Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2023 – 11:08 pm GMT

PDB ID	:	8C5W
Title	:	Crystal Structure of Penicillin-binding Protein 3 (PBP3) from Staphylococcus Epidermidis in complex with Cefotaxime
Authors	:	Schwinzer, M.; Brognaro, H.; Rohde, H.; Betzel, C.
Deposited on	:	2023-01-10
Resolution	:	2.51 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:

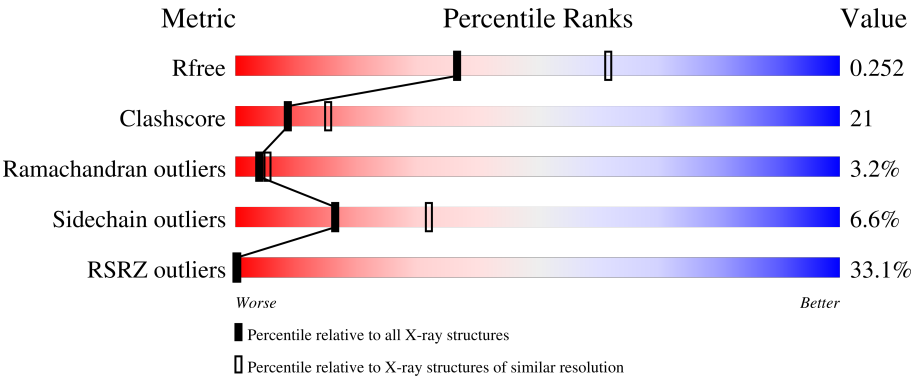
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.51 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	668	31% 56% 34% 5% 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9917 atoms, of which 4942 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.

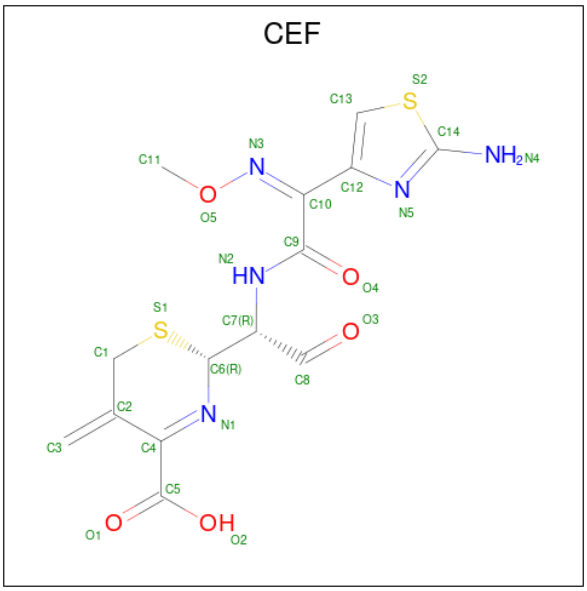
- Molecule 1 is a protein called Penicillin-binding protein 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	634	9886	3093	4942	855	980	16	0	0	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	GLY	-	expression tag	UNP Q5HNZ7
A	30	SER	-	expression tag	UNP Q5HNZ7
A	31	SER	-	expression tag	UNP Q5HNZ7
A	32	HIS	-	expression tag	UNP Q5HNZ7
A	33	HIS	-	expression tag	UNP Q5HNZ7
A	34	HIS	-	expression tag	UNP Q5HNZ7
A	35	HIS	-	expression tag	UNP Q5HNZ7
A	36	HIS	-	expression tag	UNP Q5HNZ7
A	37	HIS	-	expression tag	UNP Q5HNZ7
A	38	SER	-	expression tag	UNP Q5HNZ7
A	39	SER	-	expression tag	UNP Q5HNZ7
A	40	GLY	-	expression tag	UNP Q5HNZ7
A	41	GLU	-	expression tag	UNP Q5HNZ7
A	42	ASN	-	expression tag	UNP Q5HNZ7
A	43	LEU	-	expression tag	UNP Q5HNZ7
A	44	TYR	-	expression tag	UNP Q5HNZ7
A	45	PHE	-	expression tag	UNP Q5HNZ7
A	46	GLN	-	expression tag	UNP Q5HNZ7
A	47	SER	-	expression tag	UNP Q5HNZ7

- Molecule 2 is CEFOTAXIME, C3' cleaved, open, bound form (three-letter code: CEF) (formula: $C_{14}H_{15}N_5O_5S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	5	5	2		

- Molecule 3 is water.

