:A:542:PRO:HD2	2.53	0.43
1:A:43:VAL:O	1:A:97:SER:HA	2.18	0.43
1:A:393:VAL:HG23	1:A:478:GLN:HG3	2.01	0.43
1:A:514:GLN:CG	1:A:515:LEU:N	2.82	0.43
1:A:258:LEU:HD12	1:A:262:GLU:HB3	2.01	0.43
1:A:333:GLU:HA	4:A:1077:HOH:O	2.19	0.43
1:A:449:ALA:O	1:A:470:SER:HB2	2.19	0.43
1:A:68:ALA:HB1	1:A:72:GLY:O	2.18	0.43
1:A:397:HIS:CG	1:A:398:THR:N	2.86	0.43
1:A:819:ASN:ND2	1:A:827:ARG:NE	2.66	0.42
1:A:207:TYR:HB2	1:A:224:LEU:HB2	2.01	0.42
1:A:285:LEU:HB3	1:A:286:PRO:HD3	2.01	0.42
1:A:327:PRO:HG2	1:A:328:LEU:H	1.85	0.42
1:A:316:LYS:HG2	1:A:341:GLN:HB3	2.00	0.42
1:A:76:LEU:N	1:A:76:LEU:HD12	2.33	0.42
1:A:170:SER:C	1:A:172:THR:H	2.22	0.42
1:A:451:ARG:HB2	1:A:468:GLU:HB3	2.02	0.42
1:A:761:PHE:HD2	1:A:762:GLN:OE1	2.03	0.42
1:A:65:ALA:HA	1:A:176:LEU:HD21	2.00	0.42
1:A:173:PRO:HB2	1:A:176:LEU:HD23	2.00	0.42
1:A:202:TYR:O	1:A:535:ARG:HD2	2.20	0.42
1:A:394:TYR:CD2	1:A:479:SER:O	2.72	0.42
1:A:661:ASP:O	1:A:665:GLN:HG2	2.19	0.42
1:A:713:ASN:OD1	1:A:716:GLN:NE2	2.53	0.42
1:A:730:SER:HA	1:A:756:THR:O	2.20	0.42
1:A:825:ARG:HA	1:A:825:ARG:NE	2.20	0.42
1:A:830:PRO:HG3	4:A:1257:HOH:O	2.19	0.42
1:A:28:SER:C	1:A:30:THR:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LEU:CB	1:A:560:LEU:HD21	2.49	0.42
1:A:392:GLN:HG3	4:A:965:HOH:O	2.20	0.42
1:A:550:HIS:HA	1:A:854:SER:HB3	2.02	0.42
1:A:613:ASP:CB	1:A:621:ARG:HB2	2.49	0.42
1:A:83:GLU:HB3	4:A:1317:HOH:O	2.20	0.42
1:A:260:ARG:O	1:A:261:ASP:CB	2.68	0.42
1:A:581:TYR:HB2	1:A:585:MET:CE	2.47	0.42
1:A:208:ASN:HD21	1:A:235:ARG:HH21	1.56	0.42
1:A:29:VAL:HG13	1:A:32:VAL:CG2	2.50	0.42
1:A:292:PHE:HZ	1:A:764:LEU:HD12	1.85	0.42
1:A:40:LEU:HD13	1:A:42:LEU:HD21	2.02	0.41
1:A:74:GLY:N	1:A:179:TYR:HE2	2.01	0.41
1:A:788:ASN:CB	1:A:789:PRO:HD3	2.50	0.41
1:A:762:GLN:NE2	1:A:762:GLN:H	2.18	0.41
1:A:842:SER:HA	1:A:849:ARG:NH1	2.35	0.41
1:A:111:ILE:HA	1:A:112:PRO:HD3	1.82	0.41
