



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2024 – 03:17 AM EST

PDB ID : 3VSL
Title : Crystal structure of penicillin-binding protein 3 (PBP3) from methicillin-resistant *Staphylococcus aureus* in the cefotaxime bound form.
Authors : Yoshida, H.; Tame, J.R.; Park, S.Y.
Deposited on : 2012-04-25
Resolution : 2.40 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

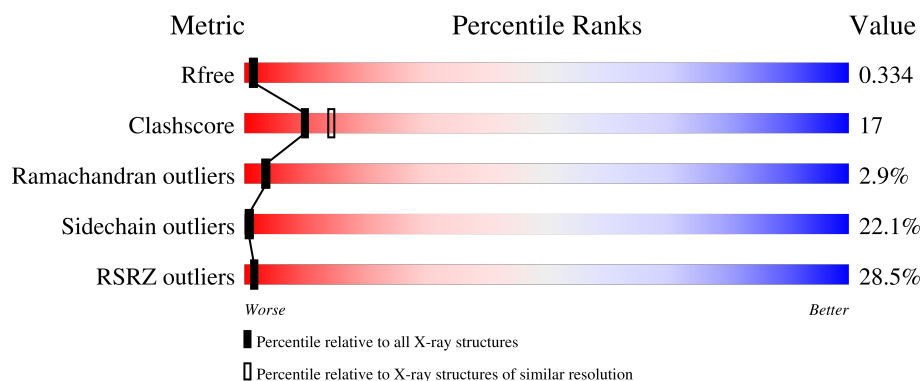
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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 $\leq 5\%$. 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	646	
1	B	646	

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:

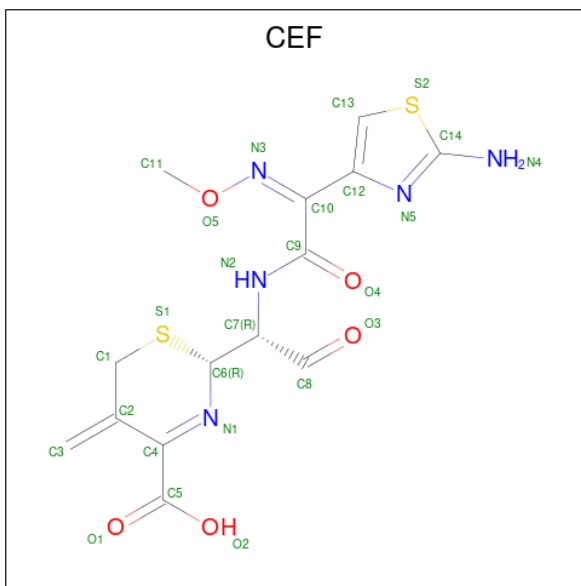
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CEF	A	701	X	-	-	-
2	CEF	B	701	X	-	-	-

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
1	A	631	Total 4943	C 3105	N 852	O 967	S 19	0	0	0
1	B	631	Total 4947	C 3107	N 853	O 968	S 19	0	0	0

- Molecule 2 is CEFOTAXIME, C3' cleaved, open, bound form (three-letter code: CEF) (formula: $C_{14}H_{15}N_5O_5S_2$).



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

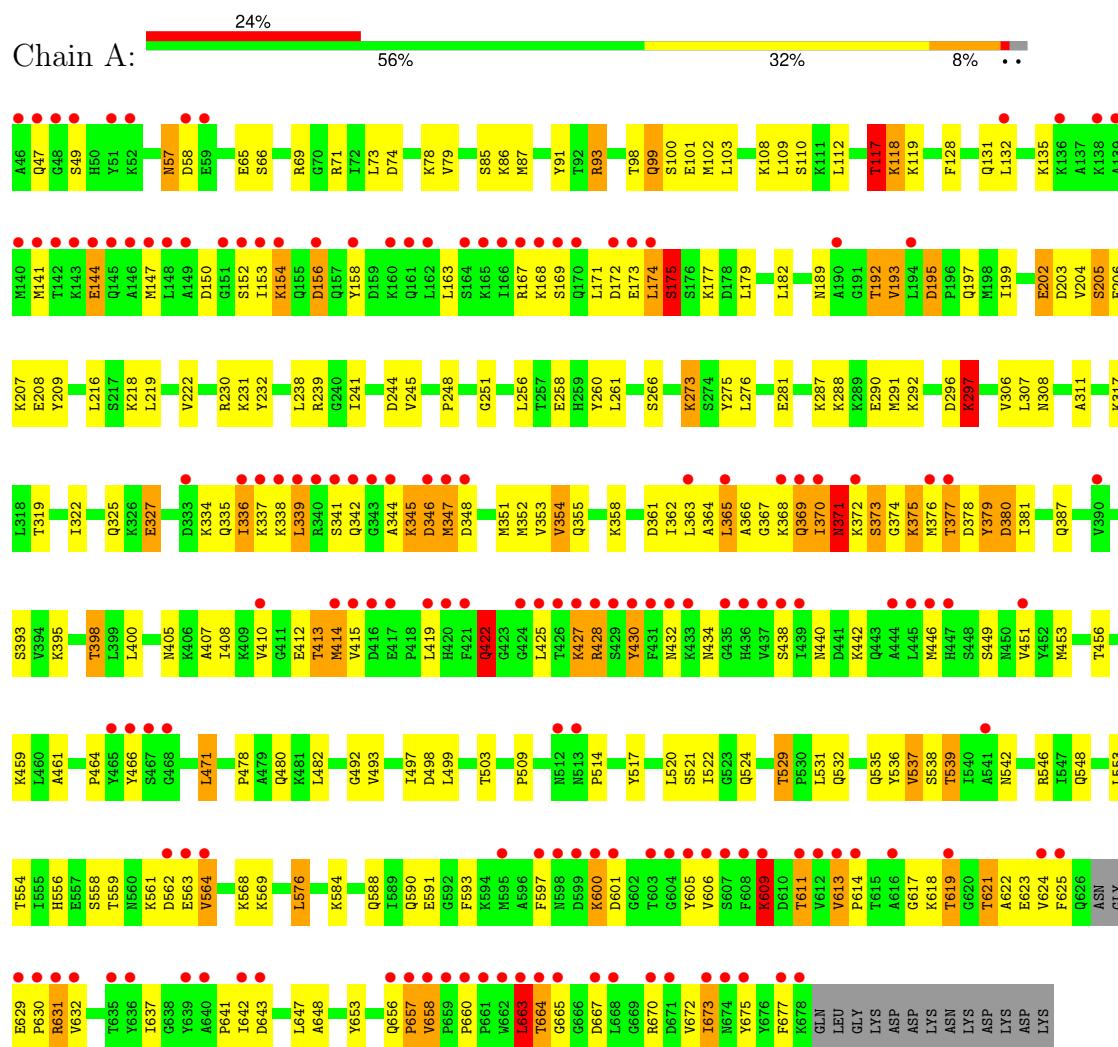
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	140	Total 140	O 140	0	0
3	B	116	Total 116	O 116	0	0

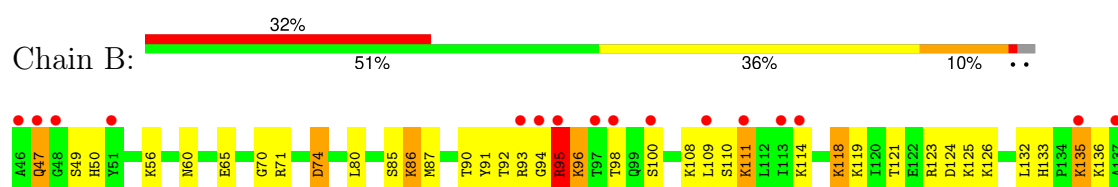
3 Residue-property plots

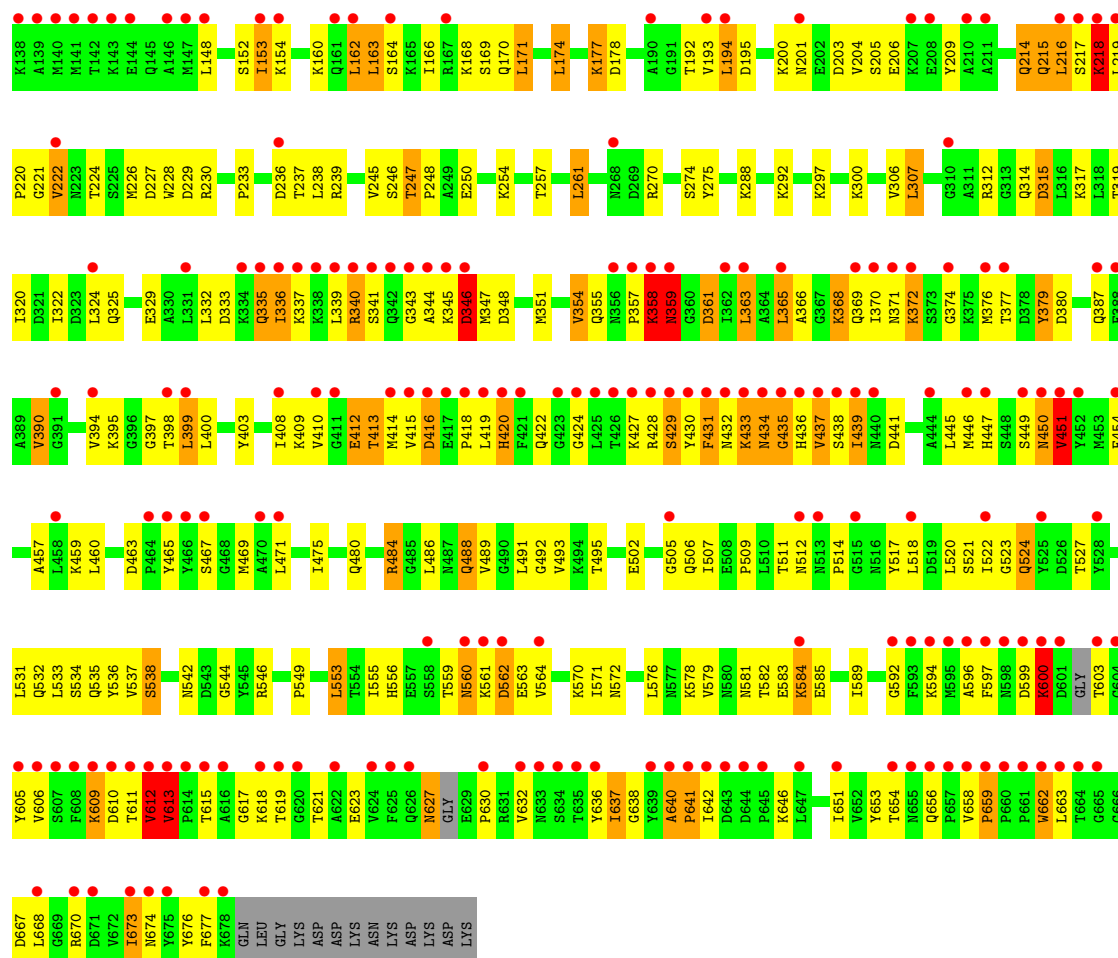
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Penicillin-binding protein 3



