Full wwPDB X-ray Structure Validation Report ⓘ

Nov 24, 2021 – 06:13 pm GMT

PDB ID	:	6Z8T
Title	:	Copper transporter OprC
Authors	:	Bhamidimarri, S.P.; van den Berg, B.
Deposited on	:	2020-06-02
Resolution	:	2.86 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 following versions of software and data (see references ⓘ) were used in the production of this report:

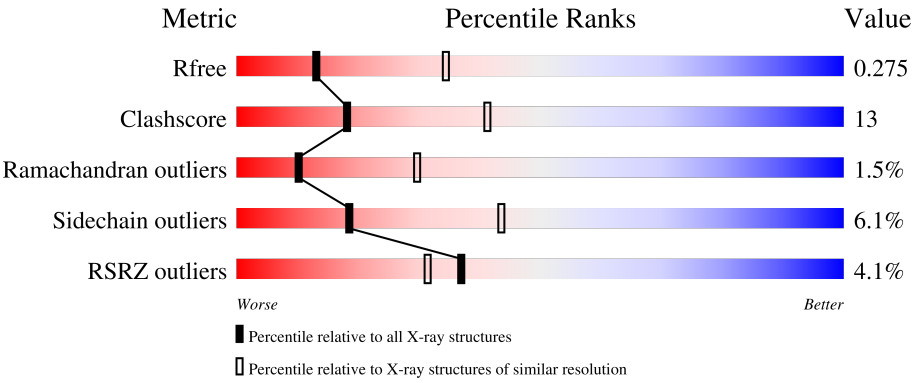
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.86 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	723	4% 63% 25% · 10%
1	B	723	3% 60% 26% · 11%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10078 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 Putative copper transport outer membrane porin OprC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	650	Total	C	N	O	S	4	1	0
			5048	3170	890	972	16			
1	B	646	Total	C	N	O	S	4	2	0
			5025	3158	886	965	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	323	ALA	HIS	engineered mutation	UNP G3XD89
B	323	ALA	HIS	engineered mutation	UNP G3XD89

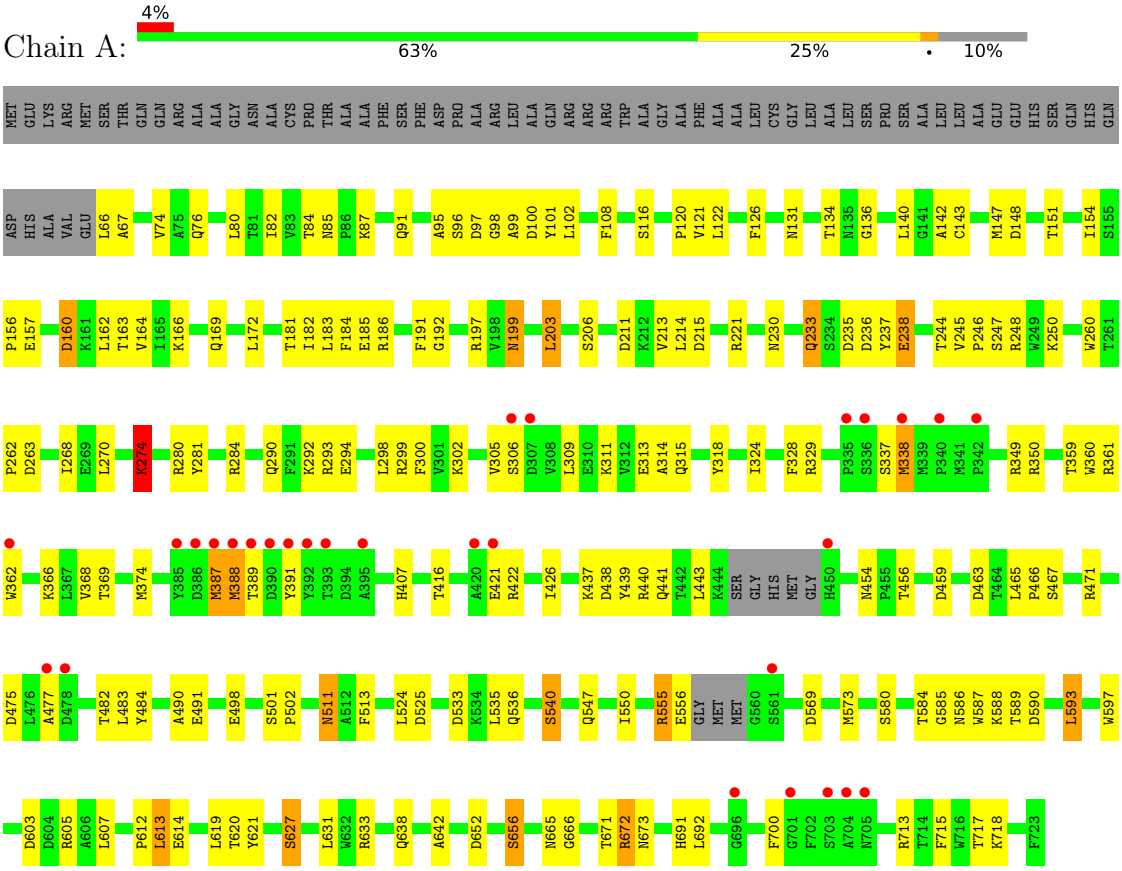
- Molecule 2 is SILVER ION (three-letter code: AG) (formula: Ag).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ag	0	0
			2	2		
2	B	3	Total	Ag	0	0
			3	3		