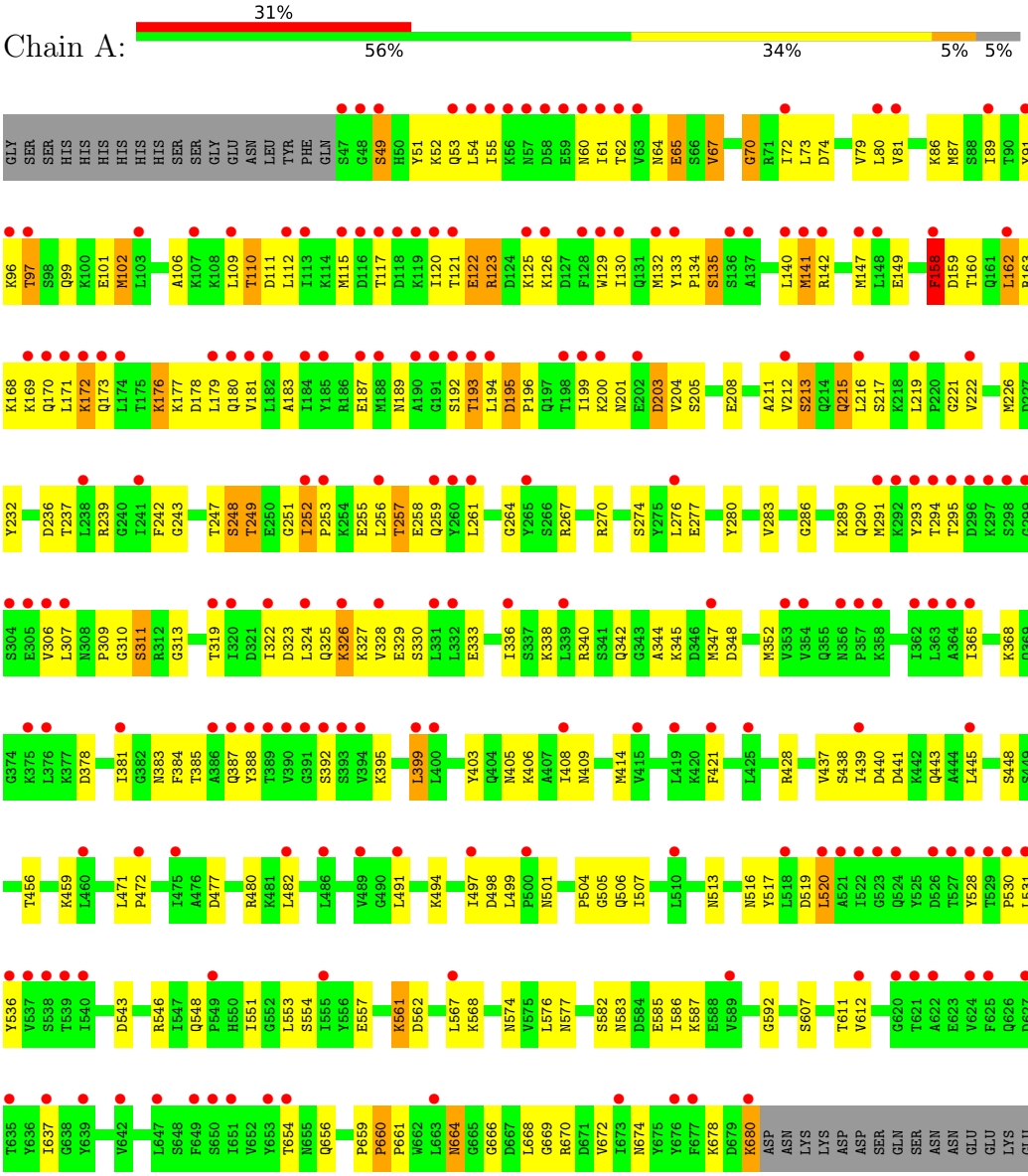
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	O	0	0
			5	5		

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: Penicillin-binding protein 3

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	83.06Å 83.06Å 308.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.75 – 2.51 46.75 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.0 (46.75-2.51) 85.9 (46.75-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.15 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.231 , 0.253 0.231 , 0.252	Depositor DCC
R_{free} test set	2000 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å^2)	71.3	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 63.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9917	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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: CEF

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	0.87	6/5022 (0.1%)	0.92	5/6772 (0.1%)

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	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	VAL	C-N	7.39	1.48	1.34
1	A	65	GLU	CD-OE2	-7.13	1.17	1.25
1	A	65	GLU	CD-OE1	-6.63	1.18	1.25
1	A	149	GLU	CD-OE1	6.05	1.32	1.25
1	A	158	PHE	CG-CD1	-5.65	1.30	1.38
1	A	158	PHE	CE2-CZ	-5.20	1.27	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	65	GLU	OE1-CD-OE2	-10.31	110.92	123.30
1	A	203	ASP	CB-CG-OD2	9.61	126.94	118.30
1	A	520	LEU	CB-CG-CD1	-6.68	99.64	111.00
1	A	637	ILE	CG1-CB-CG2	-5.72	98.82	111.40
1	A	147	MET	CG-SD-CE	5.55	109.09	100.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	230	ARG	Sidechain
1	A	632	VAL	Peptide
1	A	659	PRO	Peptide
1	A	93	ARG	Sidechain

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	4944	4942	4940	204	0
2	A	26	0	0	0	0
3	A	5	0	0	4	0
All	All	4975	4942	4940	204	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 21.