• Molecule 1: Penicillin-binding protein 3





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	143.03Å 143.03Å 189.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.86 – 2.40 48.86 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.86-2.40) 98.2 (48.86-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.247 , 0.316 0.274 , 0.334	Depositor DCC
R_{free} test set	3797 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 68.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	10198	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.46	0/5025	0.67	1/6769 (0.0%)
1	B	0.46	0/5029	0.70	0/6775
All	All	0.46	0/10054	0.69	1/13544 (0.0%)

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	8
1	B	0	11
All	All	0	19

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	ARG	NE-CZ-NH2	-5.40	117.60	120.30

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	174	LEU	Peptide
1	A	251	GLY	Peptide
1	A	296	ASP	Peptide
1	A	371	ASN	Peptide
1	A	430	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	A	657	PRO	Peptide
1	A	658	VAL	Peptide
1	A	660	PRO	Peptide
1	B	218	LYS	Peptide
1	B	346	ASP	Peptide
1	B	358	LYS	Peptide
1	B	359	ASN	Peptide
1	B	428	ARG	Peptide
1	B	429	SER	Peptide
1	B	560	ASN	Peptide
1	B	600	LYS	Peptide
1	B	612	VAL	Peptide
1	B	613	VAL	Peptide
1	B	640	ALA	Peptide

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	4943	0	4991	166	0
1	B	4947	0	4994	180	0
2	A	26	0	1	6	0
2	B	26	0	1	6	0
3	A	140	0	0	4	0
3	B	116	0	0	5	0
All	All	10198	0	9987	341	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 17.

