



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:59 AM UTC

PDB ID : 3VSL / pdb_00003vsl
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

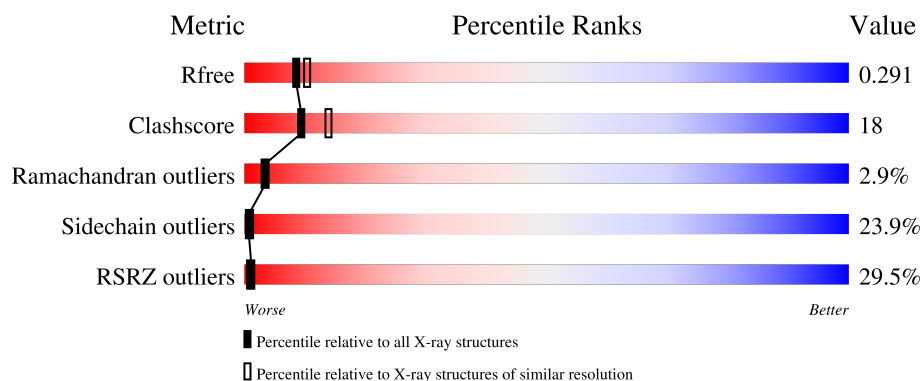
1 Overall quality at a glance

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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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	X	-	-
2	CEF	B	701	X	X	-	-

2 Entry composition [i](#)

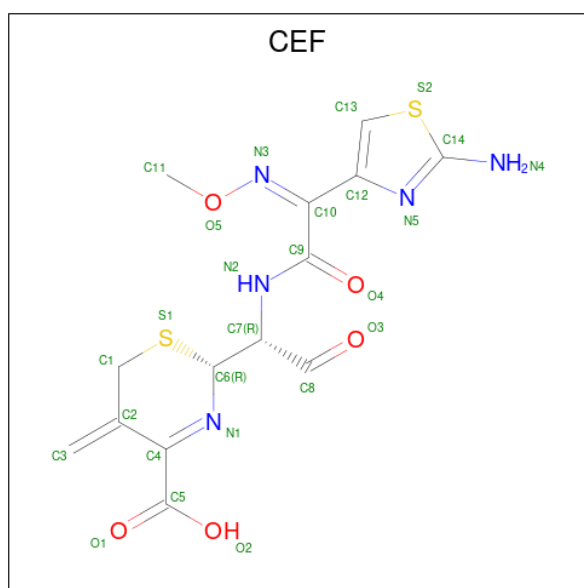
There are 3 unique types of molecules in this entry. The entry contains 10198 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Penicillin-binding protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	631	Total	C	N	O	S	0	0	0
			4943	3105	852	967	19			
1	B	631	Total	C	N	O	S	0	0	0
			4947	3107	853	968	19			

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



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

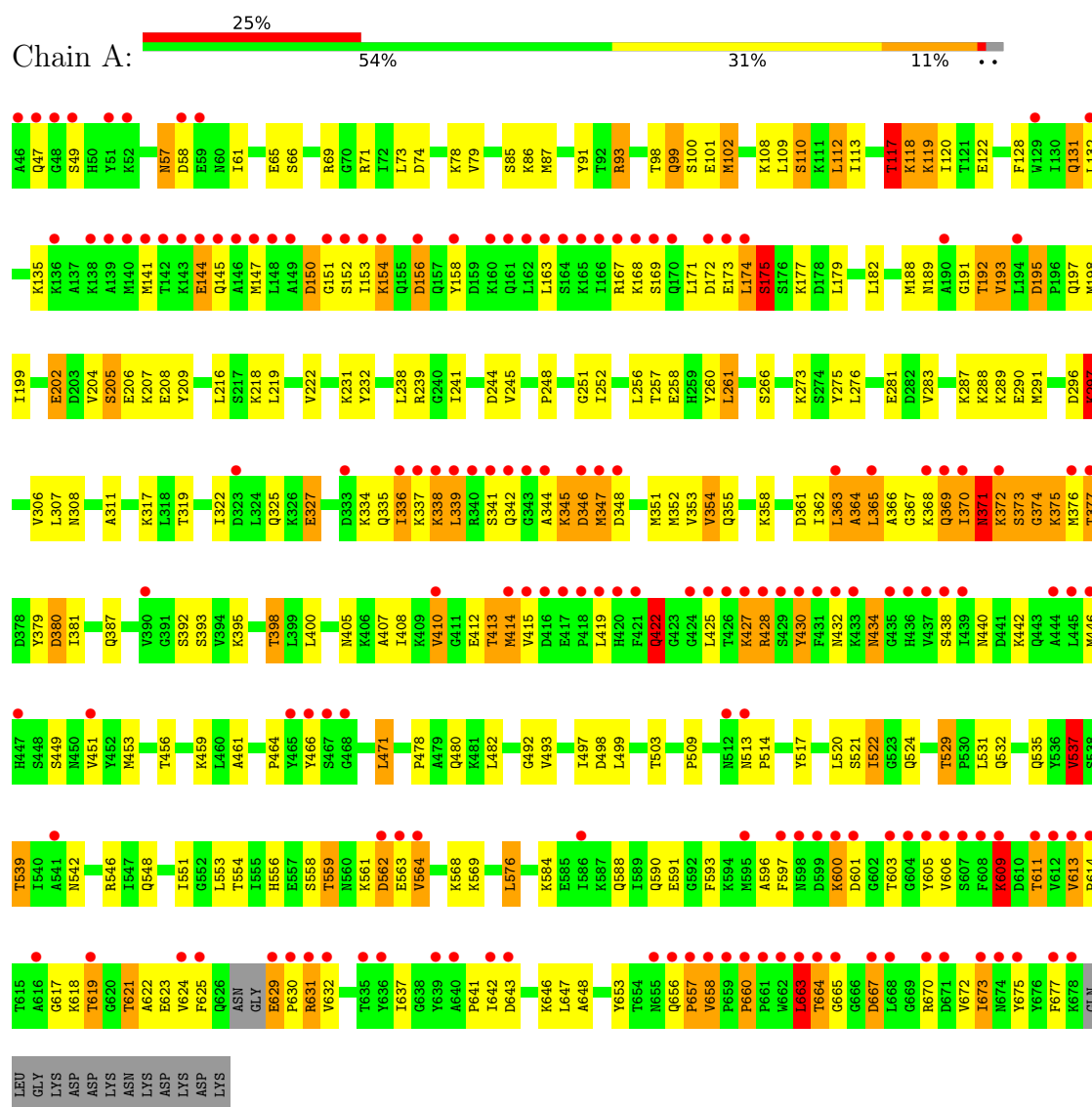
- Molecule 3 is water.