1:A:132:LEU:HG	1:A:143:PHE:HE1	1.85	0.41
1:A:347:PRO:HA	1:A:348:PRO:HD3	1.74	0.41
1:A:513:HIS:HA	1:A:517:SER:HB2	2.02	0.41
1:A:566:VAL:CG2	1:A:583:VAL:HG22	2.47	0.41
1:A:781:VAL:HG12	1:A:786:ARG:HB3	2.03	0.41
1:A:791:TRP:H	1:A:791:TRP:HD1	1.64	0.41
1:A:67:LYS:HG2	1:A:108:GLY:O	2.20	0.41
1:A:340:GLU:HG3	1:A:341:GLN:NE2	2.35	0.41
1:A:628:PRO:HA	1:A:631:VAL:HG12	2.01	0.41
1:A:43:VAL:HA	1:A:96:GLN:O	2.21	0.41
1:A:330:VAL:C	1:A:332:LYS:H	2.24	0.41
1:A:332:LYS:O	1:A:334:ILE:HD12	2.20	0.41
1:A:717:TYR:N	1:A:718:PRO:CD	2.84	0.41
1:A:294:LEU:HD23	1:A:295:ASN:N	2.35	0.41
1:A:437:LEU:HD23	1:A:472:PRO:HD3	2.03	0.41
1:A:210:LEU:N	1:A:210:LEU:CD1	2.83	0.41
1:A:365:ALA:HB1	1:A:462:LEU:HB3	2.02	0.41
1:A:114:ALA:HA	1:A:161:PHE:O	2.20	0.41
1:A:115:PHE:CE2	1:A:161:PHE:HB2	2.56	0.41
1:A:380:LEU:HD11	1:A:385:PRO:HG3	2.03	0.41
1:A:394:TYR:OH	1:A:434:MET:CG	2.69	0.41
1:A:445:THR:O	1:A:446:LYS:HD3	2.20	0.41
1:A:518:HIS:ND1	3:A:871:EGT:C16	2.52	0.41
1:A:561:ALA:HA	1:A:565:LEU:HD22	2.03	0.41
1:A:561:ALA:HA	1:A:565:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:TRP:HB3	1:A:585:MET:HE3	2.02	0.41
1:A:83:GLU:O	1:A:84:GLY:O	2.38	0.41
1:A:168:LEU:O	1:A:170:SER:N	2.54	0.41
1:A:346:PRO:HG2	1:A:771:GLU:OE2	2.21	0.41
1:A:776:HIS:NE2	1:A:849:ARG:O	2.38	0.41
1:A:169:PRO:HG3	1:A:661:ASP:OD1	2.20	0.40
1:A:183:GLU:O	1:A:187:LEU:HD22	2.21	0.40
1:A:355:LYS:HE3	1:A:355:LYS:HB3	1.96	0.40
1:A:756:THR:O	1:A:756:THR:HG22	2.21	0.40
1:A:761:PHE:O	1:A:765:ILE:HG12	2.21	0.40
1:A:437:LEU:HD12	1:A:437:LEU:HA	1.96	0.40
1:A:819:ASN:ND2	1:A:827:ARG:HH21	2.20	0.40
1:A:29:VAL:O	1:A:29:VAL:CG1	2.69	0.40
1:A:625:GLU:H	1:A:625:GLU:HG2	1.67	0.40
1:A:346:PRO:HB2	4:A:1241:HOH:O	2.21	0.40
1:A:361:ASP:HB3	1:A:464:PRO:HD2	2.04	0.40
1:A:623:VAL:O	1:A:624:ILE:CG2	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	847/857 (99%)	731 (86%)	78 (9%)	38 (4%)	2 0