All (341) 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)
2:A:701:CEF:N5	2:A:701:CEF:C14	1.72	1.45
2:B:701:CEF:N5	2:B:701:CEF:C14	1.73	1.43
2:A:701:CEF:C14	2:A:701:CEF:HN2	1.54	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:THR:HG22	1:A:532:GLN:H	1.27	0.95
1:A:600:LYS:HE3	1:A:600:LYS:H	1.35	0.89
2:B:701:CEF:C14	2:B:701:CEF:HN2	1.79	0.88
1:A:367:GLY:HA2	1:A:379:TYR:H	1.37	0.87
1:A:408:ILE:HG21	1:A:456:THR:HG22	1.62	0.80
1:A:354:VAL:H	1:A:364:ALA:HB2	1.46	0.79
1:A:99:GLN:HG2	1:A:131:GLN:HE22	1.50	0.77
1:B:94:GLY:HA3	1:B:193:VAL:HG13	1.68	0.75
1:B:329:GLU:HA	1:B:365:LEU:HD22	1.68	0.75
1:B:416:ASP:OD1	1:B:416:ASP:N	2.21	0.73
1:B:365:LEU:HG	1:B:366:ALA:N	2.05	0.71
1:A:205:SER:HB3	1:A:208:GLU:HG3	1.72	0.71
1:A:535:GLN:O	1:A:539:THR:HG22	1.91	0.70
1:A:147:MET:HA	1:A:150:ASP:HB2	1.74	0.70
1:B:446:MET:HA	1:B:596:ALA:HB2	1.74	0.70
1:A:482:LEU:HD23	1:A:520:LEU:HD23	1.74	0.69
1:A:623:GLU:OE1	2:A:701:CEF:N5	2.25	0.69
1:A:537:VAL:HG13	1:A:637:ILE:HD12	1.75	0.69
1:A:71:ARG:HH22	1:A:563:GLU:HA	1.59	0.68
1:A:336:ILE:HD13	1:A:337:LYS:HG2	1.76	0.68
1:A:427:LYS:HD3	1:A:432:ASN:HB3	1.77	0.67
1:B:354:VAL:HG13	1:B:363:LEU:HB3	1.77	0.67
1:A:410:VAL:HG23	1:A:588:GLN:HG3	1.78	0.66
1:B:49:SER:HB2	1:B:65:GLU:HB3	1.78	0.66
1:B:641:PRO:HD3	1:B:677:PHE:CZ	2.31	0.65
1:A:614:PRO:HB2	1:A:642:ILE:HD13	1.79	0.64
1:A:276:LEU:HD13	1:A:499:LEU:HD21	1.79	0.64
1:B:495:THR:HG21	1:B:531:LEU:HG	1.79	0.64
1:A:144:GLU:HA	1:A:147:MET:HG2	1.79	0.64
1:B:319:THR:HA	1:B:553:LEU:HD12	1.79	0.64
1:A:150:ASP:HB3	1:A:152:SER:H	1.63	0.63
1:A:631:ARG:HG3	1:A:657:PRO:HA	1.80	0.63
1:A:337:LYS:HA	1:A:339:LEU:HG	1.80	0.62
1:A:524:GLN:HE22	1:A:622:ALA:HA	1.64	0.61
1:A:365:LEU:HD11	1:A:380:ASP:HB3	1.81	0.61
1:B:86:LYS:HD3	1:B:201:ASN:CG	2.21	0.61
1:B:332:LEU:O	1:B:336:ILE:HG23	2.01	0.60
1:B:95:ARG:H	1:B:193:VAL:HG13	1.67	0.60
1:A:428:ARG:HH21	1:A:451:VAL:HB	1.66	0.60
1:B:340:ARG:HG2	1:B:372:LYS:HE2	1.83	0.60
1:A:529:THR:HG23	1:A:531:LEU:H	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:GLN:HE21	1:A:503:THR:HB	1.67	0.60
1:B:214:GLN:O	1:B:216:LEU:N	2.35	0.60
1:A:387:GLN:H	1:B:506:GLN:HE22	1.49	0.59
1:B:390:VAL:HG21	1:B:533:LEU:HD21	1.84	0.59
1:A:371:ASN:HA	1:A:374:GLY:H	1.67	0.59
1:A:509:PRO:HG2	1:B:368:LYS:HG2	1.83	0.59
1:B:80:LEU:O	1:B:233:PRO:HD2	2.02	0.59
1:A:352:MET:H	1:A:366:ALA:HB2	1.67	0.59
1:A:625:PHE:HD2	1:B:627:ASN:HA	1.67	0.59
1:A:658:VAL:HG11	1:A:663:LEU:HG	1.83	0.58
1:B:465:TYR:HA	1:B:469:MET:SD	2.43	0.58
1:A:442:LYS:HE2	1:A:591:GLU:HB3	1.83	0.58
1:B:95:ARG:N	1:B:193:VAL:HG13	2.18	0.58
1:B:312:ARG:NH1	1:B:562:ASP:OD1	2.36	0.58
1:B:399:LEU:HD11	1:B:441:ASP:HB2	1.86	0.58
1:A:91:TYR:HB2	1:A:199:ILE:HD11	1.86	0.58
1:A:353:VAL:HA	1:A:364:ALA:HB1	1.84	0.58
1:B:419:LEU:HB2	1:B:465:TYR:CZ	2.38	0.58
1:B:228:TRP:O	1:B:270:ARG:NH1	2.34	0.58
1:A:428:ARG:HB3	1:A:451:VAL:HG23	1.86	0.58
1:A:657:PRO:HD2	1:A:658:VAL:HG13	1.86	0.58
1:B:214:GLN:OE1	1:B:218:LYS:NZ	2.35	0.57
1:A:354:VAL:H	1:A:364:ALA:CB	2.17	0.57
1:A:625:PHE:CD2	1:B:627:ASN:HA	2.40	0.57
1:A:631:ARG:NH2	1:A:657:PRO:HB3	2.20	0.57
1:B:91:TYR:CZ	1:B:93:ARG:HB2	2.41	0.56
1:A:117:THR:O	1:A:119:LYS:N	2.33	0.56
1:B:450:ASN:HB2	3:B:899:HOH:O	2.04	0.56
1:A:248:PRO:HA	3:A:854:HOH:O	2.05	0.56
1:B:612:VAL:H	1:B:613:VAL:HG22	1.71	0.56
1:A:641:PRO:HD3	1:A:677:PHE:CE2	2.41	0.55
1:B:454:PHE:CE1	1:B:518:LEU:HB3	2.42	0.55
1:A:141:MET:HB3	1:A:144:GLU:HG3	1.88	0.55
1:B:623:GLU:OE1	2:B:701:CEF:N5	2.40	0.55
1:A:348:ASP:OD1	1:A:348:ASP:N	2.39	0.54
1:B:446:MET:HB3	1:B:600:LYS:CB	2.38	0.54
1:B:319:THR:HG22	1:B:553:LEU:HG	1.90	0.54
1:B:641:PRO:HD2	1:B:646:LYS:H	1.72	0.54
1:A:91:TYR:O	1:A:197:GLN:N	2.40	0.54
1:A:351:MET:HA	1:A:366:ALA:HB1	1.88	0.54
1:A:368:LYS:HE3	1:A:370:ILE:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:ARG:NH1	1:A:576:LEU:HD23	2.23	0.54
1:B:445:LEU:HD12	1:B:592:GLY:HA3	1.89	0.54
1:A:346:ASP:OD1	1:A:346:ASP:N	2.40	0.54
1:A:339:LEU:HD12	1:A:341:SER:HA	1.89	0.54
1:A:461:ALA:HA	1:A:478:PRO:HG3	1.90	0.54
1:B:457:ALA:HB1	1:B:517:TYR:CE2	2.43	0.53
1:A:308:ASN:HB2	3:A:933:HOH:O	2.08	0.53
1:B:335:GLN:HG3	1:B:668:LEU:HB2	1.89	0.53
1:A:258:GLU:HB2	1:B:576:LEU:HA	1.91	0.53
1:A:464:PRO:O	1:B:123:ARG:NH2	2.40	0.53
1:A:471:LEU:HG	1:A:514:PRO:HB2	1.91	0.53
1:B:372:LYS:C	1:B:374:GLY:H	2.11	0.53
2:A:701:CEF:N5	2:A:701:CEF:N4	2.45	0.53
1:B:86:LYS:NZ	1:B:227:ASP:HB2	2.22	0.53
1:B:340:ARG:CA	1:B:372:LYS:HZ1	2.21	0.53
1:B:366:ALA:HB3	1:B:379:TYR:O	2.09	0.53
1:B:365:LEU:HD12	1:B:380:ASP:OD1	2.09	0.53
1:A:232:TYR:CD1	1:A:239:ARG:HD3	2.43	0.53
1:B:615:THR:HG21	1:B:673:ILE:HD12	1.89	0.53
1:B:50:HIS:NE2	1:B:85:SER:OG	2.34	0.53
1:B:514:PRO:HA	1:B:517:TYR:HB3	1.90	0.52
1:A:87:MET:HG3	1:A:209:TYR:CE1	2.44	0.52
1:B:292:LYS:HB2	1:B:307:LEU:HD11	1.90	0.52
1:B:70:GLY:HA3	1:B:314:GLN:O	2.09	0.52
1:B:201:ASN:ND2	1:B:229:ASP:OD2	2.43	0.52
1:B:492:GLY:H	1:B:532:GLN:NE2	2.08	0.52
1:B:94:GLY:O	1:B:96:LYS:N	2.42	0.52
1:B:343:GLY:O	1:B:345:LYS:N	2.43	0.52
1:B:133:HIS:HB3	1:B:136:LYS:HB2	1.91	0.51
1:B:324:LEU:HD11	1:B:676:TYR:HD1	1.75	0.51
1:B:403:TYR:CD2	1:B:585:GLU:HB3	2.45	0.51
1:A:337:LYS:C	1:A:339:LEU:H	2.14	0.51
1:A:408:ILE:CG2	1:A:456:THR:HG22	2.38	0.51
1:A:434:ASN:OD1	1:A:434:ASN:N	2.42	0.51
1:B:636:TYR:HB2	1:B:651:ILE:HB	1.91	0.51
1:B:465:TYR:CZ	1:B:467:SER:HA	2.46	0.51
1:A:345:LYS:O	1:A:371:ASN:HB3	2.10	0.51
1:B:325:GLN:HA	1:B:363:LEU:HD21	1.92	0.51
1:B:410:VAL:HG11	1:B:584:LYS:HG3	1.93	0.51
1:A:453:MET:HB2	1:A:522:ILE:HD13	1.93	0.51
1:B:518:LEU:O	1:B:521:SER:OG	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:MET:CE	1:A:672:VAL:HG11	2.41	0.50
1:A:337:LYS:HE2	1:A:344:ALA:O	2.11	0.50
1:A:339:LEU:HB2	1:A:342:GLN:H	1.76	0.50
1:A:355:GLN:HG3	1:A:362:ILE:HD13	1.94	0.50
1:A:371:ASN:HA	1:A:374:GLY:N	2.26	0.50
2:B:701:CEF:N5	2:B:701:CEF:N4	2.47	0.50
1:B:662:TRP:HD1	1:B:663:LEU:N	2.09	0.50
1:A:348:ASP:HA	1:A:369:GLN:O	2.12	0.50
1:B:522:ILE:HD12	1:B:524:GLN:HB2	1.94	0.50
1:A:219:LEU:HB2	1:A:222:VAL:HG21	1.92	0.50
1:B:320:ILE:HD13	1:B:361:ASP:O	2.11	0.50
1:A:290:GLU:HB2	1:A:307:LEU:HB2	1.93	0.49
1:A:297:LYS:HE3	1:A:297:LYS:H	1.77	0.49
1:B:370:ILE:HB	1:B:371:ASN:HD22	1.76	0.49
1:A:428:ARG:HE	1:A:451:VAL:HB	1.77	0.49
1:B:125:LYS:HB3	1:B:171:LEU:HG	1.93	0.49
1:B:118:LYS:HG3	1:B:119:LYS:HG2	1.94	0.49
1:B:597:PHE:CZ	1:B:617:GLY:HA3	2.47	0.49
1:A:370:ILE:HD11	1:B:512:ASN:OD1	2.12	0.49
1:B:433:LYS:O	1:B:435:GLY:N	2.46	0.49
1:B:340:ARG:HA	1:B:372:LYS:NZ	2.28	0.49
1:A:86:LYS:HG2	1:A:202:GLU:C	2.33	0.49
1:B:71:ARG:NE	1:B:315:ASP:OD2	2.45	0.49
1:B:332:LEU:HD13	1:B:365:LEU:HD23	1.93	0.49
1:A:238:LEU:HD23	1:A:365:LEU:HG	1.93	0.49
1:A:273:LYS:CE	1:B:484:ARG:HH12	2.26	0.49
1:B:162:LEU:HD22	1:B:166:ILE:HD11	1.95	0.49
1:B:336:ILE:HD13	1:B:369:GLN:NE2	2.28	0.49
1:B:555:ILE:HD11	1:B:571:ILE:HD11	1.95	0.49
1:A:241:ILE:O	1:A:276:LEU:HB2	2.13	0.48
1:A:514:PRO:O	1:A:517:TYR:HB3	2.12	0.48
1:B:329:GLU:CD	1:B:365:LEU:HD13	2.33	0.48
1:A:466:TYR:CD2	1:B:163:LEU:HD23	2.48	0.48
1:A:554:THR:OG1	1:A:556:HIS:NE2	2.38	0.48
1:B:562:ASP:OD1	1:B:562:ASP:N	2.46	0.48
1:A:171:LEU:C	1:A:173:GLU:H	2.17	0.48
1:B:446:MET:HE3	1:B:600:LYS:HB2	1.95	0.48
1:A:71:ARG:HH12	1:A:563:GLU:HG3	1.78	0.48
1:A:128:PHE:CG	1:A:182:LEU:HD13	2.49	0.48
1:B:87:MET:HB2	1:B:204:VAL:HG12	1.96	0.48
1:B:247:THR:HG22	1:B:248:PRO:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:MET:HE2	1:B:600:LYS:HG3	1.94	0.48
1:A:365:LEU:HD13	1:A:366:ALA:H	1.79	0.48
1:A:631:ARG:HH21	1:A:657:PRO:HB3	1.79	0.48
1:A:653:TYR:CE2	1:A:665:GLY:HA3	2.49	0.47