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

3 Residue-property plots

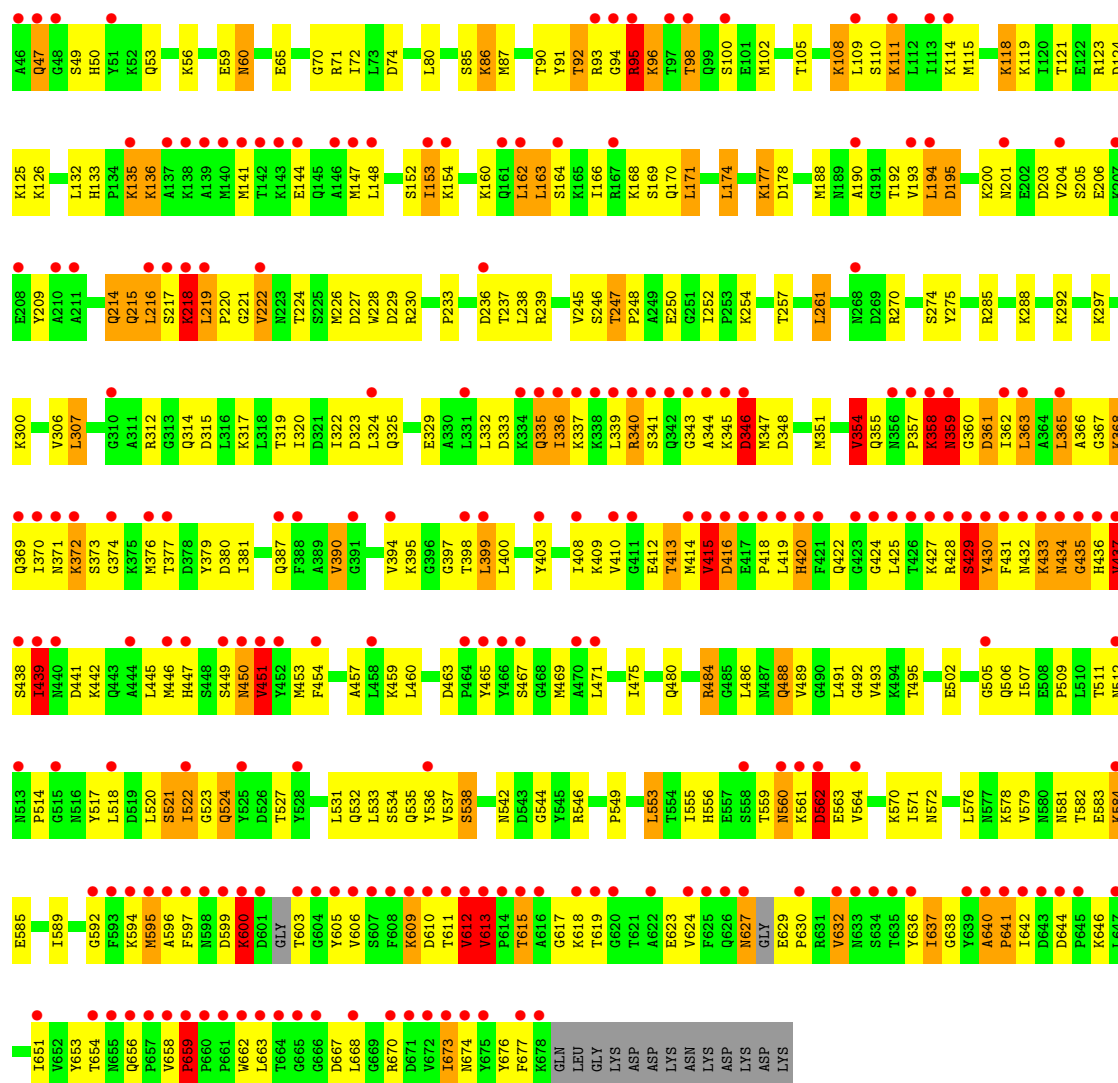
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 (Not available) , 0.291	Depositor DCC
R_{free} test set	3800 reflections (4.91%)	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	0.59	0/5025	1.04	20/6769 (0.3%)
1	B	0.59	0/5029	1.08	24/6775 (0.4%)
All	All	0.59	0/10054	1.06	44/13544 (0.3%)

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 (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	338	LYS	N-CA-C	-9.99	98.67	112.25
1	A	513	ASN	CA-C-N	9.86	129.64	119.19
1	A	513	ASN	C-N-CA	9.86	129.64	119.19
1	B	430	TYR	N-CA-C	9.40	124.15	112.87
1	B	360	GLY	N-CA-C	8.79	124.33	111.76
1	B	612	VAL	N-CA-C	-8.39	104.96	113.10
1	A	150	ASP	N-CA-C	-8.30	102.18	111.14
1	A	660	PRO	N-CA-C	8.13	120.62	110.70
1	A	364	ALA	N-CA-C	7.76	121.05	108.32
1	B	190	ALA	N-CA-C	-7.68	103.47	112.92
1	A	372	LYS	N-CA-C	-7.52	102.49	112.72
1	B	429	SER	N-CA-C	7.33	121.22	109.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	596	ALA	N-CA-C	-7.00	105.28	114.31
1	B	219	LEU	N-CA-C	-6.96	99.52	109.62
1	B	644	ASP	CA-C-N	6.92	127.30	119.83
1	B	644	ASP	C-N-CA	6.92	127.30	119.83
1	A	119	LYS	N-CA-C	-6.58	105.55	113.97
1	A	191	GLY	N-CA-C	6.43	119.83	110.63
1	A	151	GLY	N-CA-C	-6.23	106.48	115.27
1	B	659	PRO	N-CA-C	6.18	118.24	110.70
1	B	98	THR	N-CA-C	-6.17	105.50	113.16
1	A	551	ILE	N-CA-C	-6.16	105.65	113.22
1	B	600	LYS	N-CA-C	6.10	118.42	110.43
1	A	252	ILE	N-CA-C	-6.07	102.35	108.96
1	A	374	GLY	N-CA-C	-5.93	106.80	115.63
1	B	323	ASP	N-CA-C	-5.74	105.10	111.36
1	A	667	ASP	N-CA-C	-5.68	105.61	112.54
1	B	354	VAL	N-CA-C	5.63	116.58	108.48
1	B	252	ILE	CB-CA-C	-5.47	104.39	110.68
1	A	629	GLU	CA-C-N	5.46	125.63	119.90
1	A	629	GLU	C-N-CA	5.46	125.63	119.90
1	B	624	VAL	N-CA-C	5.41	115.78	107.77
1	B	415	VAL	N-CA-C	5.39	116.91	109.46
1	A	537	VAL	N-CA-CB	5.34	116.79	110.55
1	B	613	VAL	CA-C-N	-5.28	113.25	119.84
1	B	613	VAL	C-N-CA	-5.28	113.25	119.84
1	B	632	VAL	N-CA-C	5.27	115.30	108.35
1	B	367	GLY	N-CA-C	-5.26	103.42	111.10
1	B	437	VAL	N-CA-C	5.19	115.15	108.82
1	B	439	ILE	N-CA-C	5.11	116.27	109.37
1	B	195	ASP	CA-C-N	5.09	125.25	119.90
1	B	195	ASP	C-N-CA	5.09	125.25	119.90
1	A	660	PRO	CA-C-N	-5.03	113.56	119.84
1	A	660	PRO	C-N-CA	-5.03	113.56	119.84