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	38	GLN
1	A	48	ASP
1	A	73	LYS

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Mol	Chain	Res	Type
1	A	84	GLY
1	A	110	GLY
1	A	134	ASP
1	A	172	THR
1	A	328	LEU
1	A	398	THR
1	A	410	LEU
1	A	477	ASP
1	A	478	GLN
1	A	688	MET
1	A	789	PRO
1	A	845	GLY
1	A	42	LEU
1	A	55	GLY
1	A	342	ALA
1	A	479	SER
1	A	480	GLY
1	A	570	GLY
1	A	784	GLY
1	A	785	GLU
1	A	135	ILE
1	A	294	LEU
1	A	295	ASN
1	A	327	PRO
1	A	330	VAL
1	A	333	GLU
1	A	334	ILE
1	A	408	PRO
1	A	737	LYS
1	A	136	PRO
1	A	514	GLN
1	A	624	ILE
1	A	169	PRO
1	A	29	VAL

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	743/749 (99%)	660 (89%)	83 (11%)	6 3

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	25	ASP
1	A	35	ILE
1	A	41	ASP
1	A	48	ASP
1	A	54	LEU
1	A	56	ARG
1	A	67	LYS
1	A	85	ILE
1	A	104	GLU
1	A	105	TRP
1	A	135	ILE
1	A	154	LEU
1	A	156	LYS
1	A	164	ASN
1	A	165	GLN
1	A	166	THR
1	A	183	GLU
1	A	184	LEU
1	A	187	LEU
1	A	195	ARG
1	A	208	ASN
1	A	215	LYS
1	A	217	GLU
1	A	219	HIS
1	A	243	THR
1	A	248	ASN
1	A	258	LEU
1	A	269	SER
1	A	274	THR
1	A	297	THR
1	A	305	ASP
1	A	317	LEU
1	A	320	ASP
1	A	328	LEU
1	A	331	LEU
1	A	341	GLN
1	A	355	LYS

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Mol	Chain	Res	Type
1	A	362	GLU
1	A	366	ARG
1	A	390	ASP
1	A	398	THR
1	A	406	LEU
1	A	410	LEU
1	A	413	LEU
1	A	414	THR
1	A	427	LEU
1	A	452	THR
1	A	463	ARG
1	A	465	LEU
1	A	485	VAL
1	A	493	VAL
1	A	514	GLN
1	A	515	LEU
1	A	539	VAL
1	A	547	LEU
1	A	553	ASP
1	A	565	LEU
1	A	580	ARG
1	A	611	ILE
1	A	626	ASP
1	A	630	THR
1	A	634	LEU
1	A	635	GLU
1	A	638	ASP
1	A	689	GLN
1	A	722	LEU
1	A	724	LEU
1	A	743	GLU
1	A	754	LEU
1	A	785	GLU
1	A	786	ARG
1	A	788	ASN
1	A	798	LEU
1	A	799	GLU
1	A	808	LEU
1	A	810	GLN
1	A	815	LEU
1	A	822	GLU
1	A	825	ARG

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Mol	Chain	Res	Type
1	A	832	GLN
1	A	837	LEU
1	A	838	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	96	GLN
1	A	138	HIS
1	A	164	ASN
1	A	165	GLN
1	A	208	ASN
1	A	218	ASN
1	A	219	HIS
1	A	341	GLN
1	A	397	HIS
1	A	421	ASN
1	A	441	ASN
1	A	458	ASN
1	A	508	ASN
1	A	521	ASN
1	A	534	ASN
1	A	541	HIS
1	A	556	ASN
1	A	618	HIS
1	A	665	GLN
1	A	689	GLN
1	A	716	GLN
1	A	725	ASN
1	A	750	GLN
1	A	762	GLN
1	A	810	GLN
1	A	819	ASN
1	A	820	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - 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	$\#\|Z\| > 2$
3	EGT	A	871	2	24,24,24	1.17	3 (12%)	36,36,36	1.39	5 (13%)

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
3	EGT	A	871	2	-	1/4/16/16	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	871	EGT	C4-C3	2.91	1.57	1.52
3	A	871	EGT	C3-C2	2.21	1.56	1.52
3	A	871	EGT	C11-C2	2.03	1.54	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	871	EGT	C10-O1-C2	3.73	124.48	116.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	871	EGT	O1-C2-C3	-3.11	104.28	109.94
3	A	871	EGT	C4-C3-C2	-2.98	105.09	109.09
3	A	871	EGT	O1-C10-C9	2.57	120.44	116.38
3	A	871	EGT	O1-C2-C11	-2.05	102.86	107.47