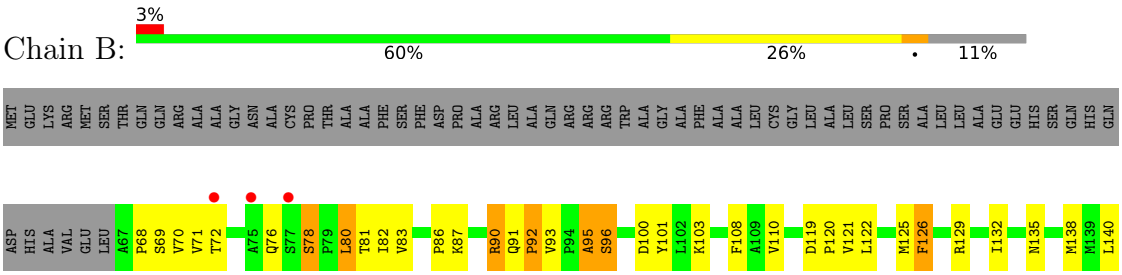
3 Residue-property plots (i)

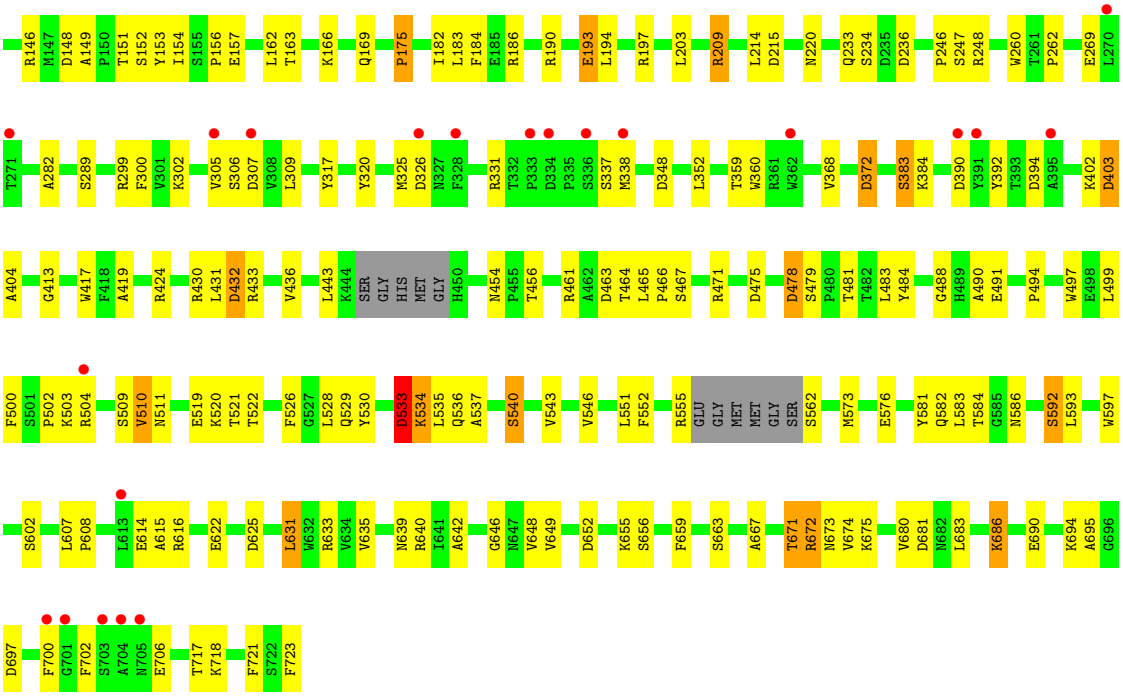
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Putative copper transport outer membrane porin OprC