All (204) 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:64:ASN:O	3:A:801:HOH:O	1.66	1.12
1:A:607:SER:OG	1:A:664:ASN:OD1	1.75	1.04
1:A:498:ASP:O	1:A:499:LEU:HD23	1.74	0.88
1:A:91:TYR:HB2	1:A:199:ILE:HD11	1.61	0.83
1:A:395:LYS:HD3	1:A:453:MET:HG3	1.59	0.81
1:A:123:ARG:HD2	1:A:123:ARG:H	1.48	0.78
1:A:117:THR:HB	1:A:120:ILE:HD12	1.65	0.77
1:A:195:ASP:OD1	1:A:195:ASP:N	2.18	0.77
1:A:252:ILE:HD11	1:A:257:THR:HG22	1.67	0.77
1:A:347:MET:HE2	1:A:656:GLN:HG2	1.67	0.76
1:A:72:ILE:HB	1:A:81:VAL:HB	1.69	0.73
1:A:67:VAL:HG21	1:A:286:GLY:HA3	1.70	0.72
1:A:255:GLU:OE1	1:A:255:GLU:N	2.20	0.71
1:A:179:LEU:H	1:A:179:LEU:HD12	1.56	0.71
1:A:123:ARG:H	1:A:123:ARG:CD	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:ILE:HD12	1:A:531:LEU:HD21	1.75	0.69
1:A:252:ILE:HD11	1:A:257:THR:CG2	2.24	0.68
1:A:583:ASN:O	1:A:587:LYS:HG3	1.94	0.66
1:A:64:ASN:HA	1:A:289:LYS:O	1.96	0.66
1:A:546:ARG:CZ	1:A:576:LEU:HD12	2.26	0.65
1:A:252:ILE:HD11	1:A:257:THR:HA	1.79	0.65
1:A:55:ILE:HB	1:A:62:THR:HB	1.79	0.64
1:A:247:THR:O	1:A:249:THR:HG23	1.98	0.64
1:A:52:LYS:N	3:A:801:HOH:O	1.88	0.63
1:A:87:MET:HB2	1:A:204:VAL:CG2	2.29	0.62
1:A:329:GLU:O	1:A:333:GLU:HG3	2.00	0.62
1:A:193:THR:HG22	1:A:194:LEU:H	1.64	0.62
1:A:252:ILE:HG23	1:A:267:ARG:HA	1.82	0.62
1:A:660:PRO:HB2	1:A:661:PRO:HD3	1.79	0.62
1:A:440:ASP:HB2	1:A:443:GLN:HG3	1.83	0.61
1:A:67:VAL:CG2	1:A:286:GLY:HA3	2.29	0.61
1:A:112:LEU:CB	1:A:212:VAL:HG12	2.30	0.61
1:A:64:ASN:OD1	1:A:290:GLN:HG2	2.01	0.61
1:A:498:ASP:OD1	1:A:551:ILE:HG22	2.01	0.61
1:A:385:THR:HG22	1:A:501:ASN:O	2.01	0.61
1:A:81:VAL:HG22	1:A:232:TYR:CE1	2.35	0.60
1:A:87:MET:C	1:A:204:VAL:HG21	2.22	0.60
1:A:607:SER:O	1:A:670:ARG:HB2	2.01	0.60
1:A:177:LYS:HE3	1:A:177:LYS:CA	2.32	0.59
1:A:177:LYS:HE3	1:A:177:LYS:HA	1.84	0.59
1:A:53:GLN:HB2	1:A:64:ASN:HD22	1.65	0.59
1:A:289:LYS:HG3	1:A:309:PRO:O	2.03	0.59
1:A:81:VAL:HG22	1:A:232:TYR:CD1	2.38	0.59
1:A:248:SER:HB3	1:A:270:ARG:HG2	1.84	0.59
1:A:166:ILE:HG12	1:A:170:GLN:HB2	1.85	0.59
1:A:162:LEU:C	1:A:164:ASP:H	2.05	0.58
1:A:482:LEU:HD23	1:A:520:LEU:HD23	1.85	0.58
1:A:381:ILE:O	1:A:385:THR:OG1	2.18	0.57
1:A:115:MET:CE	1:A:199:ILE:O	2.52	0.57
1:A:94:ASN:HB2	1:A:97:THR:OG1	2.04	0.57
1:A:159:ASP:O	1:A:162:LEU:N	2.36	0.57
1:A:87:MET:O	1:A:204:VAL:HG21	2.05	0.57
1:A:368:LYS:NZ	1:A:378:ASP:OD1	2.30	0.56
1:A:109:LEU:C	1:A:111:ASP:H	2.09	0.56
1:A:310:GLY:O	1:A:311:SER:HB3	2.06	0.56
1:A:392:SER:HB3	1:A:395:LYS:HE2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ARG:NH2	1:A:192:SER:CB	2.70	0.55
1:A:247:THR:O	1:A:249:THR:N	2.38	0.55
1:A:204:VAL:HG23	1:A:204:VAL:O	2.06	0.55
1:A:101:GLU:OE1	1:A:101:GLU:N	2.41	0.54
1:A:666:GLY:O	1:A:669:GLY:N	2.39	0.54
1:A:384:PHE:CZ	1:A:499:LEU:HD12	2.43	0.54
1:A:178:ASP:HA	1:A:181:VAL:HG12	1.90	0.54
1:A:93:ARG:HH22	1:A:192:SER:HB2	1.73	0.53
1:A:365:ILE:O	1:A:365:ILE:HG23	2.08	0.53
1:A:129:TRP:NE1	1:A:170:GLN:O	2.42	0.53
1:A:170:GLN:HA	1:A:173:GLN:HG3	1.91	0.53