1:A:605:TYR:O	1:A:609:LYS:HD2	2.14	0.47
1:B:90:THR:O	1:B:222:VAL:HA	2.14	0.47
1:A:351:MET:HA	1:A:366:ALA:CB	2.44	0.47
1:A:529:THR:HG22	1:A:532:GLN:N	2.11	0.47
1:B:578:LYS:HG2	1:B:579:VAL:O	2.15	0.47
1:B:340:ARG:HA	1:B:372:LYS:HZ1	1.79	0.47
1:B:450:ASN:OD1	1:B:450:ASN:N	2.44	0.47
1:A:144:GLU:HB2	1:A:158:TYR:CD1	2.49	0.47
1:B:506:GLN:HG2	3:B:847:HOH:O	2.14	0.47
1:B:582:THR:OG1	1:B:583:GLU:OE1	2.32	0.47
1:A:395:LYS:HG2	1:A:453:MET:HG3	1.97	0.47
1:A:600:LYS:HE3	1:A:600:LYS:N	2.17	0.47
1:B:121:THR:O	1:B:124:ASP:HB2	2.15	0.46
1:B:247:THR:OG1	1:B:250:GLU:OE1	2.32	0.46
1:A:175:SER:OG	1:A:175:SER:O	2.33	0.46
1:A:352:MET:HE2	1:A:672:VAL:HG11	1.98	0.46
1:A:548:GLN:HB2	1:A:576:LEU:HD11	1.96	0.46
1:A:93:ARG:HE	1:A:93:ARG:HB3	1.61	0.46
1:A:590:GLN:HA	1:A:593:PHE:HB2	1.96	0.46
1:A:629:GLU:HA	1:A:630:PRO:HD3	1.79	0.46
1:B:493:VAL:O	1:B:532:GLN:NE2	2.48	0.46
1:B:618:LYS:HD3	1:B:619:THR:N	2.31	0.46
1:A:73:LEU:HD23	1:A:79:VAL:HA	1.97	0.46
1:A:664:THR:HB	1:A:667:ASP:OD2	2.16	0.46
1:B:336:ILE:HD13	1:B:369:GLN:HE21	1.80	0.46
1:A:65:GLU:O	1:A:288:LYS:HB2	2.16	0.46
1:B:219:LEU:HB2	1:B:222:VAL:CG2	2.46	0.46
1:B:359:ASN:HB2	3:B:825:HOH:O	2.15	0.46
1:B:570:LYS:HD3	1:B:572:ASN:OD1	2.16	0.46
1:A:414:MET:SD	1:A:415:VAL:HG22	2.56	0.46
1:A:192:THR:HB	1:A:195:ASP:HB2	1.98	0.46
1:A:322:ILE:O	1:A:325:GLN:HB3	2.15	0.45
1:A:377:THR:HG21	1:B:511:THR:HG21	1.98	0.45
1:B:358:LYS:NZ	1:B:359:ASN:HD21	2.14	0.45
1:B:246:SER:HB2	1:B:250:GLU:HG3	1.98	0.45
1:B:394:VAL:HG13	1:B:491:LEU:HD13	1.99	0.45
1:B:641:PRO:HD3	1:B:677:PHE:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ASN:HB3	1:A:58:ASP:H	1.59	0.45
1:A:670:ARG:O	1:A:673:ILE:HG22	2.16	0.45
1:B:346:ASP:OD1	1:B:371:ASN:N	2.47	0.45
1:B:347:MET:HE1	1:B:653:TYR:HB3	1.98	0.45
1:A:398:THR:HG21	1:A:521:SER:O	2.16	0.45
1:B:148:LEU:HD23	1:B:153:ILE:O	2.16	0.45
1:A:144:GLU:H	1:A:144:GLU:HG2	1.25	0.45
1:A:412:GLU:OE2	1:A:459:LYS:NZ	2.43	0.45
1:B:523:GLY:HA2	3:B:858:HOH:O	2.16	0.45
1:B:348:ASP:OD1	1:B:348:ASP:N	2.39	0.45
1:A:379:TYR:CZ	1:B:509:PRO:HD3	2.52	0.45
1:A:428:ARG:NH1	1:A:430:TYR:HE1	2.15	0.45
1:B:257:THR:HG22	1:B:261:LEU:HD22	1.99	0.45
1:B:524:GLN:HB2	1:B:524:GLN:HE21	1.59	0.45
1:A:49:SER:OG	1:A:65:GLU:OE2	2.22	0.45
1:A:369:GLN:HE21	1:A:369:GLN:HB2	1.54	0.45
1:A:611:THR:O	1:A:613:VAL:N	2.49	0.45
2:A:701:CEF:O5	2:A:701:CEF:N2	2.50	0.45
1:B:488:GLN:O	1:B:546:ARG:HD3	2.17	0.44
1:B:594:LYS:HD3	1:B:642:ILE:HG21	1.98	0.44
1:B:618:LYS:HD3	1:B:619:THR:H	1.82	0.44
1:A:154:LYS:HD2	1:A:156:ASP:HB2	1.99	0.44
1:A:522:ILE:HD12	1:A:522:ILE:HA	1.82	0.44
1:B:325:GLN:O	1:B:329:GLU:HG3	2.16	0.44
1:A:153:ILE:HD12	1:A:158:TYR:HB2	1.98	0.44
1:A:336:ILE:HG13	1:A:369:GLN:OE1	2.18	0.44
1:B:372:LYS:HD2	1:B:372:LYS:HA	1.60	0.44
1:B:412:GLU:HG3	1:B:413:THR:N	2.32	0.44
1:A:273:LYS:CD	1:B:484:ARG:HH12	2.30	0.44
1:A:291:MET:SD	1:A:306:VAL:HG22	2.57	0.44
1:B:430:TYR:OH	1:B:447:HIS:NE2	2.49	0.44
1:B:673:ILE:HG22	1:B:677:PHE:CE1	2.53	0.44
1:A:498:ASP:OD1	1:A:498:ASP:N	2.50	0.44
1:B:74:ASP:HB2	1:B:320:ILE:O	2.17	0.44
1:B:314:GLN:HB3	1:B:556:HIS:O	2.17	0.44
1:A:492:GLY:H	1:A:532:GLN:NE2	2.16	0.44
1:A:667:ASP:HB3	1:A:670:ARG:NH1	2.33	0.44
1:A:548:GLN:HB2	1:A:576:LEU:CD1	2.48	0.43
1:B:86:LYS:HE2	1:B:86:LYS:HB3	1.70	0.43
1:B:489:VAL:O	1:B:536:TYR:HA	2.18	0.43
1:A:618:LYS:HD2	1:A:619:THR:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:VAL:HB	1:B:437:VAL:HA	1.99	0.43
1:B:431:PHE:CD1	1:B:434:ASN:HB2	2.53	0.43
1:B:512:ASN:OD1	1:B:512:ASN:N	2.52	0.43
1:A:372:LYS:HD2	1:A:372:LYS:HA	1.84	0.43
1:B:400:LEU:HB3	1:B:581:ASN:CG	2.39	0.43
1:B:621:THR:OG1	2:B:701:CEF:O1	2.28	0.43
1:A:260:TYR:HE1	1:A:281:GLU:HG2	1.83	0.43
1:A:369:GLN:HG3	1:A:376:MET:HG2	2.00	0.43
1:B:193:VAL:HG12	1:B:194:LEU:HD22	2.00	0.43
1:B:397:GLY:HA2	1:B:400:LEU:HD12	1.99	0.43
1:A:414:MET:N	3:A:902:HOH:O	2.51	0.43
1:A:597:PHE:CE2	1:A:617:GLY:HA3	2.54	0.43
1:B:216:LEU:HD21	1:B:224:THR:H	1.83	0.43
1:B:617:GLY:HA2	1:B:638:GLY:HA2	2.00	0.43
1:B:585:GLU:O	1:B:589:ILE:HD13	2.19	0.43
1:A:204:VAL:HG22	1:A:205:SER:O	2.18	0.43
1:A:422:GLN:OE1	1:A:422:GLN:N	2.52	0.43
1:A:337:LYS:NZ	1:A:371:ASN:OD1	2.52	0.42
1:A:405:ASN:O	1:A:407:ALA:N	2.51	0.42
1:B:582:THR:OG1	1:B:583:GLU:N	2.51	0.42
1:A:621:THR:HB	2:A:701:CEF:O4	2.18	0.42
1:B:171:LEU:HD12	1:B:171:LEU:HA	1.85	0.42
1:B:347:MET:CE	1:B:653:TYR:HB3	2.49	0.42
1:B:420:HIS:HB3	1:B:427:LYS:HB3	2.01	0.42
1:B:537:VAL:HB	1:B:637:ILE:HD12	1.99	0.42
1:A:287:LYS:HB2	1:A:311:ALA:HB3	2.02	0.42
1:A:375:LYS:HD2	1:A:375:LYS:HA	1.90	0.42
1:B:395:LYS:HA	1:B:398:THR:OG1	2.19	0.42
1:B:416:ASP:HB3	1:B:451:VAL:HG11	2.02	0.42
1:B:434:ASN:O	1:B:436:HIS:N	2.53	0.42
1:B:439:ILE:H	1:B:439:ILE:HG13	1.65	0.42
1:B:636:TYR:O	1:B:651:ILE:N	2.49	0.42
1:A:69:ARG:HG2	3:A:925:HOH:O	2.19	0.42
1:B:108:LYS:O	1:B:111:LYS:HG2	2.20	0.42
1:B:505:GLY:O	1:B:507:ILE:HG13	2.20	0.42
1:A:373:SER:OG	1:A:374:GLY:N	2.52	0.42
1:B:133:HIS:ND1	1:B:135:LYS:HE2	2.35	0.42
1:B:177:LYS:HG2	1:B:178:ASP:N	2.35	0.42
1:B:605:TYR:O	1:B:609:LYS:HB2	2.20	0.42
1:A:335:GLN:HA	1:A:338:LYS:HB2	2.02	0.42
1:A:336:ILE:HG13	1:A:369:GLN:CD	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:LEU:HA	1:A:342:GLN:NE2	2.35	0.42
1:B:214:GLN:OE1	1:B:215:GLN:N	2.53	0.42
1:B:659:PRO:HB3	2:B:701:CEF:N4	2.35	0.42
1:A:87:MET:HG3	1:A:209:TYR:CD1	2.55	0.42
1:A:319:THR:HB	1:A:361:ASP:HB3	2.00	0.42
1:A:327:GLU:HG3	1:A:675:TYR:CE2	2.55	0.42
1:B:247:THR:HG1	1:B:250:GLU:HG2	1.84	0.42
1:B:347:MET:HE3	1:B:656:GLN:HG2	2.02	0.42
1:B:358:LYS:HG3	1:B:359:ASN:H	1.85	0.42
1:B:400:LEU:HB3	1:B:581:ASN:OD1	2.19	0.42
1:A:347:MET:CE	1:A:656:GLN:HE21	2.33	0.42
1:A:546:ARG:CZ	1:A:576:LEU:HD23	2.50	0.42
1:A:261:LEU:HD12	1:A:261:LEU:HA	1.83	0.41
1:A:367:GLY:HA2	1:A:379:TYR:N	2.19	0.41
1:A:647:LEU:HD23	1:A:648:ALA:N	2.35	0.41
1:B:337:LYS:HD3	1:B:337:LYS:HA	2.00	0.41
1:B:92:THR:HG23	1:B:195:ASP:C	2.40	0.41
1:B:93:ARG:HG2	1:B:221:GLY:CA	2.50	0.41
1:A:147:MET:O	1:A:153:ILE:HG12	2.20	0.41
1:B:126:LYS:HG3	1:B:171:LEU:HD11	2.03	0.41
1:A:219:LEU:HB2	1:A:222:VAL:CG2	2.51	0.41
1:B:209:TYR:CE2	1:B:226:MET:HG2	2.56	0.41
1:B:354:VAL:HG22	1:B:363:LEU:HB2	2.03	0.41
1:B:534:SER:O	1:B:538:SER:HB2	2.20	0.41
1:A:336:ILE:HG21	1:A:376:MET:CE	2.50	0.41
1:A:171:LEU:HD12	1:A:174:LEU:HD22	2.02	0.41
1:A:370:ILE:O	1:A:373:SER:OG	2.37	0.41
1:B:47:GLN:NE2	1:B:560:ASN:OD1	2.53	0.41
1:B:236:ASP:HA	1:B:239:ARG:CG	2.51	0.41
1:B:432:ASN:O	1:B:433:LYS:HB2	2.21	0.41
1:B:433:LYS:HB2	1:B:433:LYS:HE2	1.93	0.41
1:B:98:THR:C	1:B:100:SER:H	2.24	0.41
1:B:612:VAL:HG21	1:B:674:ASN:HA	2.02	0.41
1:A:173:GLU:C	1:A:175:SER:N	2.74	0.41
1:A:238:LEU:HD23	1:A:238:LEU:HA	1.86	0.41
1:A:427:LYS:NZ	1:A:432:ASN:O	2.50	0.41
1:B:95:ARG:H	1:B:193:VAL:CG1	2.33	0.41
1:B:527:THR:HG21	3:B:895:HOH:O	2.21	0.41
1:A:87:MET:HG3	1:A:209:TYR:HE1	1.86	0.41
1:B:337:LYS:HZ3	1:B:340:ARG:HH11	1.68	0.41
1:B:430:TYR:CZ	1:B:431:PHE:CE2	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LYS:HD3	1:A:556:HIS:NE2	2.36	0.40
1:A:413:THR:HG23	1:A:440:ASN:HB3	2.03	0.40
1:B:86:LYS:HD3	1:B:201:ASN:ND2	2.36	0.40
1:B:174:LEU:HD12	1:B:174:LEU:HA	1.79	0.40
1:B:329:GLU:CG	1:B:365:LEU:HD13	2.51	0.40
1:A:337:LYS:HD3	1:A:339:LEU:HD11	2.03	0.40
1:B:535:GLN:HE21	1:B:549:PRO:HD3	1.87	0.40
1:B:544:GLY:O	1:B:578:LYS:HA	2.22	0.40
1:A:605:TYR:CD1	1:A:609:LYS:HA	2.56	0.40
1:B:163:LEU:HD12	1:B:163:LEU:HA	1.94	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	627/646 (97%)	554 (88%)	60 (10%)	13 (2%)	5	7
1	B	627/646 (97%)	544 (87%)	60 (10%)	23 (4%)	2	2
All	All	1254/1292 (97%)	1098 (88%)	120 (10%)	36 (3%)	3	3