• Molecule 1: Putative copper transport outer membrane porin OprC




R146 M147 D148 A149 P150 T151 S152 Y153 I154 S155 P156 E157 L162 T163 K166 Q169 P175 I182 L183 F184 E185 R186 R190 E193 L194 R197 L203 R209 L214 D215 N220 Q233 S234 D235 D236 P246 S247 R248 W260 T261 P262 E269 L270
T271 A282 S289 R299 F300 V301 K302 V305 S306 D307 V308 L309 Y317 Y320 M325 D326 N327 F328 R331 T332 P333 D334 P335 S336 S337 M338 D348 L352 T359 W360 R361 W362 V368 D372 S383 K384 D390 Y391 Y392 T393 D394 A395 K402 D403
A404 G413 W417 F418 A419 R424 R430 L431 D432 R433 V436 L443 K444 SER GLY HIS MET GLY H450 N454 P455 T456 R461 A462 D463 T464 L465 P466 S467 R471 D475 D478 S479 P480 T481 T482 L483 Y484 G488 H489 A490 E491 P494 W497 E498 L499
F500 S501 P502 K503 R504 S509 V510 N511 E519 K520 T521 T522 F526 G527 L528 Q529 Y530 D533 K534 L535 Q536 A537 S540 V543 V546 L551 F552 R555 GLU GLY MET MET GLY SER S562 M573 E576 Y581 Q582 L583 T584 G585 N586 S592 L593 W597
S602 L607 P608 L613 E614 A615 R616 E622 D625 L631 W632 R633 V634 V635 N639 R640 I641 A642 G646 N647 V648 V649 D652 K655 S656 F659 S663 A667 T671 R672 N673 V674 K675 V680 D681 N682 L683 K686 E690 K694 A695 G696
D697 F700 G701 F702 S703 A704 N705 E706 T717 K718 F721 S722 F723

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	155.52Å 196.45Å 165.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.41 – 2.86 70.41 – 2.86	Depositor EDS
% Data completeness (in resolution range)	91.2 (70.41-2.86) 96.0 (70.41-2.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.207 , 0.272 0.211 , 0.275	Depositor DCC
R_{free} test set	2808 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	69.7	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	10078	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AG

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	0.49	0/5175	0.70	4/7016 (0.1%)
1	B	0.47	0/5155	0.68	2/6990 (0.0%)
All	All	0.48	0/10330	0.69	6/14006 (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	B	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	274	LYS	CD-CE-NZ	-9.29	90.33	111.70
1	A	274	LYS	CB-CG-CD	-7.94	90.95	111.60
1	B	331	ARG	C-N-CA	-6.08	106.50	121.70
1	A	274	LYS	CB-CA-C	-6.03	98.35	110.40
1	B	80	LEU	CA-CB-CG	5.81	128.66	115.30
1	A	713	ARG	NE-CZ-NH2	-5.67	117.47	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	602	SER	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5048	0	4832	119	1
1	B	5025	0	4816	143	1
2	A	2	0	0	1	0
2	B	3	0	0	0	0
All	All	10078	0	9648	260	1

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 13.