1:A:192:SER:O	1:A:193:THR:CB	2.57	0.53
1:A:87:MET:HB2	1:A:204:VAL:HG21	1.91	0.52
1:A:179:LEU:HD12	1:A:179:LEU:N	2.22	0.52
1:A:80:LEU:HD21	1:A:322:ILE:HD13	1.91	0.52
1:A:93:ARG:O	1:A:194:LEU:HD13	2.10	0.52
1:A:112:LEU:HB2	1:A:212:VAL:HG12	1.91	0.52
1:A:251:GLY:HA3	1:A:267:ARG:O	2.09	0.52
1:A:582:SER:O	1:A:586:ILE:HD12	2.10	0.52
1:A:325:GLN:O	1:A:329:GLU:HG3	2.10	0.52
1:A:319:THR:HG22	1:A:553:LEU:HB2	1.92	0.52
1:A:395:LYS:HD3	1:A:453:MET:CG	2.37	0.52
1:A:336:ILE:HD13	1:A:370:ILE:HD11	1.90	0.51
1:A:51:TYR:HA	3:A:801:HOH:O	2.10	0.51
1:A:87:MET:HB2	1:A:204:VAL:HG23	1.92	0.51
1:A:252:ILE:CD1	1:A:257:THR:HG22	2.40	0.51
1:A:546:ARG:HD3	1:A:577:ASN:OD1	2.11	0.51
1:A:112:LEU:HD22	1:A:211:ALA:HB1	1.92	0.51
1:A:166:ILE:HD11	1:A:170:GLN:H	1.75	0.51
1:A:86:LYS:O	1:A:86:LYS:HG3	2.08	0.51
1:A:344:ALA:HB1	1:A:347:MET:HE3	1.92	0.51
1:A:171:LEU:C	1:A:173:GLN:H	2.13	0.51
1:A:115:MET:N	1:A:180:GLN:OE1	2.40	0.51
1:A:294:THR:O	1:A:301:VAL:HA	2.11	0.51
1:A:49:SER:O	1:A:65:GLU:HG3	2.10	0.50
1:A:387:GLN:OE1	1:A:506:GLN:N	2.43	0.50
1:A:120:ILE:HD11	1:A:183:ALA:HB2	1.93	0.50
1:A:179:LEU:H	1:A:179:LEU:CD1	2.22	0.50
1:A:61:ILE:HB	1:A:293:TYR:HB2	1.93	0.50
1:A:93:ARG:CZ	1:A:192:SER:HA	2.42	0.50
1:A:387:GLN:OE1	1:A:505:GLY:HA2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:GLU:OE1	1:A:568:LYS:HD2	2.11	0.49
1:A:395:LYS:NZ	1:A:450:ASN:OD1	2.45	0.49
1:A:140:LEU:HD13	1:A:165:LYS:HB3	1.94	0.49
1:A:392:SER:O	1:A:395:LYS:HG3	2.12	0.49
1:A:73:LEU:HD22	1:A:79:VAL:HG22	1.94	0.49
1:A:294:THR:HB	1:A:302:ILE:HG22	1.95	0.49
1:A:403:TYR:OH	1:A:441:ASP:OD2	2.26	0.49
1:A:310:GLY:O	1:A:311:SER:CB	2.61	0.49
1:A:51:TYR:CA	3:A:801:HOH:O	2.61	0.48
1:A:193:THR:HG22	1:A:194:LEU:N	2.27	0.48
1:A:437:VAL:HG12	1:A:439:ILE:HG23	1.95	0.48
1:A:680:LYS:N	1:A:680:LYS:HD3	2.29	0.48
1:A:158:PHE:CD2	1:A:158:PHE:C	2.85	0.48
1:A:280:TYR:HB3	1:A:283:VAL:CG2	2.43	0.48
1:A:340:ARG:HG3	1:A:345:LYS:HA	1.94	0.48
1:A:408:ILE:HG12	1:A:456:THR:HG23	1.96	0.48
1:A:660:PRO:HD2	1:A:661:PRO:HD2	1.95	0.48
1:A:371:ASP:OD1	1:A:371:ASP:C	2.52	0.48
1:A:295:THR:HA	1:A:300:ARG:O	2.14	0.47
1:A:319:THR:HG23	1:A:551:ILE:O	2.14	0.47
1:A:516:ASN:O	1:A:519:ASP:N	2.47	0.47
1:A:252:ILE:HD11	1:A:257:THR:CA	2.41	0.47
1:A:80:LEU:HD22	1:A:242:PHE:HZ	1.79	0.47
1:A:91:TYR:CE1	1:A:221:GLY:HA3	2.49	0.47
1:A:242:PHE:O	1:A:277:GLU:HG2	2.14	0.47
1:A:494:LYS:HG2	1:A:504:PRO:HB3	1.96	0.47
1:A:53:GLN:HB2	1:A:64:ASN:ND2	2.30	0.47
1:A:243:GLY:HA3	1:A:274:SER:O	2.15	0.47
1:A:477:ASP:OD1	1:A:480:ARG:NH1	2.47	0.47
1:A:668:LEU:HD12	1:A:668:LEU:O	2.15	0.47
1:A:106:ALA:O	1:A:110:THR:HG22	2.15	0.46
1:A:507:ILE:HG22	1:A:507:ILE:O	2.15	0.46
1:A:554:SER:HB2	1:A:567:LEU:HD11	1.98	0.46
1:A:660:PRO:HB2	1:A:661:PRO:CD	2.44	0.46
1:A:253:PRO:HG2	1:A:256:LEU:HD23	1.98	0.46
1:A:513:ASN:OD1	1:A:513:ASN:N	2.41	0.46
1:A:176:LYS:HD2	1:A:176:LYS:H	1.81	0.45
1:A:257:THR:O	1:A:259:GLN:N	2.49	0.45
1:A:115:MET:HE2	1:A:199:ILE:O	2.15	0.45
1:A:93:ARG:HH22	1:A:192:SER:CB	2.30	0.45