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	LYS
1	A	373	SER
1	B	95	ARG
1	B	215	GLN
1	B	344	ALA
1	B	434	ASN
1	B	561	LYS
1	B	562	ASP

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Mol	Chain	Res	Type
1	A	172	ASP
1	A	175	SER
1	A	297	LYS
1	A	609	LYS
1	B	275	TYR
1	B	359	ASN
1	B	433	LYS
1	B	435	GLY
1	B	609	LYS
1	A	422	GLN
1	A	663	LEU
1	B	203	ASP
1	B	220	PRO
1	B	357	PRO
1	B	599	ASP
1	B	630	PRO
1	A	117	THR
1	A	167	ARG
1	B	358	LYS
1	B	424	GLY
1	B	451	VAL
1	B	640	ALA
1	A	275	TYR
1	B	659	PRO
1	A	193	VAL
1	B	641	PRO
1	A	564	VAL
1	B	418	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	546/559 (98%)	429 (79%)	117 (21%)	1	1
1	B	547/559 (98%)	422 (77%)	125 (23%)	0	1
All	All	1093/1118 (98%)	851 (78%)	242 (22%)	1	1

All (242) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	57	ASN
1	A	66	SER
1	A	74	ASP
1	A	78	LYS
1	A	85	SER
1	A	93	ARG
1	A	98	THR
1	A	99	GLN
1	A	100	SER
1	A	101	GLU
1	A	102	MET
1	A	103	LEU
1	A	108	LYS
1	A	109	LEU
1	A	110	SER
1	A	112	LEU
1	A	117	THR
1	A	118	LYS
1	A	132	LEU
1	A	135	LYS
1	A	144	GLU
1	A	154	LYS
1	A	156	ASP
1	A	163	LEU
1	A	168	LYS
1	A	169	SER
1	A	175	SER
1	A	177	LYS
1	A	179	LEU
1	A	189	ASN
1	A	192	THR
1	A	193	VAL
1	A	195	ASP
1	A	202	GLU
1	A	203	ASP
1	A	205	SER
1	A	206	GLU
1	A	207	LYS
1	A	216	LEU
1	A	218	LYS
1	A	231	LYS

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Mol	Chain	Res	Type
1	A	244	ASP
1	A	245	VAL
1	A	256	LEU
1	A	266	SER
1	A	273	LYS
1	A	292	LYS
1	A	297	LYS
1	A	327	GLU
1	A	334	LYS
1	A	336	ILE
1	A	339	LEU
1	A	345	LYS
1	A	346	ASP
1	A	347	MET
1	A	354	VAL
1	A	358	LYS
1	A	363	LEU
1	A	365	LEU
1	A	369	GLN
1	A	370	ILE
1	A	371	ASN
1	A	375	LYS
1	A	377	THR
1	A	378	ASP
1	A	379	TYR
1	A	380	ASP
1	A	381	ILE
1	A	393	SER
1	A	398	THR
1	A	400	LEU
1	A	413	THR
1	A	414	MET
1	A	419	LEU
1	A	422	GLN
1	A	425	LEU
1	A	427	LYS
1	A	428	ARG
1	A	438	SER
1	A	446	MET
1	A	449	SER
1	A	471	LEU
1	A	480	GLN

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Mol	Chain	Res	Type
1	A	493	VAL
1	A	497	ILE
1	A	529	THR
1	A	536	TYR
1	A	537	VAL
1	A	538	SER
1	A	539	THR
1	A	542	ASN
1	A	553	LEU
1	A	558	SER
1	A	559	THR
1	A	561	LYS
1	A	562	ASP
1	A	564	VAL
1	A	568	LYS
1	A	569	LYS
1	A	576	LEU
1	A	584	LYS
1	A	600	LYS
1	A	601	ASP
1	A	606	VAL
1	A	609	LYS
1	A	611	THR
1	A	613	VAL
1	A	619	THR
1	A	621	THR
1	A	624	VAL
1	A	631	ARG
1	A	632	VAL
1	A	643	ASP
1	A	663	LEU
1	A	664	THR
1	A	673	ILE
1	B	47	GLN
1	B	56	LYS
1	B	60	ASN
1	B	74	ASP
1	B	86	LYS
1	B	95	ARG
1	B	96	LYS
1	B	109	LEU
1	B	110	SER

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Mol	Chain	Res	Type
1	B	111	LYS
1	B	114	LYS
1	B	118	LYS
1	B	132	LEU
1	B	135	LYS
1	B	152	SER
1	B	153	ILE
1	B	154	LYS
1	B	160	LYS
1	B	162	LEU
1	B	163	LEU
1	B	164	SER
1	B	168	LYS
1	B	169	SER
1	B	170	GLN
1	B	171	LEU
1	B	174	LEU
1	B	177	LYS
1	B	192	THR
1	B	194	LEU
1	B	200	LYS
1	B	205	SER
1	B	206	GLU
1	B	214	GLN
1	B	216	LEU
1	B	217	SER
1	B	218	LYS
1	B	222	VAL
1	B	230	ARG
1	B	237	THR
1	B	238	LEU
1	B	245	VAL
1	B	247	THR
1	B	254	LYS
1	B	261	LEU
1	B	274	SER
1	B	288	LYS
1	B	297	LYS
1	B	300	LYS
1	B	306	VAL
1	B	307	LEU
1	B	315	ASP

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Mol	Chain	Res	Type
1	B	317	LYS
1	B	322	ILE
1	B	333	ASP
1	B	335	GLN
1	B	336	ILE
1	B	339	LEU
1	B	340	ARG
1	B	341	SER
1	B	346	ASP
1	B	351	MET
1	B	354	VAL
1	B	355	GLN
1	B	361	ASP
1	B	363	LEU
1	B	365	LEU
1	B	368	LYS
1	B	372	LYS
1	B	376	MET
1	B	377	THR
1	B	379	TYR
1	B	387	GLN
1	B	390	VAL
1	B	399	LEU
1	B	408	ILE
1	B	409	LYS
1	B	412	GLU
1	B	413	THR
1	B	414	MET
1	B	416	ASP
1	B	420	HIS
1	B	422	GLN
1	B	429	SER
1	B	431	PHE
1	B	437	VAL
1	B	438	SER
1	B	439	ILE
1	B	449	SER
1	B	450	ASN
1	B	451	VAL
1	B	459	LYS
1	B	460	LEU
1	B	463	ASP

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Mol	Chain	Res	Type
1	B	471	LEU
1	B	475	ILE
1	B	480	GLN
1	B	484	ARG
1	B	486	LEU
1	B	488	GLN
1	B	502	GLU
1	B	520	LEU
1	B	524	GLN
1	B	538	SER
1	B	542	ASN
1	B	553	LEU
1	B	559	THR
1	B	563	GLU
1	B	564	VAL
1	B	584	LYS
1	B	600	LYS
1	B	603	THR
1	B	606	VAL
1	B	610	ASP
1	B	611	THR
1	B	612	VAL
1	B	613	VAL
1	B	627	ASN
1	B	632	VAL
1	B	637	ILE
1	B	654	THR
1	B	658	VAL
1	B	662	TRP
1	B	667	ASP
1	B	670	ARG
1	B	673	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	145	GLN
1	A	387	GLN
1	A	590	GLN
1	A	656	GLN
1	B	47	GLN