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	871	EGT	C12-C11-C2-O1

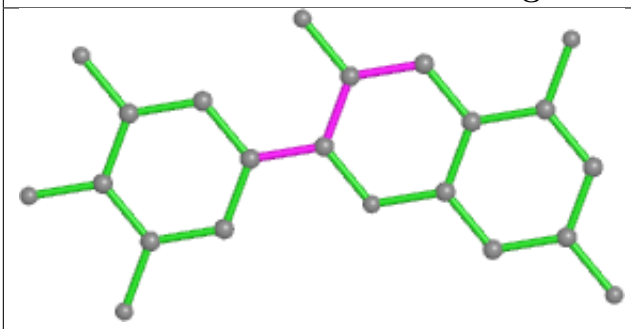
There are no ring outliers.

1 monomer is involved in 13 short contacts:

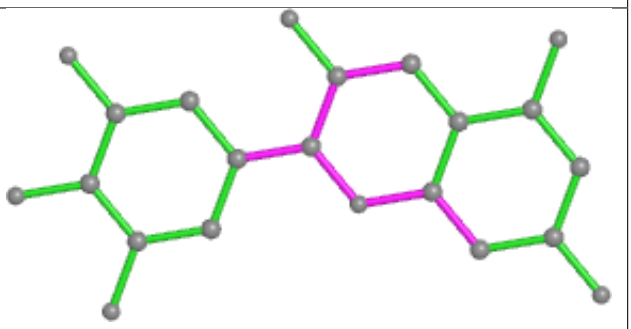
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	871	EGT	13	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

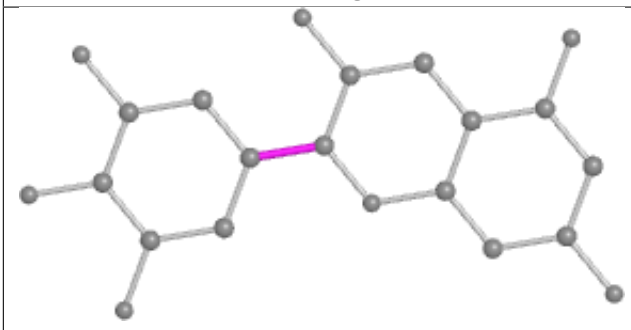
Ligand EGT A 871



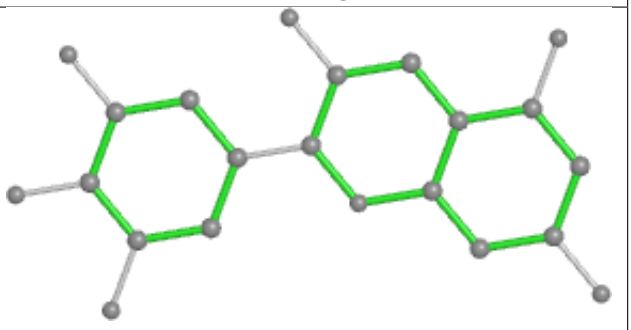
Bond lengths



Bond angles



Torsions



Rings

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	849/857 (99%)	-0.09	26 (3%) 49 55	12, 28, 57, 73	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	40	LEU	7.4
1	A	44	GLY	6.4
1	A	45	SER	6.1
1	A	43	VAL	6.1
1	A	36	ILE	5.8
1	A	784	GLY	5.8
1	A	393	VAL	4.4
1	A	32	VAL	4.3
1	A	35	ILE	3.7
1	A	46	THR	3.5
1	A	335	PHE	3.4
1	A	410	LEU	3.4
1	A	318	PRO	3.2
1	A	39	GLY	3.1
1	A	514	GLN	2.9
1	A	409	ASN	2.5
1	A	42	LEU	2.4
1	A	330	VAL	2.4
1	A	481	ALA	2.4
1	A	33	GLY	2.4
1	A	630	THR	2.3
1	A	395	GLY	2.3
1	A	34	GLY	2.2
1	A	297	THR	2.1
1	A	480	GLY	2.1
1	A	296	PHE	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 monosaccharides in this entry.

