



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:00 PM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

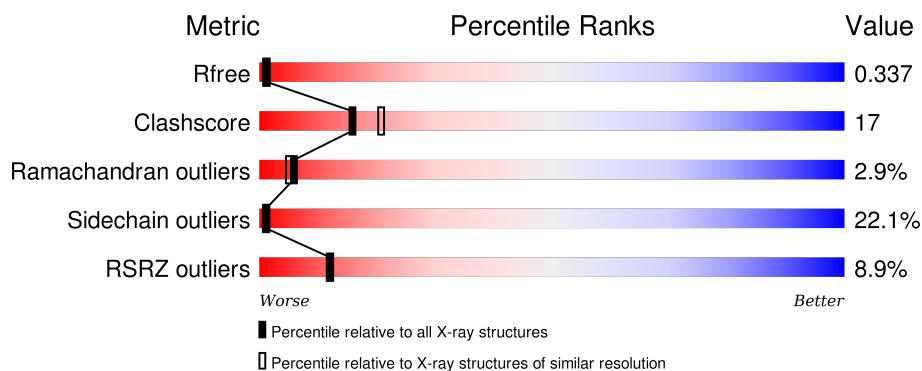
1 Overall quality at a glance

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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	-	-	-

2 Entry composition [i](#)

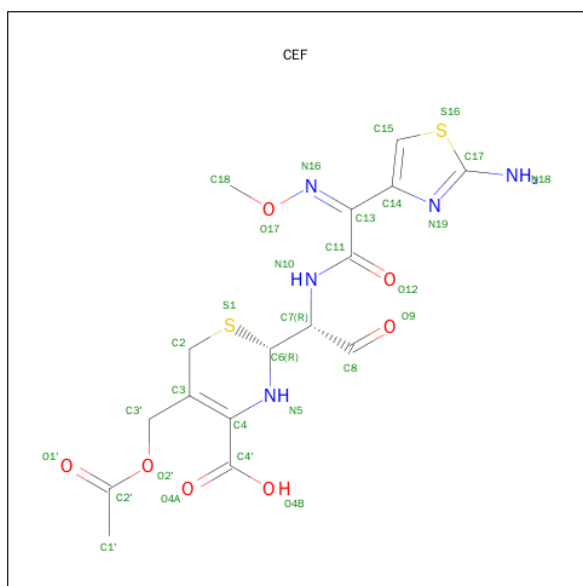
There are 3 unique types of molecules in this entry. The entry contains 10198 atoms, of which 0 are hydrogens and 0 are deuteriums.