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Mol	Chain	Res	Type
1	B	201	ASN
1	B	335	GLN
1	B	359	ASN
1	B	371	ASN
1	B	387	GLN
1	B	432	ASN
1	B	436	HIS
1	B	480	GLN
1	B	488	GLN
1	B	524	GLN
1	B	542	ASN
1	B	560	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CEF	A	701	1	21,27,27	9.09	13 (61%)	19,37,37	5.62	12 (63%)
2	CEF	B	701	1	21,27,27	9.13	13 (61%)	19,37,37	4.60	13 (68%)

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	1/1/7/9	6/14/38/38	0/1/2/2
2	CEF	B	701	1	1/1/7/9	6/14/38/38	0/1/2/2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	CEF	C4-N1	33.63	1.60	1.28
2	B	701	CEF	C4-N1	33.58	1.60	1.28
2	B	701	CEF	C10-N3	13.86	1.50	1.29
2	A	701	CEF	C10-N3	12.82	1.48	1.29
2	A	701	CEF	C12-C10	-11.52	1.30	1.47
2	B	701	CEF	C12-C10	-10.88	1.31	1.47
2	B	701	CEF	C1-S1	-10.58	1.60	1.82
2	A	701	CEF	C1-S1	-10.32	1.61	1.82
2	B	701	CEF	C3-C2	7.23	1.47	1.32
2	A	701	CEF	C3-C2	7.20	1.47	1.32
2	B	701	CEF	C9-N2	5.95	1.46	1.34
2	A	701	CEF	C9-N2	5.80	1.46	1.34
2	B	701	CEF	C4-C2	5.27	1.63	1.46
2	A	701	CEF	C4-C2	4.96	1.62	1.46
2	A	701	CEF	C12-N5	4.93	1.52	1.37
2	B	701	CEF	C12-N5	4.76	1.52	1.37
2	B	701	CEF	C4-C5	-4.48	1.39	1.48
2	A	701	CEF	C4-C5	-4.18	1.39	1.48
2	A	701	CEF	O5-N3	-3.81	1.31	1.40
2	B	701	CEF	O5-N3	-3.25	1.33	1.40
2	A	701	CEF	C14-N4	-2.93	1.26	1.35
2	B	701	CEF	C14-N4	-2.91	1.26	1.35
2	B	701	CEF	C1-C2	-2.50	1.47	1.50
2	B	701	CEF	C10-C9	2.47	1.55	1.50
2	A	701	CEF	C1-C2	-2.40	1.47	1.50
2	A	701	CEF	C13-S2	-2.16	1.67	1.70

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	CEF	C12-C13-S2	-11.91	97.16	111.79
2	A	701	CEF	N4-C14-N5	-11.15	109.06	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	CEF	C1-S1-C6	10.07	112.81	94.36
2	B	701	CEF	N4-C14-N5	-10.03	110.47	123.19
2	B	701	CEF	C11-O5-N3	9.66	120.11	108.32
2	A	701	CEF	C11-O5-N3	7.86	117.92	108.32
2	B	701	CEF	C1-C2-C3	-7.80	106.99	121.59
2	B	701	CEF	C1-S1-C6	6.54	106.34	94.36
2	A	701	CEF	C1-C2-C3	-6.10	110.19	121.59
2	A	701	CEF	C12-C10-C9	-5.63	107.78	118.17
2	B	701	CEF	C12-C10-C9	-5.27	108.44	118.17
2	A	701	CEF	C10-C9-N2	5.18	122.93	114.40
2	A	701	CEF	C6-N1-C4	4.84	120.56	116.33
2	B	701	CEF	C12-C13-S2	-4.75	105.96	111.79
2	A	701	CEF	C7-N2-C9	-3.83	114.40	121.97
2	B	701	CEF	O2-C5-C4	3.68	125.76	116.02
2	A	701	CEF	C9-C10-N3	-3.41	103.90	120.64
2	A	701	CEF	O4-C9-N2	-3.18	117.50	123.09
2	B	701	CEF	C9-C10-N3	-3.03	105.73	120.64
2	A	701	CEF	O2-C5-O1	-2.40	118.19	123.90
2	B	701	CEF	C10-C9-N2	2.35	118.27	114.40
2	B	701	CEF	O3-C8-C7	-2.20	119.05	124.86
2	B	701	CEF	O2-C5-O1	-2.19	118.68	123.90
2	B	701	CEF	O4-C9-N2	-2.19	119.24	123.09
2	B	701	CEF	O1-C5-C4	-2.12	115.55	120.92

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	701	CEF	C7
2	B	701	CEF	C6

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	CEF	C9-C10-N3-O5
2	B	701	CEF	N1-C4-C5-O1
2	B	701	CEF	N1-C4-C5-O2
2	B	701	CEF	C12-C10-N3-O5
2	B	701	CEF	C12-C10-C9-O4
2	A	701	CEF	C12-C10-N3-O5
2	A	701	CEF	N1-C4-C5-O2
2	A	701	CEF	N1-C4-C5-O1
2	A	701	CEF	N3-C10-C9-O4

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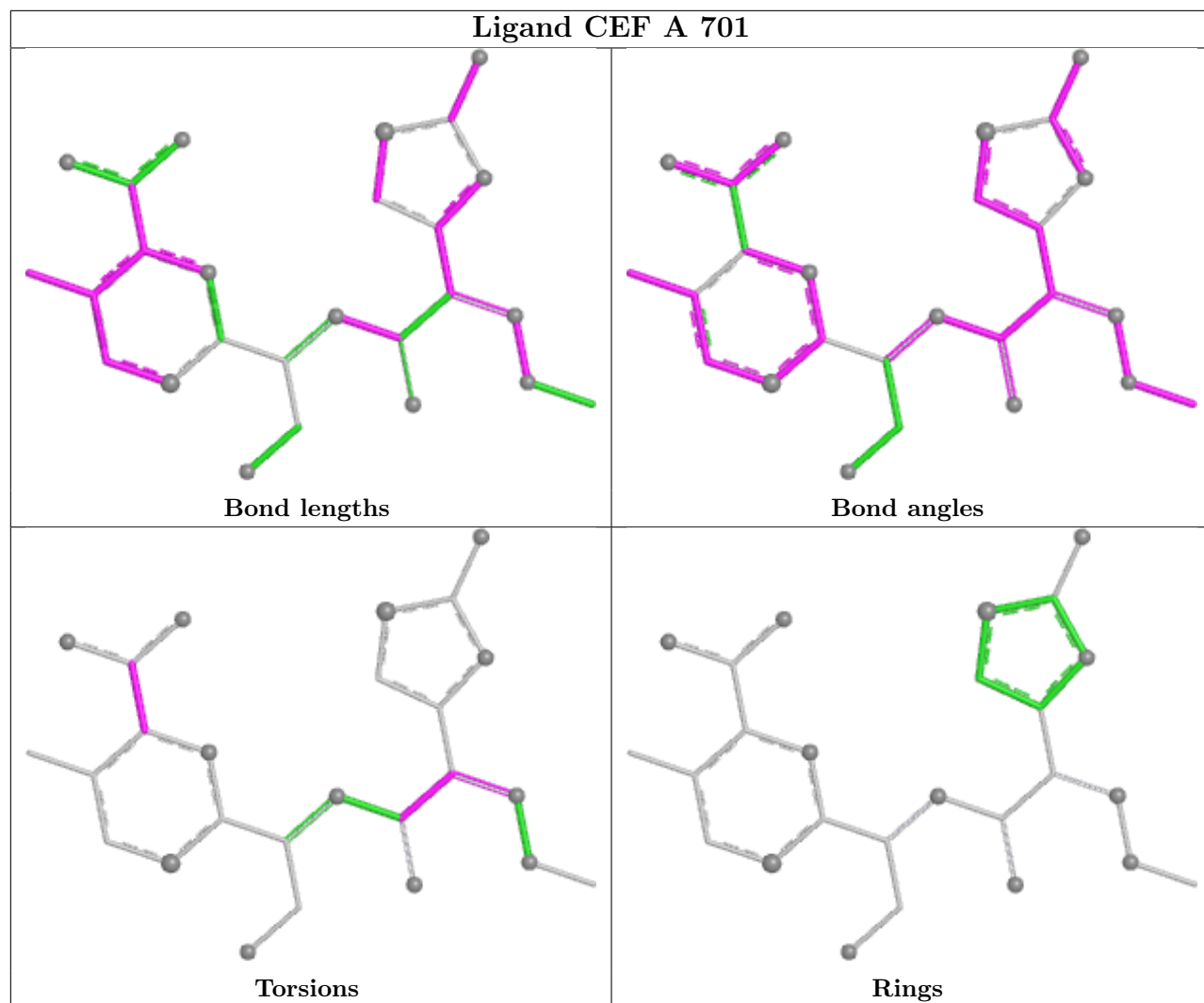
Mol	Chain	Res	Type	Atoms
2	B	701	CEF	N3-C10-C9-O4
2	B	701	CEF	C8-C7-N2-C9
2	A	701	CEF	N3-C10-C9-N2