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	177	0
1	B	4947	0	4994	188	0
2	A	26	0	1	6	0
2	B	26	0	1	5	0
3	A	140	0	0	4	0
3	B	116	0	0	5	0
All	All	10198	0	9987	359	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 18.

All (359) 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:352:MET:HE1	1:A:672:VAL:HG11	1.58	0.86
1:A:141:MET:HE3	1:A:144:GLU:HG3	1.61	0.82
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:102:MET:HG2	1:A:188:MET:HE2	1.67	0.77
1:A:99:GLN:HG2	1:A:131:GLN:HE22	1.50	0.77
1:B:446:MET:HE2	1:B:600:LYS:HG3	1.66	0.76
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:347:MET:HE2	1:B:653:TYR:HB3	1.69	0.73
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:B:442:LYS:HD3	1:B:595:MET:HE1	1.74	0.70
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:86:LYS:HD3	1:B:201:ASN:CG	2.21	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:347:MET:HE2	1:A:656:GLN:HE21	1.63	0.62
1:A:337:LYS:HA	1:A:339:LEU:HG	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:B:214:GLN:OE1	1:B:218:LYS:NZ	2.35	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:347:MET:HE3	1:B:656:GLN:HG2	1.85	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:372:LYS:C	1:B:374:GLY:H	2.11	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:A:395:LYS:HB3	1:A:453:MET:HE3	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:LYS:C	1:A:339:LEU:H	2.14	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
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:A:86:LYS:HG2	1:A:202:GLU:C	2.33	0.53
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
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:329:GLU:CD	1:B:365:LEU:HD13	2.33	0.53
1:B:366:ALA:HB3	1:B:379:TYR:O	2.09	0.53
1:B:147:MET:HE2	1:B:153:ILE:HD13	1.91	0.53
1:B:365:LEU:HD12	1:B:380:ASP:OD1	2.09	0.53
1:A:171:LEU:C	1:A:173:GLU:H	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:412:GLU:OE2	1:A:459:LYS:NZ	2.43	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
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:A:392:SER:HB3	1:A:395:LYS:HZ2	1.77	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:91:TYR:CE1	1:A:188:MET:HE3	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:B:400:LEU:HB3	1:B:581:ASN:CG	2.39	0.47
1:A:653:TYR:CE2	1:A:665:GLY:HA3	2.49	0.47
1:B:247:THR:OG1	1:B:250:GLU:OE1	2.32	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:B:60:ASN:OD1	1:B:292:LYS:NZ	2.45	0.47
1:A:529:THR:HG22	1:A:532:GLN:N	2.11	0.47
1:B:141:MET:HE3	1:B:144:GLU:HB2	1.96	0.47
1:B:578:LYS:HG2	1:B:579:VAL:O	2.15	0.47
1:B:209:TYR:HH	1:B:224:THR:HG23	1.80	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:336:ILE:HG13	1:A:369:GLN:CD	2.40	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: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:B:395:LYS:HD3	1:B:453:MET:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:92:THR:HG23	1:B:195:ASP:C	2.40	0.46
1:A:173:GLU:C	1:A:175:SER:N	2.74	0.46
1:A:192:THR:HB	1:A:195:ASP:HB2	1.98	0.46
1:B:98:THR:C	1:B:100:SER:H	2.24	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:A:559:THR:HG1	1:A:562:ASP:H	1.63	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
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:A:49:SER:OG	1:A:65:GLU:OE2	2.22	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: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: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:B:579:VAL:C	1:B:581:ASN:H	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:340:ARG:HA	1:B:372:LYS:HZ3	1.83	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
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:A:175:SER:O	1:A:175:SER:OG	2.33	0.43
1:A:372:LYS:HD2	1:A:372:LYS:HA	1.84	0.43
1:A:198:MET:HE2	1:A:198:MET:HB2	1.90	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:337:LYS:HZ3	1:B:340:ARG:HH11	1.66	0.43
1:B:372:LYS:C	1:B:374:GLY:N	2.77	0.43
1:B:442:LYS:CD	1:B:595:MET:HE1	2.47	0.43
1:B:512:ASN:OD1	1:B:512:ASN:N	2.52	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:B:371:ASN:C	1:B:373:SER:N	2.77	0.43
1:A:257:THR:O	1:A:258:GLU:C	2.62	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:LYS:HZ2	1:B:484:ARG:HH22	1.66	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: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:446:MET:C	1:B:600:LYS:HD2	2.44	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: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:105:THR:HB	1:B:188:MET:HE1	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:612:VAL:HG21	1:B:674:ASN:HA	2.02	0.41
1:A:110:SER:C	1:A:112:LEU:H	2.28	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:430:TYR:CZ	1:B:431:PHE:CE2	3.09	0.41
1:A:317:LYS:HD3	1:A:556:HIS:NE2	2.36	0.40
1:A:371:ASN:HD22	1:A:371:ASN:C	2.28	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:362:ILE:C	1:A:363:LEU:HD23	2.47	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 [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	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
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

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Mol	Chain	Res	Type
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%)	423 (78%)	123 (22%)	1	1
1	B	547/559 (98%)	409 (75%)	138 (25%)	0	1
All	All	1093/1118 (98%)	832 (76%)	261 (24%)	1	1

All (261) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	57	ASN
1	A	61	ILE
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	108	LYS
1	A	109	LEU
1	A	110	SER
1	A	112	LEU
1	A	113	ILE
1	A	117	THR
1	A	118	LYS
1	A	120	ILE
1	A	122	GLU