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			

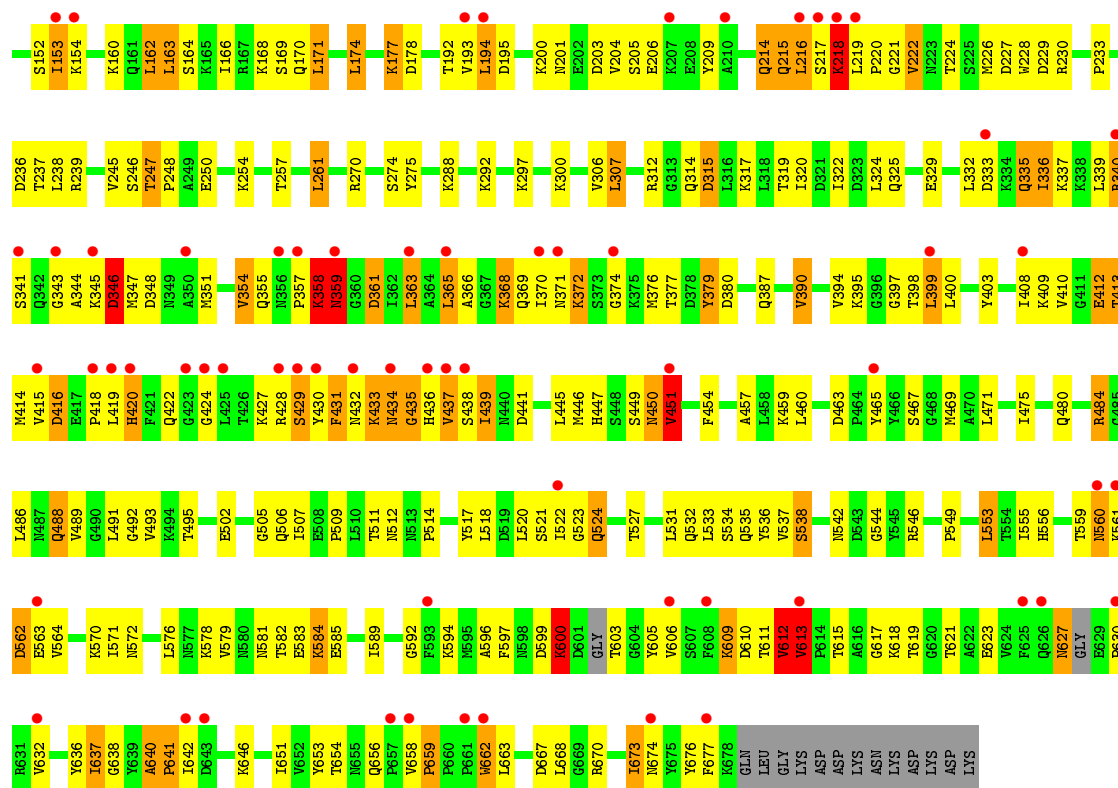
- Molecule 2 is CEFOTAXIME GROUP (three-letter code: CEF) (formula: $C_{16}H_{19}N_5O_7S_2$).