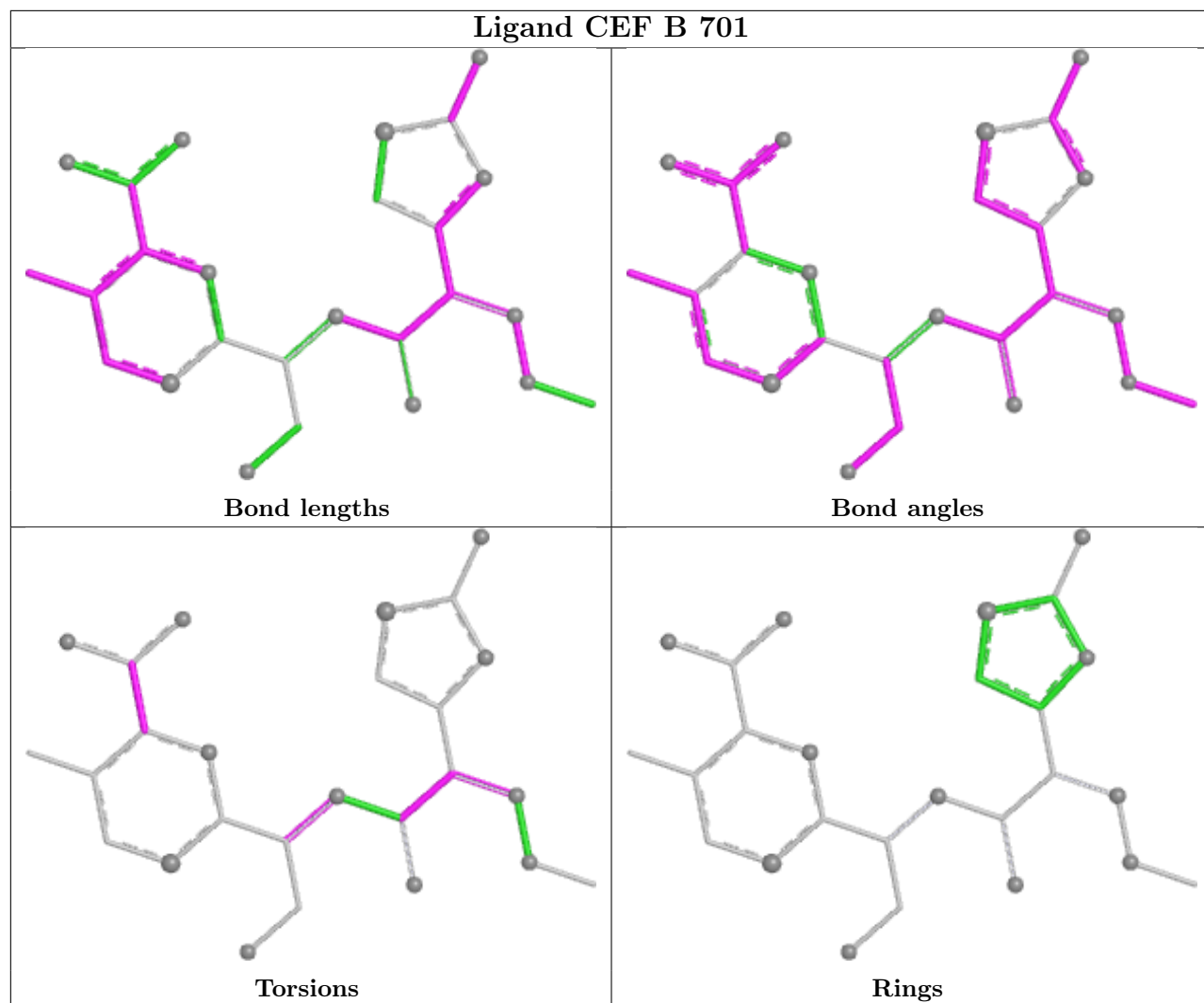
There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	CEF	6	0
2	B	701	CEF	6	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 than 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.





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, 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(Å ²)	Q<0.9
1	A	631/646 (97%)	1.16	153 (24%)	2 2	27, 61, 117, 146	0
1	B	631/646 (97%)	1.46	207 (32%)	1 1	29, 70, 124, 161	0
All	All	1262/1292 (97%)	1.31	360 (28%)	1 1	27, 66, 121, 161	0

All (360) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	625	PHE	8.2
1	A	174	LEU	8.1
1	A	168	LYS	7.0
1	A	658	VAL	6.6
1	B	437	VAL	6.5
1	B	425	LEU	6.2
1	B	606	VAL	6.1
1	B	430	TYR	5.7
1	A	339	LEU	5.5
1	B	612	VAL	5.4
1	B	658	VAL	5.4
1	B	662	TRP	5.4
1	B	603	THR	5.3
1	B	663	LEU	5.1
1	B	643	ASP	5.0
1	B	674	ASN	4.9
1	B	661	PRO	4.9
1	B	657	PRO	4.8
1	B	429	SER	4.7
1	A	660	PRO	4.7
1	B	363	LEU	4.6
1	B	217	SER	4.5
1	A	166	ILE	4.5
1	B	611	THR	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	357	PRO	4.5
1	B	218	LYS	4.5
1	A	616	ALA	4.5
1	A	562	ASP	4.5
1	B	371	ASN	4.4
1	B	608	PHE	4.4
1	A	343	GLY	4.4
1	A	341	SER	4.4
1	A	142	THR	4.4
1	B	619	THR	4.4
1	B	216	LEU	4.4
1	A	415	VAL	4.4
1	A	344	ALA	4.3
1	B	344	ALA	4.3
1	A	48	GLY	4.3
1	B	374	GLY	4.3
1	A	657	PRO	4.2
1	B	642	ILE	4.2
1	B	659	PRO	4.2
1	B	438	SER	4.2
1	A	598	ASN	4.2
1	A	431	PHE	4.2
1	A	661	PRO	4.1
1	A	609	LYS	4.1
1	A	365	LEU	4.1
1	A	606	VAL	4.1
1	B	613	VAL	4.1
1	B	601	ASP	4.1
1	B	593	PHE	4.1
1	B	626	GLN	4.0
1	A	136	LYS	4.0
1	A	369	GLN	4.0
1	A	139	ALA	4.0
1	A	194	LEU	3.9
1	B	660	PRO	3.9
1	B	604	GLY	3.9
1	B	436	HIS	3.9
1	B	93	ARG	3.9
1	B	451	VAL	3.8
1	A	426	THR	3.8
1	B	677	PHE	3.8
1	B	632	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	343	GLY	3.8
1	B	370	ILE	3.8
1	B	194	LEU	3.7
1	B	193	VAL	3.7
1	B	614	PRO	3.7
1	A	337	LYS	3.7
1	A	46	ALA	3.7
1	A	167	ARG	3.7
1	B	465	TYR	3.6
1	A	51	TYR	3.6
1	A	432	ASN	3.5
1	B	47	GLN	3.5
1	A	143	LYS	3.5
1	B	454	PHE	3.5
1	A	428	ARG	3.5
1	A	151	GLY	3.5
1	A	564	VAL	3.5
1	B	408	ILE	3.5
1	A	372	LYS	3.4
1	B	345	LYS	3.4
1	B	423	GLY	3.4
1	B	471	LEU	3.4
1	A	613	VAL	3.4
1	A	158	TYR	3.4
1	A	47	GLN	3.4
1	A	659	PRO	3.4
1	A	165	LYS	3.4
1	B	595	MET	3.4
1	B	622	ALA	3.3
1	B	428	ARG	3.3
1	B	135	LYS	3.3
1	B	51	TYR	3.3
1	B	365	LEU	3.3
1	A	414	MET	3.3
1	B	431	PHE	3.3
1	B	605	TYR	3.3
1	A	512	ASN	3.3
1	A	429	SER	3.3
1	A	438	SER	3.3
1	A	607	SER	3.3
1	A	656	GLN	3.3
1	B	310	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	417	GLU	3.3
1	B	421	PHE	3.3
1	B	356	ASN	3.2
1	B	522	ILE	3.2
1	A	162	LEU	3.2
1	B	111	LYS	3.2
1	A	611	THR	3.2
1	A	416	ASP	3.2
1	A	340	ARG	3.2
1	B	415	VAL	3.2
1	A	347	MET	3.2
1	B	414	MET	3.2
1	A	662	TRP	3.2
1	A	625	PHE	3.2
1	A	631	ARG	3.2
1	A	370	ILE	3.2
1	A	663	LEU	3.2
1	B	518	LEU	3.2
1	B	656	GLN	3.2
1	B	424	GLY	3.2
1	A	642	ILE	3.2
1	A	430	TYR	3.2
1	A	675	TYR	3.2
1	B	98	THR	3.2
1	A	465	TYR	3.1
1	B	139	ALA	3.1
1	B	418	PRO	3.1
1	A	170	GLN	3.1
1	A	149	ALA	3.1
1	B	142	THR	3.1
1	B	426	THR	3.1
1	B	615	THR	3.1
1	B	342	GLN	3.1
1	B	466	TYR	3.1
1	A	153	ILE	3.0
1	B	143	LYS	3.0
1	B	609	LYS	3.0
1	B	147	MET	3.0
1	B	419	LEU	3.0
1	B	470	ALA	3.0
1	B	339	LEU	3.0
1	A	435	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	334	LYS	3.0
1	A	624	VAL	3.0
1	B	624	VAL	3.0
1	A	670	ARG	3.0
1	A	145	GLN	3.0
1	A	425	LEU	3.0
1	B	164	SER	3.0
1	B	596	ALA	3.0
1	B	639	TYR	2.9
1	A	346	ASP	2.9
1	B	46	ALA	2.9
1	A	368	LYS	2.9
1	A	420	HIS	2.9
1	A	156	ASP	2.9
1	B	210	ALA	2.9
1	B	597	PHE	2.9
1	A	144	GLU	2.9
1	B	447	HIS	2.9
1	A	664	THR	2.9
1	B	336	ILE	2.9
1	A	608	PHE	2.9
1	A	629	GLU	2.9
1	A	612	VAL	2.9
1	A	599	ASP	2.9
1	B	207	LYS	2.9
1	B	153	ILE	2.8
1	B	410	VAL	2.8
1	A	190	ALA	2.8
1	B	337	LYS	2.8
1	B	640	ALA	2.8
1	A	603	THR	2.8
1	A	419	LEU	2.8
1	A	141	MET	2.8
1	B	387	GLN	2.8
1	B	594	LYS	2.8
1	A	601	ASP	2.8
1	B	641	PRO	2.8
1	A	154	LYS	2.8
1	A	172	ASP	2.8
1	B	137	ALA	2.8
1	B	399	LEU	2.8
1	A	390	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	632	VAL	2.8
1	A	667	ASP	2.7
1	A	619	THR	2.7
1	B	512	ASN	2.7
1	A	614	PRO	2.7
1	A	678	LYS	2.7
1	A	437	VAL	2.7
1	A	595	MET	2.7
1	A	674	ASN	2.7
1	A	336	ILE	2.7
1	B	208	GLU	2.7
1	B	372	LYS	2.7
1	B	505	GLY	2.7
1	B	678	LYS	2.7
1	A	146	ALA	2.7
1	B	645	PRO	2.7
1	A	605	TYR	2.7
1	B	636	TYR	2.7
1	B	154	LYS	2.7
1	A	173	GLU	2.7
1	B	435	GLY	2.7
1	A	421	PHE	2.7
1	A	427	LYS	2.6
1	A	436	HIS	2.6
1	B	598	ASN	2.6
1	B	630	PRO	2.6
1	A	677	PHE	2.6
1	B	458	LEU	2.6
1	A	377	THR	2.6
1	A	630	PRO	2.6
1	B	416	ASP	2.6
1	B	113	ILE	2.6
1	B	654	THR	2.6
1	A	604	GLY	2.6
1	B	94	GLY	2.6
1	A	49	SER	2.6
1	A	348	ASP	2.6
1	A	671	ASP	2.6
1	A	59	GLU	2.6
1	B	376	MET	2.6
1	A	138	LYS	2.6
1	A	338	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	100	SER	2.6
1	A	439	ILE	2.6
1	B	562	ASP	2.6
1	B	359	ASN	2.6
1	B	148	LEU	2.5
1	B	433	LYS	2.5
1	B	600	LYS	2.5
1	A	447	HIS	2.5
1	A	466	TYR	2.5
1	B	450	ASN	2.5
1	A	376	MET	2.5
1	B	561	LYS	2.5
1	B	464	PRO	2.5
1	B	161	GLN	2.5
1	B	434	ASN	2.5
1	A	451	VAL	2.5
1	A	169	SER	2.5
1	B	440	ASN	2.5
1	B	211	ALA	2.5
1	A	417	GLU	2.5
1	A	342	GLN	2.5
1	A	147	MET	2.5
1	A	424	GLY	2.5
1	B	358	LYS	2.5
1	B	398	THR	2.5
1	A	636	TYR	2.5
1	B	675	TYR	2.5
1	B	324	LEU	2.4
1	A	152	SER	2.4
1	B	446	MET	2.4
1	B	411	GLY	2.4
1	A	363	LEU	2.4
1	B	647	LEU	2.4
1	A	563	GLU	2.4
1	A	446	MET	2.4
1	A	467	SER	2.4
1	B	114	LYS	2.4
1	B	48	GLY	2.4
1	B	592	GLY	2.4
1	B	219	LEU	2.4
1	B	138	LYS	2.4
1	B	616	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	673	ILE	2.4
1	B	467	SER	2.4
1	B	664	THR	2.4
1	A	58	ASP	2.4
1	B	671	ASP	2.4
1	B	432	ASN	2.4
1	B	584	LYS	2.4
1	B	618	LYS	2.4
1	B	651	ILE	2.4
1	B	633	ASN	2.3
1	B	95	ARG	2.3
1	A	468	GLY	2.3
1	B	391	GLY	2.3
1	A	643	ASP	2.3
1	B	190	ALA	2.3
1	B	444	ALA	2.3
1	B	331	LEU	2.3
1	A	597	PHE	2.3
1	A	160	LYS	2.3
1	B	141	MET	2.3
1	B	144	GLU	2.3
1	B	362	ILE	2.3
1	B	109	LEU	2.3
1	B	525	TYR	2.3
1	A	444	ALA	2.3
1	A	600	LYS	2.2
1	B	607	SER	2.2
1	B	670	ARG	2.2
1	A	513	ASN	2.2
1	B	439	ILE	2.2
1	B	668	LEU	2.2
1	B	341	SER	2.2
1	B	635	THR	2.2
1	B	346	ASP	2.2
1	B	513	ASN	2.2
1	A	161	GLN	2.2
1	A	668	LEU	2.2
1	B	620	GLY	2.2
1	B	634	SER	2.2
1	B	335	GLN	2.2
1	A	148	LEU	2.2
1	A	665	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	167	ARG	2.2
1	B	449	SER	2.2
1	A	333	ASP	2.2
1	B	201	ASN	2.2
1	B	655	ASN	2.2
1	A	410	VAL	2.2
1	B	146	ALA	2.2
1	B	420	HIS	2.2
1	A	639	TYR	2.1
1	A	140	MET	2.1
1	B	369	GLN	2.1
1	B	610	ASP	2.1
1	A	433	LYS	2.1
1	A	541	ALA	2.1
1	B	388	PHE	2.1
1	B	268	ASN	2.1
1	B	427	LYS	2.1
1	B	644	ASP	2.1
1	B	222	VAL	2.1
1	B	564	VAL	2.1
1	A	445	LEU	2.1
1	B	515	GLY	2.1
1	B	452	TYR	2.1
1	B	528	TYR	2.1
1	A	635	THR	2.1
1	B	162	LEU	2.1
1	B	394	VAL	2.1
1	B	665	GLY	2.1
1	B	97	THR	2.1
1	A	164	SER	2.1
1	B	558	SER	2.1
1	B	599	ASP	2.1
1	A	132	LEU	2.0
1	A	640	ALA	2.0
1	A	52	LYS	2.0
1	B	377	THR	2.0
1	B	236	ASP	2.0
1	B	560	ASN	2.0
1	B	340	ARG	2.0
1	B	338	LYS	2.0
1	B	140	MET	2.0
1	A	673	ILE	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](#)