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Mol	Chain	Res	Type
1	A	131	GLN
1	A	132	LEU
1	A	135	LYS
1	A	144	GLU
1	A	145	GLN
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	205	SER
1	A	206	GLU
1	A	207	LYS
1	A	216	LEU
1	A	218	LYS
1	A	231	LYS
1	A	244	ASP
1	A	245	VAL
1	A	256	LEU
1	A	261	LEU
1	A	266	SER
1	A	283	VAL
1	A	289	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

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Mol	Chain	Res	Type
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	380	ASP
1	A	381	ILE
1	A	393	SER
1	A	398	THR
1	A	400	LEU
1	A	410	VAL
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	434	ASN
1	A	438	SER
1	A	446	MET
1	A	449	SER
1	A	471	LEU
1	A	480	GLN
1	A	493	VAL
1	A	497	ILE
1	A	522	ILE
1	A	529	THR
1	A	537	VAL
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

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Mol	Chain	Res	Type
1	A	600	LYS
1	A	601	ASP
1	A	603	THR
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	646	LYS
1	A	663	LEU
1	A	664	THR
1	A	673	ILE
1	B	47	GLN
1	B	53	GLN
1	B	56	LYS
1	B	59	GLU
1	B	60	ASN
1	B	72	ILE
1	B	86	LYS
1	B	92	THR
1	B	95	ARG
1	B	96	LYS
1	B	102	MET
1	B	108	LYS
1	B	109	LEU
1	B	110	SER
1	B	111	LYS
1	B	114	LYS
1	B	115	MET
1	B	118	LYS
1	B	132	LEU
1	B	135	LYS
1	B	136	LYS
1	B	152	SER
1	B	153	ILE
1	B	154	LYS
1	B	160	LYS

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Mol	Chain	Res	Type
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	285	ARG
1	B	288	LYS
1	B	297	LYS
1	B	300	LYS
1	B	306	VAL
1	B	307	LEU
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

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Mol	Chain	Res	Type
1	B	351	MET
1	B	354	VAL
1	B	355	GLN
1	B	361	ASP
1	B	362	ILE
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	381	ILE
1	B	387	GLN
1	B	390	VAL
1	B	399	LEU
1	B	408	ILE
1	B	409	LYS
1	B	413	THR
1	B	414	MET
1	B	415	VAL
1	B	416	ASP
1	B	420	HIS
1	B	422	GLN
1	B	425	LEU
1	B	429	SER
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
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

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Mol	Chain	Res	Type
1	B	521	SER
1	B	522	ILE
1	B	524	GLN
1	B	538	SER
1	B	542	ASN
1	B	553	LEU
1	B	559	THR
1	B	562	ASP
1	B	563	GLU
1	B	564	VAL
1	B	584	LYS
1	B	595	MET
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	615	THR
1	B	627	ASN
1	B	629	GLU
1	B	632	VAL
1	B	637	ILE
1	B	654	THR
1	B	658	VAL
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 (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	131	GLN
1	A	145	GLN
1	A	387	GLN
1	A	501	ASN
1	A	506	GLN
1	A	548	GLN
1	A	590	GLN
1	A	656	GLN

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Mol	Chain	Res	Type
1	B	47	GLN
1	B	53	GLN
1	B	201	ASN
1	B	314	GLN
1	B	335	GLN
1	B	359	ASN
1	B	371	ASN
1	B	387	GLN
1	B	404	GLN
1	B	432	ASN
1	B	436	HIS
1	B	480	GLN
1	B	487	ASN
1	B	488	GLN
1	B	501	ASN
1	B	516	ASN
1	B	524	GLN
1	B	542	ASN
1	B	560	ASN
1	B	626	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CEF	B	701	1	24,27,27	11.02	16 (66%)	25,37,37	9.27	19 (76%)
2	CEF	A	701	1	24,27,27	10.93	16 (66%)	25,37,37	10.05	18 (72%)

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	B	701	1	1/1/7/9	9/18/38/38	0/1/2/2
2	CEF	A	701	1	1/1/7/9	8/18/38/38	0/1/2/2

All (32) 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	C14-N5	29.34	1.73	1.31
2	A	701	CEF	C14-N5	28.95	1.72	1.31
2	B	701	CEF	C13-C12	20.14	1.72	1.36
2	A	701	CEF	C13-C12	19.68	1.71	1.36
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	A	701	CEF	C10-C12	-9.04	1.30	1.46
2	B	701	CEF	C10-C12	-8.51	1.31	1.46
2	B	701	CEF	C10-N3	8.11	1.50	1.29
2	A	701	CEF	C10-N3	7.48	1.48	1.29
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	A	701	CEF	C12-N5	6.67	1.52	1.38
2	B	701	CEF	C12-N5	6.43	1.52	1.38
2	B	701	CEF	C9-N2	5.95	1.46	1.34
2	A	701	CEF	C14-S2	-5.90	1.66	1.74
2	B	701	CEF	C14-S2	-5.87	1.66	1.74
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	B	701	CEF	C4-C5	-4.48	1.39	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	CEF	C4-C5	-4.18	1.39	1.48
2	A	701	CEF	C14-N4	-4.14	1.26	1.34
2	B	701	CEF	C14-N4	-4.10	1.26	1.34
2	A	701	CEF	O5-N3	-3.81	1.31	1.40
2	B	701	CEF	C10-C9	3.56	1.55	1.48
2	B	701	CEF	O5-N3	-3.25	1.33	1.40
2	A	701	CEF	C10-C9	2.91	1.54	1.48
2	B	701	CEF	C1-C2	-2.50	1.47	1.50
2	A	701	CEF	C1-C2	-2.40	1.47	1.50

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	CEF	C13-S2-C14	38.73	105.53	88.84
2	B	701	CEF	C13-S2-C14	37.12	104.84	88.84
2	A	701	CEF	S2-C14-N5	-15.17	102.58	114.54
2	A	701	CEF	N4-C14-N5	-12.90	109.06	124.05
2	B	701	CEF	S2-C14-N5	-12.40	104.77	114.54
2	B	701	CEF	N4-C14-N5	-11.69	110.47	124.05
2	A	701	CEF	C12-C13-S2	-11.32	97.16	110.24
2	A	701	CEF	C1-S1-C6	10.07	112.81	94.36
2	B	701	CEF	C11-O5-N3	9.66	120.11	108.32
2	B	701	CEF	C13-C12-C10	-9.50	108.69	125.69
2	A	701	CEF	S2-C14-N4	-8.52	111.08	120.99
2	A	701	CEF	C13-C12-C10	-8.48	110.52	125.69
2	B	701	CEF	S2-C14-N4	-8.45	111.17	120.99
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	C13-C12-N5	-5.75	107.53	115.43
2	A	701	CEF	C10-C9-N2	5.49	122.93	114.27
2	B	701	CEF	C13-C12-N5	-5.35	108.07	115.43
2	A	701	CEF	C6-N1-C4	4.84	120.56	116.33
2	A	701	CEF	C7-N2-C9	-3.83	114.40	121.97
2	B	701	CEF	C12-C13-S2	-3.70	105.96	110.24
2	B	701	CEF	C14-N5-C12	-3.68	105.16	110.57
2	A	701	CEF	C10-C12-N5	-3.68	110.49	119.39
2	B	701	CEF	O2-C5-C4	3.68	125.76	116.02
2	B	701	CEF	C10-C12-N5	-3.51	110.91	119.39
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	CEF	C9-C10-N3	-3.03	105.73	120.64
2	B	701	CEF	C10-C9-N2	2.54	118.27	114.27
2	A	701	CEF	C14-N5-C12	-2.47	106.95	110.57
2	A	701	CEF	O2-C5-O1	-2.40	118.19	123.90
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 (17) torsion outliers are listed below:

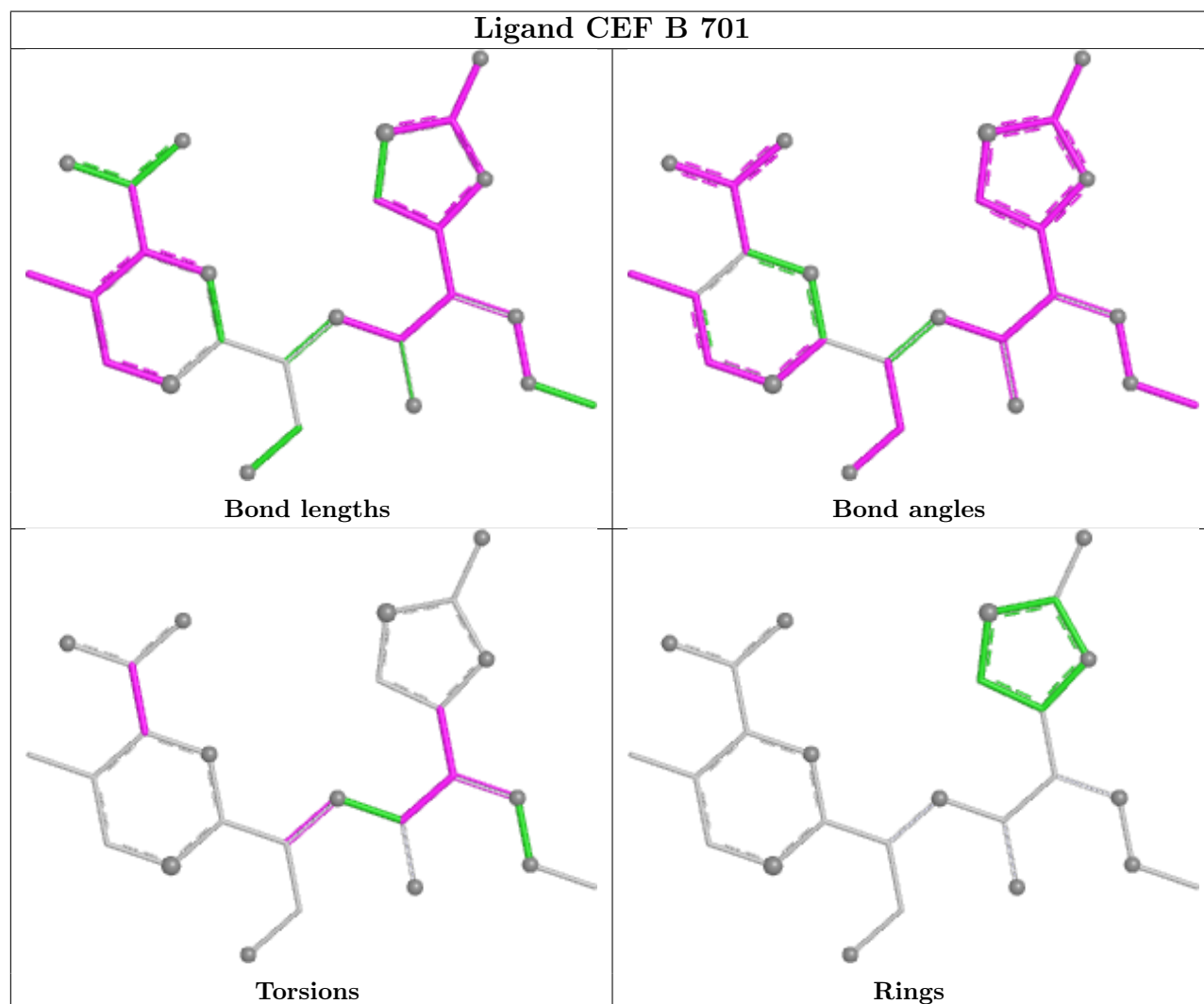
Mol	Chain	Res	Type	Atoms
2	A	701	CEF	C9-C10-N3-O5
2	A	701	CEF	C12-C10-N3-O5
2	A	701	CEF	N3-C10-C12-N5
2	B	701	CEF	N1-C4-C5-O1
2	B	701	CEF	N1-C4-C5-O2
2	B	701	CEF	C12-C10-N3-O5
2	B	701	CEF	C9-C10-C12-C13
2	B	701	CEF	N3-C10-C12-N5
2	B	701	CEF	C12-C10-C9-N2
2	B	701	CEF	C12-C10-C9-O4
2	A	701	CEF	N1-C4-C5-O2
2	A	701	CEF	N1-C4-C5-O1
2	A	701	CEF	N3-C10-C9-O4
2	A	701	CEF	C9-C10-C12-C13
2	B	701	CEF	N3-C10-C9-O4
2	B	701	CEF	C8-C7-N2-C9
2	A	701	CEF	N3-C10-C9-N2