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



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	2.01 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.247 , 0.316 0.281 , 0.337	Depositor DCC
R_{free} test set	3797 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 67.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 75968 reflections (0.001%)	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 9.87% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	181	0
2	A	26	0	12	5	0
2	B	26	0	12	6	0
3	A	140	0	0	4	0
3	B	116	0	0	5	0
All	All	10198	0	10009	340	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 (340) 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:N19	2:A:701:CEF:C17	1.72	1.45
2:B:701:CEF:N19	2:B:701:CEF:C17	1.73	1.43
1:A:529:THR:HG22	1:A:532:GLN:H	1.27	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:LYS:H	1:A:600:LYS:HE3	1.35	0.89
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:N19	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:442:LYS:HE2	1:A:591:GLU:HB3	1.83	0.58
1:B:399:LEU:HD11	1:B:441:ASP:HB2	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:A:91:TYR:HB2	1:A:199:ILE:HD11	1.86	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:631:ARG:NH2	1:A:657:PRO:HB3	2.20	0.57
1:A:625:PHE:CD2	1:B:627:ASN:HA	2.40	0.57
1:B:91:TYR:CZ	1:B:93:ARG:HB2	2.41	0.56
1:B:659:PRO:HB3	2:B:701:CEF:HN81	1.71	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:N19	2.40	0.55
1:B:446:MET:HB3	1:B:600:LYS:CB	2.38	0.54
1:A:348:ASP:N	1:A:348:ASP:OD1	2.39	0.54
1:B:641:PRO:HD2	1:B:646:LYS:H	1.72	0.54
1:B:319:THR:HG22	1:B:553:LEU:HG	1.90	0.54
1:A:368:LYS:HE3	1:A:370:ILE:HG23	1.89	0.54
1:A:351:MET:HA	1:A:366:ALA:HB1	1.88	0.54
1:A:91:TYR:O	1:A:197:GLN:N	2.40	0.54
1:A:546:ARG:NH1	1:A:576:LEU:HD23	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:372:LYS:C	1:B:374:GLY:H	2.11	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:A:258:GLU:HB2	1:B:576:LEU:HA	1.91	0.53
2:A:701:CEF:N18	2:A:701:CEF:N19	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:B:615:THR:HG21	1:B:673:ILE:HD12	1.89	0.53
1:A:232:TYR:CD1	1:A:239:ARG:HD3	2.43	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: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:B:133:HIS:HB3	1:B:136:LYS:HB2	1.91	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:B:636:TYR:HB2	1:B:651:ILE:HB	1.91	0.51
1:A:434:ASN:N	1:A:434:ASN:OD1	2.42	0.51
1:B:465:TYR:CZ	1:B:467:SER:HA	2.46	0.51
1:B:325:GLN:HA	1:B:363:LEU:HD21	1.92	0.51
1:A:345:LYS:O	1:A:371:ASN:HB3	2.10	0.51
1:B:410:VAL:HG11	1:B:584:LYS:HG3	1.93	0.51
1:B:518:LEU:O	1:B:521:SER:OG	2.27	0.51
1:A:453:MET:HB2	1:A:522:ILE:HD13	1.93	0.51
1:A:352:MET:CE	1:A:672:VAL:HG11	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:LYS:HE2	1:A:344:ALA:O	2.11	0.50
2:B:701:CEF:N19	2:B:701:CEF:N18	2.47	0.50
1:A:339:LEU:HB2	1:A:342:GLN:H	1.76	0.50
1:A:371:ASN:HA	1:A:374:GLY:N	2.26	0.50
1:A:355:GLN:HG3	1:A:362:ILE:HD13	1.94	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:B:320:ILE:HD13	1:B:361:ASP:O	2.11	0.50
1:A:219:LEU:HB2	1:A:222:VAL:HG21	1.92	0.50
1:A:290:GLU:HB2	1:A:307:LEU:HB2	1.93	0.49