1:A:370:ILE:HG22	1:A:371:ASP:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:MET:HE1	1:A:199:ILE:O	2.17	0.44
1:A:141:MET:HG3	1:A:158:PHE:CE2	2.53	0.44
1:A:54:LEU:HA	1:A:62:THR:O	2.18	0.44
1:A:112:LEU:CD1	1:A:212:VAL:HG12	2.48	0.44
1:A:94:ASN:HB3	1:A:96:LYS:H	1.82	0.44
1:A:414:MET:HE1	1:A:459:LYS:HD2	1.99	0.44
1:A:680:LYS:HD3	1:A:680:LYS:H	1.82	0.44
1:A:192:SER:O	1:A:193:THR:HB	2.18	0.44
1:A:53:GLN:O	1:A:54:LEU:HD12	2.18	0.43
1:A:133:TYR:N	1:A:134:PRO:CD	2.82	0.43
1:A:327:LYS:O	1:A:330:SER:HB3	2.18	0.43
1:A:403:TYR:CD2	1:A:585:GLU:HG2	2.52	0.43
1:A:96:LYS:O	1:A:97:THR:HG23	2.18	0.43
1:A:109:LEU:HD11	1:A:222:VAL:HG21	2.01	0.43
1:A:205:SER:O	1:A:208:GLU:N	2.50	0.43
1:A:89:ILE:HD13	1:A:212:VAL:HG21	2.01	0.43
1:A:132:MET:O	1:A:133:TYR:CD1	2.71	0.43
1:A:228:TRP:O	1:A:270:ARG:NH1	2.52	0.43
1:A:93:ARG:NH2	1:A:192:SER:HB2	2.34	0.42
1:A:93:ARG:NH2	1:A:192:SER:HA	2.34	0.42
1:A:491:LEU:HB3	1:A:528:TYR:CE2	2.54	0.42
1:A:516:ASN:O	1:A:517:TYR:C	2.56	0.42
1:A:213:SER:HA	1:A:216:LEU:HG	2.01	0.42
1:A:236:ASP:O	1:A:237:THR:C	2.56	0.42
1:A:216:LEU:HD22	1:A:222:VAL:O	2.19	0.42
1:A:141:MET:HG2	1:A:162:LEU:HG	2.01	0.42
1:A:383:ASN:HA	1:A:530:PRO:HG2	2.02	0.42
1:A:399:LEU:HD13	1:A:453:MET:HE1	2.02	0.42
1:A:405:ASN:O	1:A:406:LYS:HB2	2.19	0.42
1:A:307:LEU:C	1:A:307:LEU:HD13	2.39	0.42
1:A:194:LEU:O	1:A:196:PRO:HD3	2.19	0.42
1:A:122:GLU:HA	1:A:125:LYS:HD3	2.02	0.42
1:A:189:ASN:O	1:A:189:ASN:OD1	2.37	0.42
1:A:548:GLN:OE1	1:A:574:ASN:HB2	2.20	0.42
1:A:129:TRP:HE3	1:A:130:ILE:HD13	1.85	0.41
1:A:348:ASP:OD1	1:A:348:ASP:N	2.52	0.41
1:A:122:GLU:H	1:A:122:GLU:CD	2.24	0.41
1:A:176:LYS:H	1:A:176:LYS:CD	2.33	0.41
1:A:203:ASP:O	1:A:203:ASP:OD2	2.38	0.41
1:A:215:GLN:O	1:A:219:LEU:HD22	2.20	0.41
1:A:471:LEU:O	1:A:472:PRO:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:ASP:N	1:A:441:ASP:OD1	2.54	0.41
1:A:612:VAL:HG12	1:A:674:ASN:HA	2.02	0.41
1:A:70:GLY:H	1:A:313:GLY:HA3	1.86	0.41
1:A:133:TYR:C	1:A:135:SER:N	2.74	0.41
1:A:421:PHE:CD2	1:A:471:LEU:HD21	2.56	0.41
1:A:668:LEU:O	1:A:672:VAL:HG23	2.21	0.41
1:A:158:PHE:C	1:A:158:PHE:HD2	2.24	0.41
1:A:291:MET:SD	1:A:306:VAL:HA	2.61	0.41
1:A:388:TYR:CD2	1:A:654:THR:HG21	2.56	0.41
1:A:406:LYS:HA	1:A:406:LYS:HD3	1.92	0.41
1:A:561:LYS:O	1:A:562:ASP:HB2	2.19	0.41
1:A:295:THR:HG22	1:A:301:VAL:HG22	2.03	0.41
1:A:94:ASN:C	1:A:96:LYS:H	2.24	0.41
1:A:121:THR:HB	1:A:123:ARG:HD3	2.03	0.41
1:A:237:THR:OG1	1:A:326:LYS:HE3	2.22	0.40
1:A:409:ASN:OD1	1:A:409:ASN:N	2.53	0.40
1:A:319:THR:CG2	1:A:553:LEU:HB2	2.51	0.40
1:A:338:LYS:O	1:A:342:GLN:HG3	2.22	0.40
1:A:445:LEU:HD12	1:A:592:GLY:HA3	2.04	0.40
1:A:200:LYS:CE	1:A:203:ASP:OD2	2.70	0.40
1:A:183:ALA:O	1:A:187:GLU:HG2	2.21	0.40
1:A:261:LEU:N	1:A:261:LEU:HD12	2.37	0.40
1:A:276:LEU:HD23	1:A:276:LEU:HA	1.85	0.40
1:A:324:LEU:O	1:A:328:VAL:HG23	2.21	0.40
1:A:93:ARG:HD2	1:A:102:MET:CE	2.51	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	632/668 (95%)	528 (84%)	84 (13%)	20 (3%)	4 5