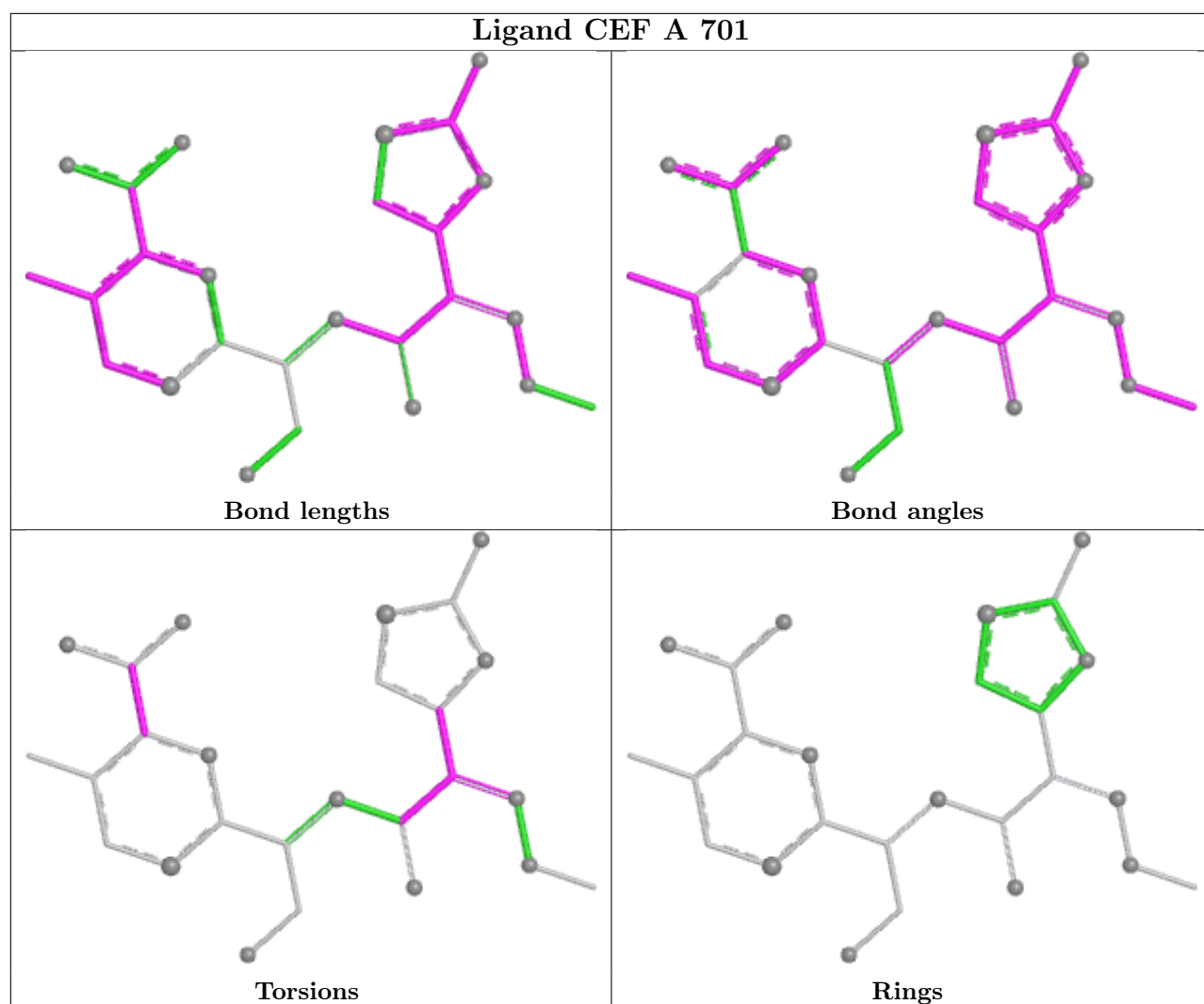
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	CEF	5	0
2	A	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%)	1.24	159 (25%)  	27, 61, 117, 146	0
1	B	631/646 (97%)	1.54	213 (33%)  	29, 70, 124, 161	0
All	All	1262/1292 (97%)	1.39	372 (29%)  	27, 66, 121, 161	0