1:A:297:LYS:H	1:A:297:LYS:HE3	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:B:332:LEU:HD13	1:B:365:LEU:HD23	1.93	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:336:ILE:HD13	1:B:369:GLN:NE2	2.28	0.49
1:A:238:LEU:HD23	1:A:365:LEU:HG	1.93	0.49
1:B:162:LEU:HD22	1:B:166:ILE:HD11	1.95	0.49
1:A:273:LYS:CE	1:B:484:ARG:HH12	2.26	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:B:329:GLU:CD	1:B:365:LEU:HD13	2.33	0.48
1:A:514:PRO:O	1:A:517:TYR:HB3	2.12	0.48
1:B:562:ASP:N	1:B:562:ASP:OD1	2.46	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:446:MET:HE3	1:B:600:LYS:HB2	1.95	0.48
1:A:171:LEU:C	1:A:173:GLU:H	2.17	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:446:MET:HE2	1:B:600:LYS:HG3	1.94	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:A:631:ARG:HH21	1:A:657:PRO:HB3	1.79	0.48
1:A:365:LEU:HD13	1:A:366:ALA:H	1.79	0.48
1:A:653:TYR:CE2	1:A:665:GLY:HA3	2.49	0.47
1:B:90:THR:O	1:B:222:VAL:HA	2.14	0.47
1:A:605:TYR:O	1:A:609:LYS:HD2	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:N	1:B:450:ASN:OD1	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:600:LYS:N	1:A:600:LYS:HE3	2.17	0.47
1:A:395:LYS:HG2	1:A:453:MET:HG3	1.97	0.47
1:B:247:THR:OG1	1:B:250:GLU:OE1	2.32	0.46
1:B:121:THR:O	1:B:124:ASP:HB2	2.15	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:175:SER:O	1:A:175:SER:OG	2.33	0.46
1:B:493:VAL:O	1:B:532:GLN:NE2	2.48	0.46
1:A:629:GLU:HA	1:A:630:PRO:HD3	1.79	0.46
1:A:590:GLN:HA	1:A:593:PHE:HB2	1.96	0.46
1:A:93:ARG:HB3	1:A:93:ARG:HE	1.61	0.46
1:B:618:LYS:HD3	1:B:619:THR:N	2.31	0.46
1:B:336:ILE:HD13	1:B:369:GLN:HE21	1.80	0.46
1:A:664:THR:HB	1:A:667:ASP:OD2	2.16	0.46
1:A:73:LEU:HD23	1:A:79:VAL:HA	1.97	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:A:65:GLU:O	1:A:288:LYS:HB2	2.16	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:B:358:LYS:NZ	1:B:359:ASN:HD21	2.14	0.45
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: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:B:346:ASP:OD1	1:B:371:ASN:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:ARG:O	1:A:673:ILE:HG22	2.16	0.45
1:A:57:ASN:HB3	1:A:58:ASP:H	1.59	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:HG2	1:A:144:GLU:H	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:B:524:GLN:HB2	1:B:524:GLN:HE21	1.59	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
2:A:701:CEF:O17	2:A:701:CEF:N10	2.50	0.45
1:A:369:GLN:HB2	1:A:369:GLN:HE21	1.54	0.45
1:A:49:SER:OG	1:A:65:GLU:OE2	2.22	0.45
1:A:611:THR:O	1:A:613:VAL:N	2.49	0.45
1:B:618:LYS:HD3	1:B:619:THR:H	1.82	0.44
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:325:GLN:O	1:B:329:GLU:HG3	2.16	0.44
1:A:522:ILE:HD12	1:A:522:ILE:HA	1.82	0.44
1:A:154:LYS:HD2	1:A:156:ASP:HB2	1.99	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:B:673:ILE:HG22	1:B:677:PHE:CE1	2.53	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:314:GLN:HB3	1:B:556:HIS:O	2.17	0.44
1:B:74:ASP:HB2	1:B:320:ILE:O	2.17	0.44
1:A:498:ASP:OD1	1:A:498:ASP:N	2.50	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:B:86:LYS:HB3	1:B:86:LYS:HE2	1.70	0.43
1:A:548:GLN:HB2	1:A:576:LEU:CD1	2.48	0.43
1:B:489:VAL:O	1:B:536:TYR:HA	2.18	0.43
1:B:512:ASN:OD1	1:B:512:ASN:N	2.52	0.43