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	SER
1	A	135	SER
1	A	193	THR
1	A	257	THR
1	A	311	SER
1	A	99	GLN
1	A	168	LYS
1	A	70	GLY
1	A	102	MET
1	A	172	LYS
1	A	258	GLU
1	A	110	THR
1	A	248	SER
1	A	122	GLU
1	A	126	LYS
1	A	163	ARG
1	A	217	SER
1	A	660	PRO
1	A	167	GLY
1	A	264	GLY

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	544/586 (93%)	508 (93%)	36 (7%)	16 32

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	74	ASP
1	A	97	THR
1	A	123	ARG
1	A	141	MET

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Mol	Chain	Res	Type
1	A	142	ARG
1	A	158	PHE
1	A	160	THR
1	A	162	LEU
1	A	169	LYS
1	A	172	LYS
1	A	176	LYS
1	A	195	ASP
1	A	201	ASN
1	A	213	SER
1	A	215	GLN
1	A	226	MET
1	A	239	ARG
1	A	249	THR
1	A	252	ILE
1	A	323	ASP
1	A	326	LYS
1	A	352	MET
1	A	371	ASP
1	A	399	LEU
1	A	428	ARG
1	A	438	SER
1	A	448	SER
1	A	451	VAL
1	A	536	TYR
1	A	543	ASP
1	A	561	LYS
1	A	611	THR
1	A	664	ASN
1	A	678	LYS
1	A	680	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	161	GLN
1	A	656	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	CEF	A	701	1	19,27,27	1.28	2 (10%)	14,37,37	3.93	9 (64%)

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	CEF	A	701	1	-	7/14/38/38	0/1/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	CEF	C13-S2	3.10	1.75	1.70
2	A	701	CEF	C10-N3	2.63	1.33	1.29

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	CEF	O5-N3-C10	8.33	120.45	111.28
2	A	701	CEF	C11-O5-N3	8.25	117.99	108.40
2	A	701	CEF	C1-S1-C6	5.08	104.44	94.47
2	A	701	CEF	N4-C14-N5	3.75	128.04	123.19
2	A	701	CEF	C12-C13-S2	-3.06	108.03	111.79
2	A	701	CEF	O2-C5-O1	3.05	130.60	123.61
2	A	701	CEF	O1-C5-C4	-2.61	113.97	120.86
2	A	701	CEF	C10-C9-N2	2.18	118.00	114.38
2	A	701	CEF	C2-C1-S1	-2.02	107.48	111.65

There are no chirality outliers.

All (7) torsion outliers are listed below:

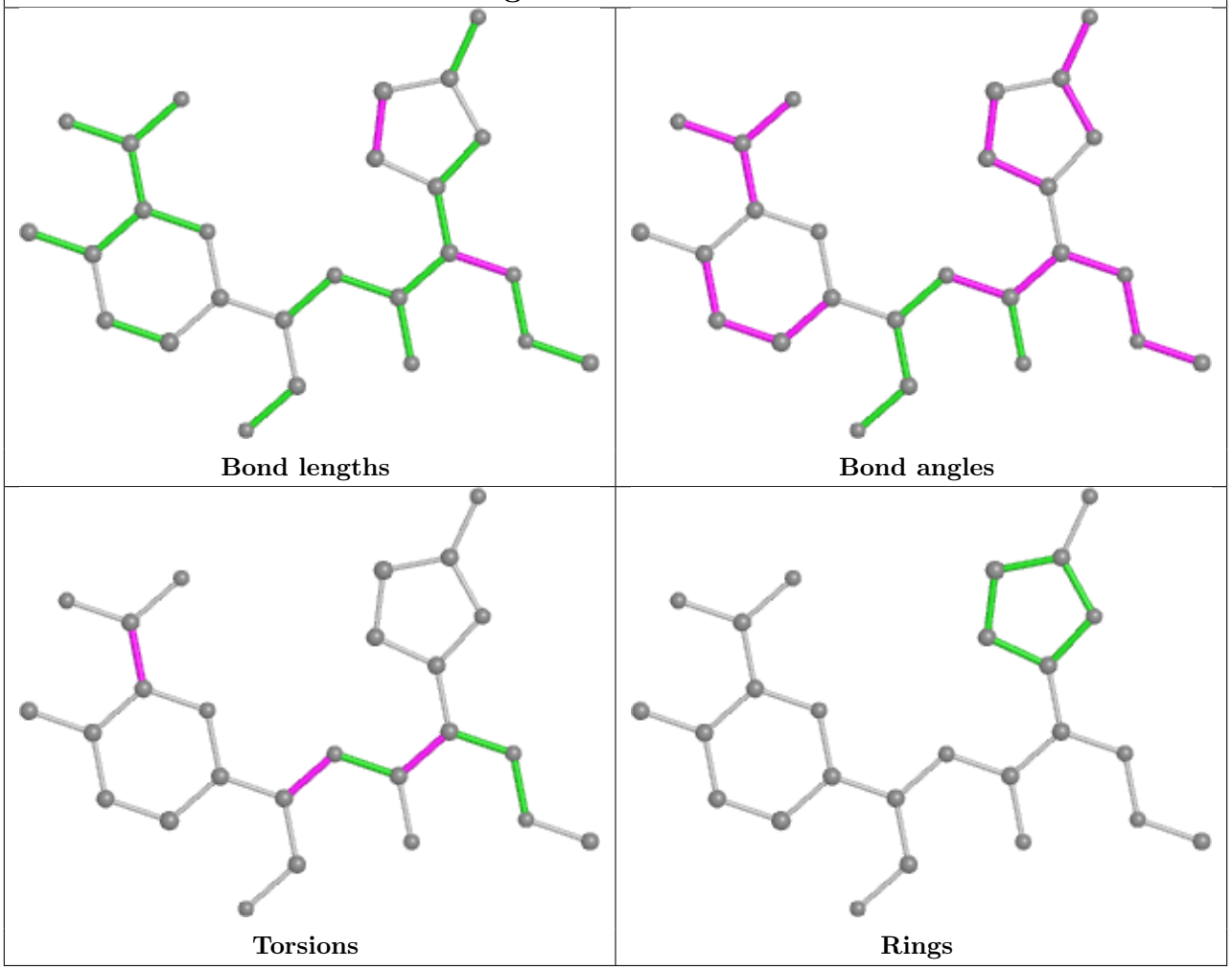
Mol	Chain	Res	Type	Atoms
2	A	701	CEF	C6-C7-N2-C9
2	A	701	CEF	C12-C10-C9-O4
2	A	701	CEF	N3-C10-C9-O4
2	A	701	CEF	N3-C10-C9-N2
2	A	701	CEF	N1-C4-C5-O2
2	A	701	CEF	N1-C4-C5-O1
2	A	701	CEF	C12-C10-C9-N2

There are no ring outliers.