All (372) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	625	PHE	8.3
1	A	174	LEU	8.1
1	A	168	LYS	6.8
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	5.8
1	A	339	LEU	5.6
1	B	662	TRP	5.6
1	B	612	VAL	5.4
1	B	658	VAL	5.4
1	B	603	THR	5.4
1	B	663	LEU	5.2
1	B	643	ASP	4.9
1	B	661	PRO	4.9
1	B	674	ASN	4.9
1	B	657	PRO	4.9
1	B	429	SER	4.8
1	A	660	PRO	4.8
1	B	363	LEU	4.7
1	A	166	ILE	4.6
1	B	217	SER	4.6
1	B	611	THR	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	608	PHE	4.5
1	B	357	PRO	4.5
1	A	616	ALA	4.5
1	B	216	LEU	4.5
1	A	343	GLY	4.4
1	A	341	SER	4.4
1	B	371	ASN	4.4
1	A	142	THR	4.4
1	B	619	THR	4.4
1	B	218	LYS	4.4
1	A	415	VAL	4.4
1	A	562	ASP	4.4
1	A	344	ALA	4.4
1	B	344	ALA	4.3
1	A	48	GLY	4.3
1	B	374	GLY	4.3
1	B	642	ILE	4.3
1	A	431	PHE	4.3
1	A	657	PRO	4.3
1	B	438	SER	4.2
1	B	659	PRO	4.2
1	B	593	PHE	4.2
1	A	365	LEU	4.2
1	A	598	ASN	4.2
1	A	661	PRO	4.2
1	A	606	VAL	4.2
1	B	613	VAL	4.2
1	A	609	LYS	4.1
1	B	626	GLN	4.0
1	B	601	ASP	4.0
1	A	139	ALA	4.0
1	A	369	GLN	4.0
1	A	194	LEU	4.0
1	A	136	LYS	4.0
1	B	660	PRO	3.9
1	B	604	GLY	3.9
1	B	436	HIS	3.9
1	B	451	VAL	3.9
1	B	677	PHE	3.9
1	A	426	THR	3.9
1	B	370	ILE	3.8
1	B	194	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	632	VAL	3.8
1	B	343	GLY	3.8
1	B	193	VAL	3.8
1	B	93	ARG	3.8
1	B	614	PRO	3.8
1	A	46	ALA	3.7
1	B	465	TYR	3.7
1	A	51	TYR	3.7
1	A	337	LYS	3.7
1	B	454	PHE	3.6
1	A	167	ARG	3.6
1	A	432	ASN	3.6
1	B	47	GLN	3.6
1	B	408	ILE	3.5
1	A	564	VAL	3.5
1	B	471	LEU	3.5
1	A	151	GLY	3.5
1	A	143	LYS	3.5
1	A	158	TYR	3.5
1	B	423	GLY	3.5
1	A	613	VAL	3.5
1	B	51	TYR	3.4
1	B	431	PHE	3.4
1	B	595	MET	3.4
1	A	47	GLN	3.4
1	B	365	LEU	3.4
1	A	372	LYS	3.4
1	A	659	PRO	3.4
1	B	345	LYS	3.4
1	B	622	ALA	3.4
1	B	605	TYR	3.4
1	A	428	ARG	3.4
1	B	421	PHE	3.4
1	A	414	MET	3.4
1	A	662	TRP	3.4
1	A	429	SER	3.4
1	A	438	SER	3.4
1	A	607	SER	3.4
1	A	512	ASN	3.3
1	A	165	LYS	3.3
1	A	162	LEU	3.3
1	B	310	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	522	ILE	3.3
1	A	625	PHE	3.3
1	B	135	LYS	3.3
1	A	656	GLN	3.3
1	A	611	THR	3.3
1	B	356	ASN	3.3
1	A	663	LEU	3.3
1	B	518	LEU	3.3
1	B	428	ARG	3.3
1	B	415	VAL	3.3
1	A	347	MET	3.3
1	A	370	ILE	3.3
1	B	414	MET	3.3
1	A	430	TYR	3.3
1	A	675	TYR	3.3
1	A	642	ILE	3.3
1	A	465	TYR	3.2
1	B	98	THR	3.2
1	B	424	GLY	3.2
1	B	111	LYS	3.2
1	B	656	GLN	3.2
1	A	416	ASP	3.2
1	B	417	GLU	3.2
1	B	139	ALA	3.2
1	A	340	ARG	3.2
1	B	418	PRO	3.2
1	B	466	TYR	3.2
1	A	170	GLN	3.1
1	A	631	ARG	3.1
1	A	153	ILE	3.1
1	B	142	THR	3.1
1	B	426	THR	3.1
1	B	615	THR	3.1
1	A	149	ALA	3.1
1	B	419	LEU	3.1
1	B	342	GLN	3.1
1	B	147	MET	3.1
1	B	339	LEU	3.1
1	B	470	ALA	3.1
1	A	425	LEU	3.1
1	A	435	GLY	3.1
1	A	624	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	624	VAL	3.1
1	B	639	TYR	3.0
1	B	164	SER	3.0
1	B	143	LYS	3.0
1	B	609	LYS	3.0
1	A	145	GLN	3.0
1	B	596	ALA	3.0
1	B	597	PHE	3.0
1	B	46	ALA	3.0
1	A	608	PHE	3.0
1	B	334	LYS	3.0
1	A	420	HIS	3.0
1	B	210	ALA	3.0
1	B	336	ILE	2.9
1	A	664	THR	2.9
1	B	447	HIS	2.9
1	A	670	ARG	2.9
1	A	346	ASP	2.9
1	B	153	ILE	2.9
1	A	612	VAL	2.9
1	A	368	LYS	2.9
1	A	419	LEU	2.9
1	A	156	ASP	2.9
1	B	410	VAL	2.9
1	A	603	THR	2.9
1	A	190	ALA	2.9
1	B	640	ALA	2.9
1	A	141	MET	2.9
1	B	399	LEU	2.9
1	A	599	ASP	2.9
1	B	387	GLN	2.9
1	A	144	GLU	2.9
1	B	207	LYS	2.8
1	B	641	PRO	2.8
1	B	137	ALA	2.8
1	A	629	GLU	2.8
1	B	337	LYS	2.8
1	A	390	VAL	2.8
1	A	632	VAL	2.8
1	A	619	THR	2.8
1	A	601	ASP	2.8
1	B	594	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	336	ILE	2.8
1	B	512	ASN	2.8
1	A	437	VAL	2.8
1	A	614	PRO	2.8
1	A	595	MET	2.8
1	A	154	LYS	2.8
1	A	172	ASP	2.8
1	A	421	PHE	2.8
1	B	505	GLY	2.8
1	A	605	TYR	2.8
1	B	636	TYR	2.8
1	A	674	ASN	2.8
1	A	146	ALA	2.8
1	A	667	ASP	2.8
1	A	677	PHE	2.8
1	B	645	PRO	2.7
1	A	678	LYS	2.7
1	B	435	GLY	2.7
1	B	458	LEU	2.7
1	B	372	LYS	2.7
1	B	678	LYS	2.7
1	A	436	HIS	2.7
1	B	113	ILE	2.7
1	B	630	PRO	2.7
1	B	598	ASN	2.7
1	A	377	THR	2.7
1	B	654	THR	2.7
1	B	208	GLU	2.7
1	A	604	GLY	2.7
1	B	94	GLY	2.7
1	A	630	PRO	2.7
1	B	154	LYS	2.7
1	A	49	SER	2.7
1	A	427	LYS	2.6
1	A	439	ILE	2.6
1	B	376	MET	2.6
1	B	148	LEU	2.6
1	A	173	GLU	2.6
1	B	100	SER	2.6
1	A	466	TYR	2.6
1	B	416	ASP	2.6
1	B	359	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	447	HIS	2.6
1	A	348	ASP	2.6
1	A	671	ASP	2.6
1	A	376	MET	2.6
1	B	450	ASN	2.6
1	A	138	LYS	2.6
1	A	338	LYS	2.6
1	B	464	PRO	2.6
1	B	562	ASP	2.6
1	A	59	GLU	2.6
1	A	451	VAL	2.6
1	B	434	ASN	2.6
1	B	161	GLN	2.6
1	A	169	SER	2.6
1	B	433	LYS	2.6
1	B	600	LYS	2.6
1	A	636	TYR	2.6
1	B	675	TYR	2.6
1	B	324	LEU	2.5
1	B	440	ASN	2.5
1	B	211	ALA	2.5
1	B	561	LYS	2.5
1	B	398	THR	2.5
1	A	147	MET	2.5
1	A	424	GLY	2.5
1	A	363	LEU	2.5
1	B	647	LEU	2.5
1	A	342	GLN	2.5
1	A	152	SER	2.5
1	B	446	MET	2.5
1	B	411	GLY	2.5
1	B	219	LEU	2.5
1	A	467	SER	2.5
1	A	446	MET	2.5
1	B	48	GLY	2.5
1	B	592	GLY	2.5
1	B	673	ILE	2.5
1	B	358	LYS	2.5
1	B	616	ALA	2.5
1	B	467	SER	2.5
1	B	664	THR	2.5
1	A	417	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	651	ILE	2.4
1	B	432	ASN	2.4
1	B	114	LYS	2.4
1	A	597	PHE	2.4
1	B	633	ASN	2.4
1	A	563	GLU	2.4
1	B	138	LYS	2.4
1	A	468	GLY	2.4
1	B	391	GLY	2.4
1	A	58	ASP	2.4
1	B	671	ASP	2.4
1	B	331	LEU	2.4
1	B	190	ALA	2.4
1	B	444	ALA	2.4
1	B	584	LYS	2.4
1	B	618	LYS	2.4
1	B	362	ILE	2.4
1	B	109	LEU	2.4
1	B	525	TYR	2.4
1	B	141	MET	2.4
1	A	643	ASP	2.3
1	A	444	ALA	2.3
1	B	95	ARG	2.3
1	B	607	SER	2.3
1	B	439	ILE	2.3
1	B	668	LEU	2.3
1	A	160	LYS	2.3
1	A	513	ASN	2.3
1	B	635	THR	2.3
1	B	341	SER	2.3
1	A	668	LEU	2.3
1	B	144	GLU	2.3
1	B	513	ASN	2.3
1	A	161	GLN	2.3
1	B	620	GLY	2.3
1	B	634	SER	2.3
1	A	148	LEU	2.3
1	A	600	LYS	2.3
1	A	639	TYR	2.3
1	A	665	GLY	2.2
1	B	335	GLN	2.2
1	B	449	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	346	ASP	2.2
1	B	388	PHE	2.2
1	A	410	VAL	2.2
1	B	670	ARG	2.2
1	B	146	ALA	2.2
1	B	201	ASN	2.2
1	B	655	ASN	2.2
1	B	420	HIS	2.2
1	A	140	MET	2.2
1	A	541	ALA	2.2
1	B	369	GLN	2.2
1	B	452	TYR	2.2
1	B	528	TYR	2.2
1	A	445	LEU	2.2
1	A	333	ASP	2.2
1	B	222	VAL	2.2
1	B	564	VAL	2.2
1	B	268	ASN	2.2
1	A	635	THR	2.2
1	B	162	LEU	2.2
1	B	515	GLY	2.2
1	B	610	ASP	2.2
1	B	167	ARG	2.2
1	A	433	LYS	2.2
1	B	394	VAL	2.1
1	A	132	LEU	2.1
1	B	97	THR	2.1
1	B	665	GLY	2.1
1	A	164	SER	2.1
1	B	558	SER	2.1
1	B	644	ASP	2.1
1	B	427	LYS	2.1
1	A	640	ALA	2.1
1	B	377	THR	2.1
1	A	129	TRP	2.1
1	B	560	ASN	2.1
1	A	673	ILE	2.1
1	B	599	ASP	2.1
1	B	140	MET	2.1
1	A	52	LYS	2.1
1	B	236	ASP	2.1
1	B	403	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	163	LEU	2.0
1	B	666	GLY	2.0
1	B	338	LYS	2.0
1	A	323	ASP	2.0
1	B	536	TYR	2.0
1	B	204	VAL	2.0
1	B	340	ARG	2.0
1	B	672	VAL	2.0
1	A	655	ASN	2.0
1	B	627	ASN	2.0
1	A	586	ILE	2.0
1	A	418	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