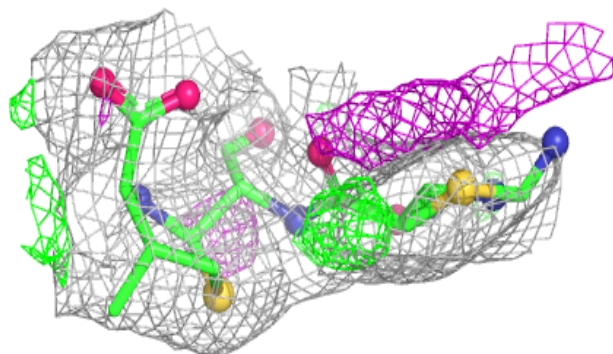
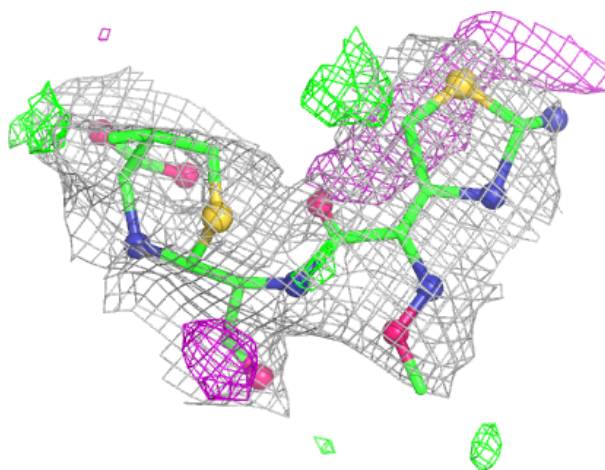
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CEF	A	701	26/26	0.78	0.21	68,89,111,143	0
2	CEF	B	701	26/26	0.81	0.21	77,99,154,157	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.

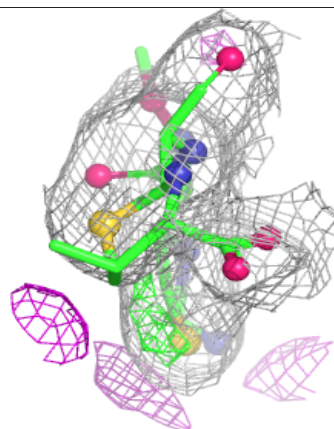
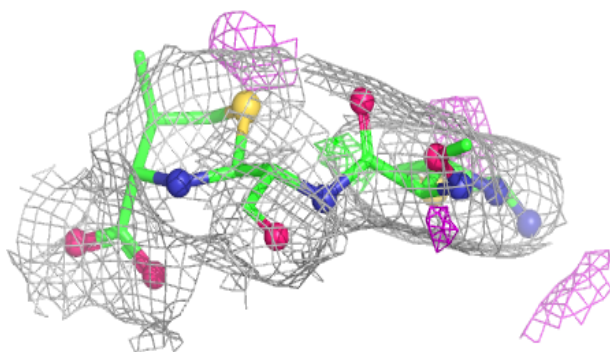
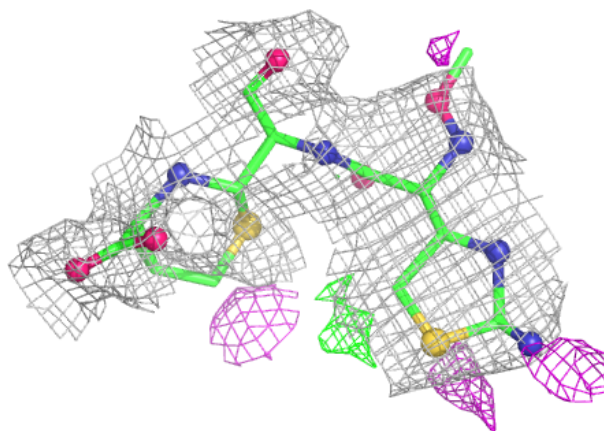
Electron density around CEF A 701:

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



Electron density around CEF B 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 [i](#)

There are no such residues in this entry.