No monomer is involved in short contacts.

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 CEF A 701



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	634/668 (94%)	1.67	210 (33%)	0	0	70, 94, 144, 178	0

All (210) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	293	TYR	10.9
1	A	306	VAL	9.9
1	A	302	ILE	9.6
1	A	47	SER	9.6
1	A	56	LYS	9.5
1	A	61	ILE	9.4
1	A	292	LYS	8.7
1	A	54	LEU	8.7
1	A	174	LEU	7.9
1	A	55	ILE	7.7
1	A	305	GLU	7.6
1	A	120	ILE	7.4
1	A	57	ASN	7.2
1	A	63	VAL	6.7
1	A	303	SER	6.7
1	A	58	ASP	6.6
1	A	307	LEU	6.6
1	A	297	LYS	6.5
1	A	62	THR	6.0
1	A	304	SER	5.9
1	A	118	ASP	5.9
1	A	260	TYR	5.6
1	A	170	GLN	5.4
1	A	256	LEU	5.4
1	A	296	ASP	5.3
1	A	136	SER	5.2
1	A	301	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	298	SER	5.1
1	A	128	PHE	5.1
1	A	192	SER	5.0
1	A	166	ILE	4.9
1	A	130	ILE	4.8
1	A	194	LEU	4.8
1	A	222	VAL	4.8
1	A	300	ARG	4.8
1	A	185	TYR	4.7
1	A	59	GLU	4.7
1	A	299	GLY	4.7
1	A	199	ILE	4.7
1	A	291	MET	4.6
1	A	133	TYR	4.6
1	A	109	LEU	4.6
1	A	137	ALA	4.6
1	A	140	LEU	4.5
1	A	103	LEU	4.5
1	A	673	ILE	4.3
1	A	95	ARG	4.2
1	A	259	GLN	4.2
1	A	265	TYR	4.1
1	A	132	MET	4.0
1	A	169	LYS	4.0
1	A	141	MET	4.0
1	A	294	THR	4.0
1	A	119	LYS	4.0
1	A	165	LYS	4.0
1	A	191	GLY	3.9
1	A	393	SER	3.9
1	A	531	LEU	3.9
1	A	173	GLN	3.9
1	A	125	LYS	3.9
1	A	91	TYR	3.8
1	A	181	VAL	3.8
1	A	179	LEU	3.8
1	A	533	LEU	3.8
1	A	113	ILE	3.6
1	A	129	TRP	3.6
1	A	389	THR	3.6
1	A	326	LYS	3.6
1	A	184	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	363	LEU	3.6
1	A	362	ILE	3.5
1	A	518	LEU	3.5
1	A	534	SER	3.5
1	A	392	SER	3.3
1	A	388	TYR	3.3
1	A	528	TYR	3.3
1	A	530	PRO	3.2
1	A	116	ASP	3.2
1	A	60	ASN	3.2
1	A	212	VAL	3.2
1	A	527	THR	3.2
1	A	523	GLY	3.2
1	A	188	MET	3.2
1	A	126	LYS	3.2
1	A	171	LEU	3.2
1	A	472	PRO	3.1
1	A	536	TYR	3.1
1	A	117	THR	3.1
1	A	187	GLU	3.1
1	A	261	LEU	3.1
1	A	48	GLY	3.1
1	A	53	GLN	3.1
1	A	347	MET	3.1
1	A	391	GLY	3.0
1	A	625	PHE	3.0
1	A	637	ILE	3.0
1	A	529	THR	3.0
1	A	650	SER	3.0
1	A	322	ILE	3.0
1	A	538	SER	3.0
1	A	89	ILE	3.0
1	A	320	ILE	3.0
1	A	624	VAL	3.0
1	A	121	THR	3.0
1	A	419	LEU	3.0
1	A	49	SER	2.9
1	A	642	VAL	2.9
1	A	390	VAL	2.9
1	A	295	THR	2.9
1	A	510	LEU	2.9
1	A	537	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	167	GLY	2.9
1	A	158	PHE	2.8
1	A	475	ILE	2.8
1	A	172	LYS	2.8
1	A	387	GLN	2.8
1	A	400	LEU	2.8
1	A	539	THR	2.8
1	A	162	LEU	2.8
1	A	376	LEU	2.8
1	A	115	MET	2.8
1	A	142	ARG	2.7
1	A	182	LEU	2.7
1	A	521	ALA	2.7
1	A	276	LEU	2.7
1	A	328	VAL	2.7
1	A	332	LEU	2.7
1	A	520	LEU	2.7
1	A	81	VAL	2.7
1	A	252	ILE	2.7
1	A	647	LEU	2.7
1	A	524	GLN	2.6
1	A	365	ILE	2.6
1	A	651	ILE	2.6
1	A	370	ILE	2.6
1	A	336	ILE	2.6
1	A	540	ILE	2.6
1	A	622	ALA	2.5
1	A	491	LEU	2.5
1	A	93	ARG	2.5
1	A	190	ALA	2.5
1	A	386	ALA	2.5
1	A	394	VAL	2.5
1	A	193	THR	2.5
1	A	653	TYR	2.5
1	A	198	THR	2.5
1	A	486	LEU	2.5
1	A	399	LEU	2.5
1	A	489	VAL	2.4
1	A	353	VAL	2.4
1	A	375	LYS	2.4
1	A	200	LYS	2.4
1	A	357	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	635	THR	2.4
1	A	80	LEU	2.4
1	A	72	ILE	2.4
1	A	381	ILE	2.4
1	A	216	LEU	2.4
1	A	148	LEU	2.4
1	A	621	THR	2.3
1	A	532	GLN	2.3
1	A	180	GLN	2.3
1	A	415	VAL	2.3
1	A	439	ILE	2.3
1	A	421	PHE	2.3
1	A	677	PHE	2.3
1	A	627	ASP	2.3
1	A	500	PRO	2.3
1	A	354	VAL	2.3
1	A	241	ILE	2.3
1	A	219	LEU	2.3
1	A	680	LYS	2.2
1	A	460	LEU	2.2
1	A	535	GLN	2.2
1	A	358	LYS	2.2
1	A	147	MET	2.2
1	A	482	LEU	2.2
1	A	620	GLY	2.2
1	A	612	VAL	2.2
1	A	425	LEU	2.2
1	A	373	GLN	2.2
1	A	408	ILE	2.2
1	A	497	ILE	2.2
1	A	445	LEU	2.2
1	A	663	LEU	2.2
1	A	364	ALA	2.2
1	A	238	LEU	2.2
1	A	634	SER	2.2
1	A	639	TYR	2.1
1	A	526	ASP	2.1
1	A	549	PRO	2.1
1	A	96	LYS	2.1
1	A	522	ILE	2.1
1	A	649	PHE	2.1
1	A	567	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	589	VAL	2.1
1	A	319	THR	2.1
1	A	356	ASN	2.1
1	A	451	VAL	2.1
1	A	555	ILE	2.0
1	A	253	PRO	2.0
1	A	97	THR	2.0
1	A	331	LEU	2.0
1	A	339	LEU	2.0
1	A	107	LYS	2.0
1	A	654	THR	2.0
1	A	112	LEU	2.0
1	A	324	LEU	2.0
1	A	676	TYR	2.0
1	A	202	GLU	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)