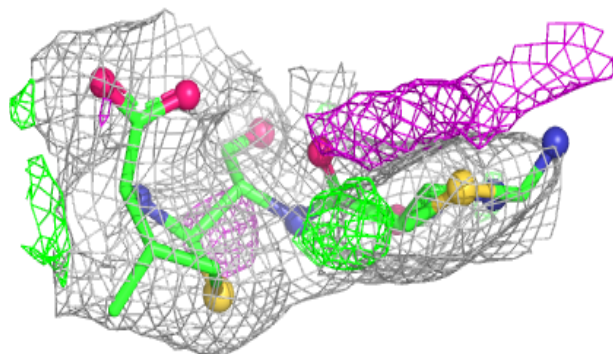
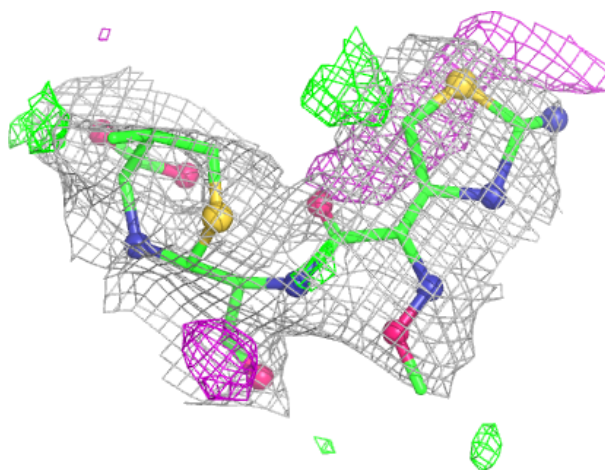
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	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.

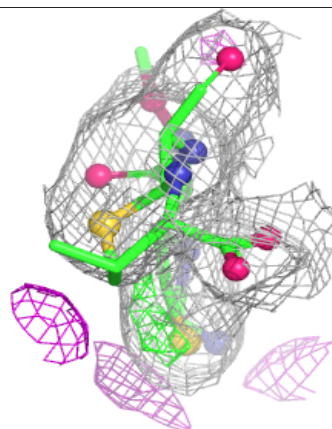
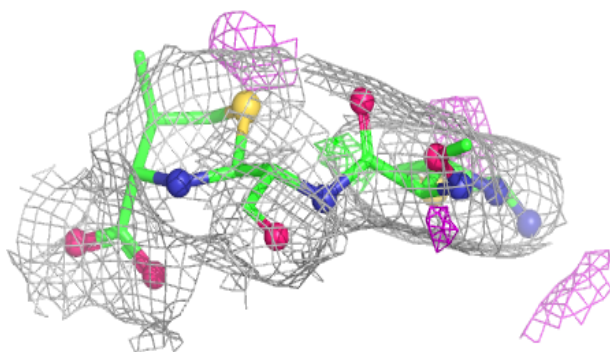
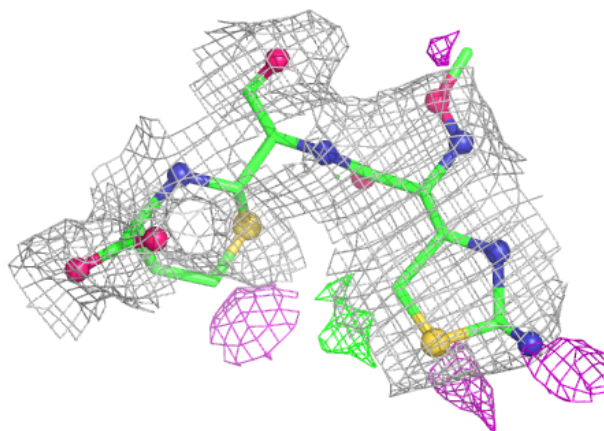
Electron density around CEF A 701:

$2mF_o-DF_c$ (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.