1:B:431:PHE:CD1	1:B:434:ASN:HB2	2.53	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:A:618:LYS:HD2	1:A:619:THR:H	1.82	0.43
1:A:372:LYS:HA	1:A:372:LYS:HD2	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:O4B	2.28	0.43
1:B:193:VAL:HG12	1:B:194:LEU:HD22	2.00	0.43
1:A:369:GLN:HG3	1:A:376:MET:HG2	2.00	0.43
1:B:397:GLY:HA2	1:B:400:LEU:HD12	1.99	0.43
1:A:260:TYR:HE1	1:A:281:GLU:HG2	1.83	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: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: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:B:582:THR:OG1	1:B:583:GLU:N	2.51	0.42
1:A:405:ASN:O	1:A:407:ALA:N	2.51	0.42
1:A:621:THR:HB	2:A:701:CEF:O12	2.18	0.42
1:B:171:LEU:HA	1:B:171:LEU:HD12	1.85	0.42
1:B:347:MET:CE	1:B:653:TYR:HB3	2.49	0.42
1:B:537:VAL:HB	1:B:637:ILE:HD12	1.99	0.42
1:B:420:HIS:HB3	1:B:427:LYS:HB3	2.01	0.42
1:A:287:LYS:HB2	1:A:311:ALA:HB3	2.02	0.42
1:B:395:LYS:HA	1:B:398:THR:OG1	2.19	0.42
1:A:375:LYS:HA	1:A:375:LYS:HD2	1.90	0.42
1:B:416:ASP:HB3	1:B:451:VAL:HG11	2.02	0.42
1:B:636:TYR:O	1:B:651:ILE:N	2.49	0.42
1:B:434:ASN:O	1:B:436:HIS:N	2.53	0.42
1:B:439:ILE:HG13	1:B:439:ILE:H	1.65	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:336:ILE:HG13	1:A:369:GLN:CD	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:GLN:HA	1:A:338:LYS:HB2	2.02	0.42
1:A:87:MET:HG3	1:A:209:TYR:CD1	2.55	0.42
1:B:247:THR:HG1	1:B:250:GLU:HG2	1.84	0.42
1:B:358:LYS:HG3	1:B:359:ASN:H	1.85	0.42
1:B:347:MET:HE3	1:B:656:GLN:HG2	2.02	0.42
1:B:400:LEU:HB3	1:B:581:ASN:OD1	2.19	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:A:546:ARG:CZ	1:A:576:LEU:HD23	2.50	0.42
1:A:347:MET:CE	1:A:656:GLN:HE21	2.33	0.42
1:A:367:GLY:HA2	1:A:379:TYR:N	2.19	0.41
1:B:337:LYS:HA	1:B:337:LYS:HD3	2.00	0.41
1:A:647:LEU:HD23	1:A:648:ALA:N	2.35	0.41
1:A:261:LEU:HD12	1:A:261:LEU:HA	1.83	0.41
1:B:93:ARG:HG2	1:B:221:GLY:CA	2.50	0.41
1:B:92:THR:HG23	1:B:195:ASP:C	2.40	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:522:ILE:HD13	2:B:701:CEF:H181	2.01	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:370:ILE:O	1:A:373:SER:OG	2.37	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:A:171:LEU:HD12	1:A:174:LEU:HD22	2.02	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:612:VAL:HG21	1:B:674:ASN:HA	2.02	0.41
1:B:98:THR:C	1:B:100:SER:H	2.24	0.41
1:B:95:ARG:H	1:B:193:VAL:CG1	2.33	0.41
1:A:427:LYS:NZ	1:A:432:ASN:O	2.50	0.41
1:A:238:LEU:HA	1:A:238:LEU:HD23	1.86	0.41
1:A:173:GLU:C	1:A:175:SER:N	2.74	0.41
1:B:527:THR:HG21	3:B:895:HOH:O	2.21	0.41
1:B:337:LYS:HZ3	1:B:340:ARG:HH11	1.68	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:B:329:GLU:CG	1:B:365:LEU:HD13	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:LYS:HD3	1:B:201:ASN:ND2	2.36	0.40
1:A:317:LYS:HD3	1:A:556:HIS:NE2	2.36	0.40
1:B:174:LEU:HD12	1:B:174:LEU:HA	1.79	0.40
1:A:413:THR:HG23	1:A:440:ASN:HB3	2.03	0.40
1:A:337:LYS:HD3	1:A:339:LEU:HD11	2.03	0.40
1:B:544:GLY:O	1:B:578:LYS:HA	2.22	0.40
1:B:535:GLN:HE21	1:B:549:PRO:HD3	1.87	0.40
1:B:163:LEU:HD12	1:B:163:LEU:HA	1.94	0.40
1:A:605:TYR:CD1	1:A:609:LYS:HA	2.56	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%)	9	10
1	B	627/646 (97%)	544 (87%)	60 (10%)	23 (4%)	4	3
All	All	1254/1292 (97%)	1098 (88%)	120 (10%)	36 (3%)	6	5