6.4 Ligands (i)

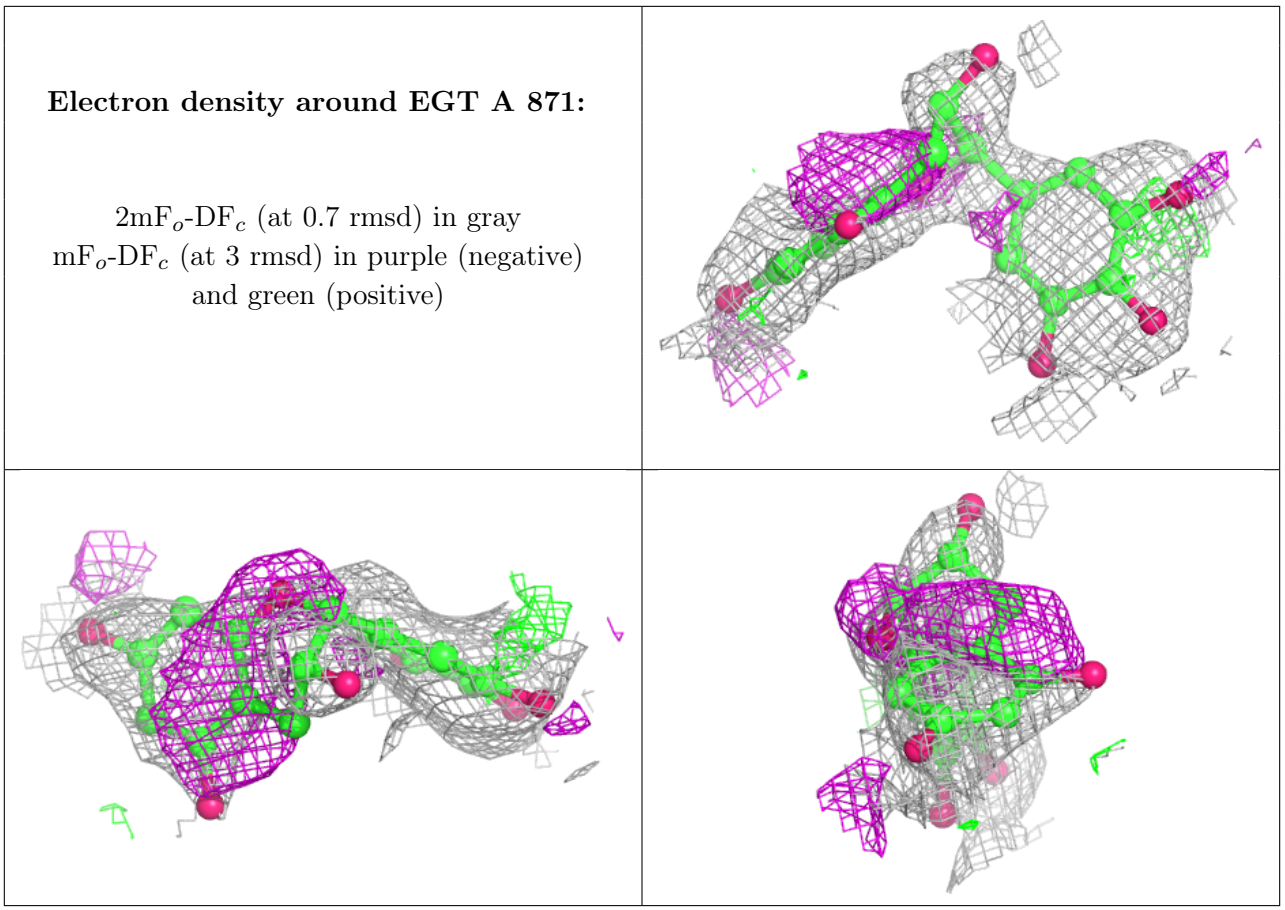
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EGT	A	871	22/22	0.74	0.39	43,47,51,51	0
2	FE2	A	858	1/1	0.99	0.07	32,32,32,32	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around EGT A 871:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.