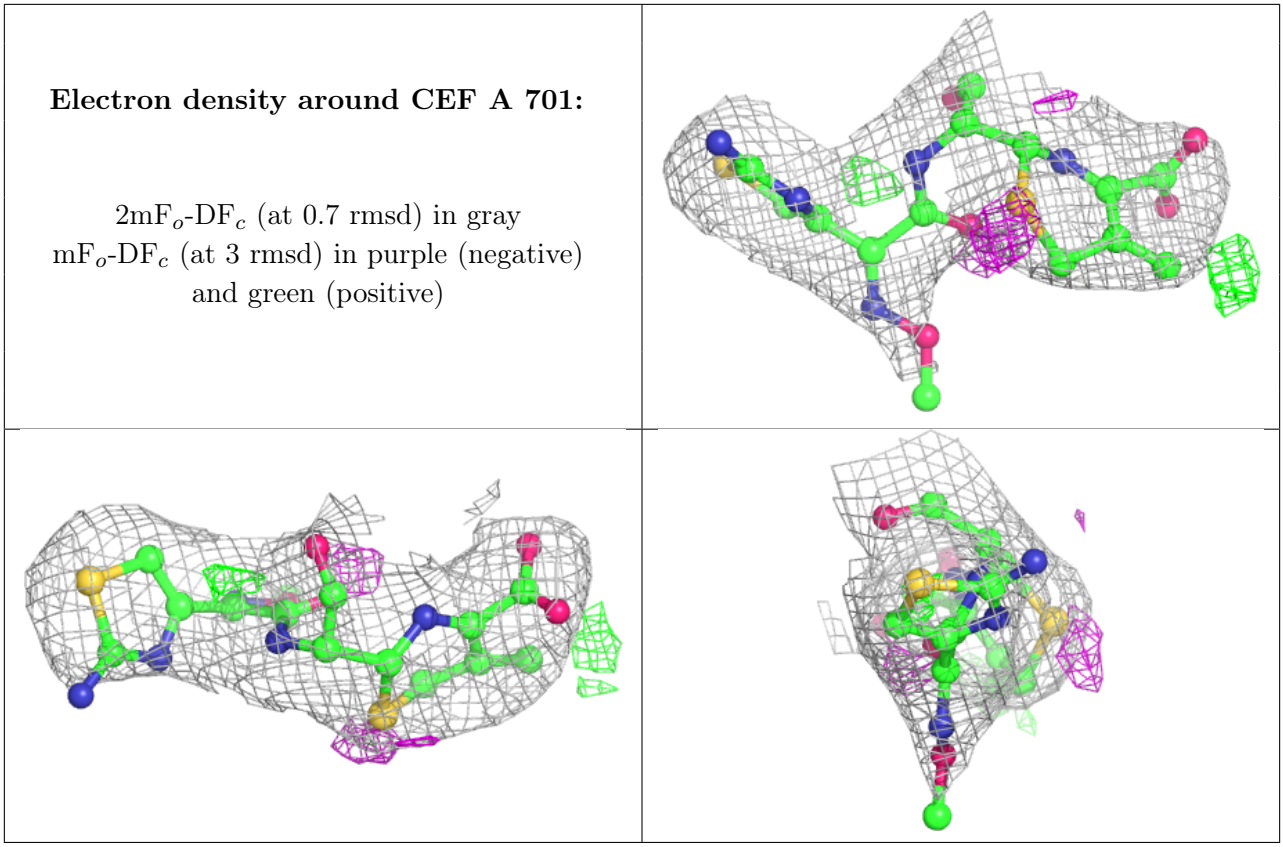
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	CEF	A	701	26/26	0.91	0.30	72,96,121,124	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 CEF A 701:

$2mF_o$-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.