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

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Mol	Chain	Res	Type
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%)	1	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

Some 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 carbohydrates 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	18,27,31	7.50	13 (72%)	16,37,42	6.59	11 (68%)
2	CEF	B	701	1	18,27,31	7.69	13 (72%)	16,37,42	5.70	12 (75%)

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	1/1/7/11	0/10/38/43	0/1/2/2
2	CEF	B	701	1	1/1/7/11	0/10/38/43	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	C14-C13	-10.42	1.30	1.48
2	B	701	CEF	C14-C13	-9.85	1.31	1.48
2	B	701	CEF	C2-S1	-9.20	1.60	1.82
2	A	701	CEF	C2-S1	-8.97	1.61	1.82
2	B	701	CEF	C4'-C4	-7.55	1.39	1.52
2	A	701	CEF	C4'-C4	-7.18	1.39	1.52
2	A	701	CEF	O17-N16	-4.26	1.31	1.40
2	B	701	CEF	O17-N16	-3.64	1.33	1.40
2	B	701	CEF	C2-C3	-3.17	1.47	1.51
2	A	701	CEF	C2-C3	-3.07	1.47	1.51
2	A	701	CEF	C17-N18	-2.90	1.26	1.35
2	B	701	CEF	C17-N18	-2.87	1.26	1.35
2	A	701	CEF	C3'-C3	-2.36	1.47	1.51
2	B	701	CEF	C3'-C3	-2.32	1.47	1.51
2	A	701	CEF	C15-S16	-2.16	1.67	1.70
2	B	701	CEF	C13-C11	2.50	1.55	1.50
2	B	701	CEF	C14-N19	4.76	1.52	1.37
2	A	701	CEF	C14-N19	4.93	1.52	1.37
2	A	701	CEF	C11-N10	5.79	1.46	1.34
2	B	701	CEF	C11-N10	5.95	1.46	1.34
2	B	701	CEF	C4-N5	7.69	1.60	1.34
2	A	701	CEF	C4-N5	7.70	1.60	1.34
2	A	701	CEF	C13-N16	11.19	1.48	1.29
2	B	701	CEF	C13-N16	12.09	1.50	1.29
2	A	701	CEF	C3-C4	21.83	1.62	1.34
2	B	701	CEF	C3-C4	22.58	1.63	1.34

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	CEF	C3'-C3-C4	-12.21	107.85	123.48
2	A	701	CEF	C14-C15-S16	-11.91	97.16	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	CEF	C3'-C3-C4	-11.87	108.28	123.48
2	A	701	CEF	N18-C17-N19	-10.59	109.06	122.92
2	B	701	CEF	N18-C17-N19	-9.51	110.47	122.92
2	B	701	CEF	C3-C2-S1	-6.64	109.00	117.17
2	A	701	CEF	C2-C3-C4	-5.98	113.45	123.50
2	B	701	CEF	C2-C3-C4	-5.38	114.45	123.50
2	B	701	CEF	C14-C15-S16	-4.75	105.96	111.79
2	A	701	CEF	C7-N10-C11	-4.62	114.40	122.01
2	A	701	CEF	C3-C2-S1	-4.34	111.83	117.17
2	B	701	CEF	C3'-C3-C2	-4.06	106.99	113.22
2	A	701	CEF	C11-C13-N16	-3.71	103.90	121.44
2	B	701	CEF	C11-C13-N16	-3.33	105.73	121.44
2	A	701	CEF	O12-C11-N10	-3.07	117.50	123.01
2	B	701	CEF	O9-C8-C7	-2.18	119.05	125.74
2	B	701	CEF	O12-C11-N10	-2.10	119.24	123.01
2	B	701	CEF	C13-C11-N10	2.27	118.27	114.41
2	A	701	CEF	C13-C11-N10	5.03	122.93	114.41
2	B	701	CEF	C2-S1-C6	6.21	106.34	94.36
2	A	701	CEF	C18-O17-N16	8.25	117.92	108.47
2	A	701	CEF	C2-S1-C6	9.57	112.81	94.36
2	B	701	CEF	C18-O17-N16	10.17	120.11	108.47

All (2) chirality outliers are listed below:

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

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	CEF	5	0
2	B	701	CEF	6	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	631/646 (97%)	0.45	37 (5%) 26 26	27, 61, 117, 146	0
1	B	631/646 (97%)	0.69	75 (11%) 6 6	29, 70, 124, 161	0
All	All	1262/1292 (97%)	0.57	112 (8%) 12 12	27, 66, 121, 161	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	217	SER	11.7
1	B	425	LEU	10.5
1	A	174	LEU	9.7
1	B	218	LYS	9.4
1	A	562	ASP	7.5
1	B	432	ASN	6.8
1	B	424	GLY	6.7
1	B	658	VAL	5.9
1	B	216	LEU	5.8
1	B	436	HIS	5.6
1	B	94	GLY	5.5
1	A	340	ARG	5.4
1	B	423	GLY	5.3
1	B	194	LEU	5.2
1	B	429	SER	5.2
1	B	418	PRO	5.0
1	B	657	PRO	5.0
1	B	98	THR	4.9
1	A	661	PRO	4.8
1	B	625	PHE	4.8
1	A	435	GLY	4.7
1	B	661	PRO	4.7
1	B	111	LYS	4.6
1	B	437	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	154	LYS	4.5
1	A	658	VAL	4.4
1	B	438	SER	4.3
1	B	47	GLN	4.3
1	B	374	GLY	4.3
1	A	343	GLY	4.2
1	B	113	ILE	4.1
1	B	451	VAL	4.1
1	B	343	GLY	4.1
1	A	439	ILE	4.0
1	B	643	ASP	3.9
1	B	561	LYS	3.8
1	B	428	ARG	3.7
1	B	96	LYS	3.6
1	B	674	ASN	3.6
1	A	47	GLN	3.5
1	A	657	PRO	3.5
1	A	341	SER	3.5
1	B	93	ARG	3.4
1	B	465	TYR	3.4
1	B	677	PHE	3.2
1	B	626	GLN	3.2
1	A	451	VAL	3.1
1	B	363	LEU	3.1
1	B	193	VAL	3.1
1	B	345	LYS	3.1
1	B	434	ASN	3.1
1	B	109	LEU	3.1
1	A	95	ARG	3.0
1	B	593	PHE	3.0
1	A	433	LYS	2.9
1	A	415	VAL	2.9
1	A	434	ASN	2.8
1	B	630	PRO	2.8
1	A	432	ASN	2.8
1	A	660	PRO	2.8
1	B	207	LYS	2.8
1	A	438	SER	2.7
1	A	59	GLU	2.7
1	B	522	ILE	2.7
1	B	219	LEU	2.7
1	B	153	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	95	ARG	2.6
1	B	365	LEU	2.6
1	B	560	ASN	2.5
1	A	663	LEU	2.5
1	A	154	LYS	2.5
1	A	158	TYR	2.5
1	A	598	ASN	2.5
1	A	675	TYR	2.4
1	A	561	LYS	2.4
1	B	370	ILE	2.4
1	B	340	ARG	2.3
1	B	662	TRP	2.3
1	A	564	VAL	2.3
1	A	339	LEU	2.3
1	B	341	SER	2.3
1	B	359	ASN	2.3
1	B	112	LEU	2.3
1	A	431	PHE	2.3
1	B	420	HIS	2.3
1	B	430	TYR	2.3
1	B	632	VAL	2.3
1	B	333	ASP	2.2
1	A	156	ASP	2.2
1	B	563	GLU	2.2
1	B	100	SER	2.2
1	B	608	PHE	2.2
1	B	148	LEU	2.2
1	B	613	VAL	2.2
1	A	151	GLY	2.2
1	B	408	ILE	2.2
1	B	357	PRO	2.2
1	B	210	ALA	2.1
1	A	48	GLY	2.1
1	B	371	ASN	2.1
1	A	168	LYS	2.1
1	B	642	ILE	2.1
1	A	560	ASN	2.1
1	B	356	ASN	2.1
1	B	399	LEU	2.1
1	A	173	GLU	2.1
1	A	149	ALA	2.0
1	B	350	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	415	VAL	2.0
1	B	606	VAL	2.0
1	A	428	ARG	2.0
1	B	419	LEU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	CEF	A	701	26/30	0.80	0.22	0.10	68,89,111,143	0
2	CEF	B	701	26/30	0.85	0.20	-0.49	77,99,154,157	0

6.5 Other polymers [i](#)

There are no such residues in this entry.