All (260) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:GLN:NE2	1:B:663:SER:HB3	1.78	0.96
1:A:421:GLU:HG3	1:A:422:ARG:HG3	1.50	0.93
1:B:72:THR:HB	1:B:631:LEU:HD13	1.62	0.81
1:A:359:THR:HB	1:A:368:VAL:HG12	1.61	0.80
1:B:503:LYS:HE2	1:B:503:LYS:HA	1.63	0.79
1:A:456:THR:HG21	1:A:513:PHE:CD2	2.19	0.78
1:B:236:ASP:HA	1:B:247:SER:HB3	1.67	0.77
1:B:91:GLN:NE2	1:B:663:SER:CB	2.49	0.76
1:B:521:THR:HG22	1:B:546:VAL:HG22	1.67	0.75
1:A:498:GLU:HG2	1:A:550:ILE:HG21	1.69	0.75
1:B:91:GLN:HE22	1:B:663:SER:CB	2.00	0.74
1:B:135:ASN:HD21	1:B:186:ARG:HB2	1.52	0.74
1:A:163:THR:HG23	1:A:183:LEU:HB2	1.70	0.74
1:B:479:SER:HB2	1:B:481:THR:HG22	1.69	0.73
1:A:233:GLN:HB3	1:A:250:LYS:HG3	1.69	0.73
1:B:91:GLN:HE22	1:B:663:SER:HB3	1.51	0.73
1:B:533:ASP:O	1:B:535:LEU:N	2.21	0.72
1:B:151:THR:HA	1:B:154:ILE:HD12	1.70	0.71
1:A:206:SER:HB2	1:A:715:PHE:H	1.57	0.70
1:A:555:ARG:HH11	1:A:556:GLU:H	1.40	0.69
1:A:131:ASN:HB2	1:A:181:THR:HG22	1.75	0.69
1:B:260:TRP:CE2	1:B:262:PRO:HG3	2.29	0.68
1:B:203:LEU:HB2	1:B:718:LYS:HG3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ILE:HD11	1:B:166:LYS:HE3	1.74	0.68
1:A:203:LEU:HB3	1:A:211:ASP:HB2	1.77	0.67
1:B:149:ALA:O	1:B:152:SER:HB3	1.94	0.67
1:B:543:VAL:HG12	1:B:573:MET:HB3	1.77	0.67
1:A:389:THR:HG23	1:A:391:TYR:H	1.59	0.67
1:B:616:ARG:HE	1:B:633:ARG:HD2	1.59	0.67
1:B:132:ILE:CD1	1:B:182:ILE:HD13	2.25	0.67
1:B:132:ILE:HD11	1:B:182:ILE:HD13	1.77	0.66
1:A:274:LYS:HD2	1:A:274:LYS:N	2.09	0.66
1:B:80:LEU:HD21	1:B:169:GLN:HG3	1.77	0.65
1:A:439:TYR:O	1:A:441:GLN:NE2	2.29	0.65
1:A:95:ALA:HB1	1:A:116:SER:HB2	1.79	0.65
1:A:143:CYS:HG	2:A:801:AG:AG	1.66	0.64
1:B:91:GLN:HE21	1:B:663:SER:HB3	1.60	0.64
1:B:300:PHE:HE1	1:B:302:LYS:HB2	1.63	0.64
1:B:359:THR:HG23	1:B:368:VAL:HG22	1.79	0.64
1:B:91:GLN:O	1:B:93:VAL:N	2.31	0.64
1:A:235:ASP:HA	1:A:248:ARG:HG3	1.80	0.63
1:B:91:GLN:HB3	1:B:92:PRO:HD3	1.80	0.63
1:B:138:MET:HG3	1:B:317:TYR:OH	1.99	0.63
1:B:78:SER:HA	1:B:529:GLN:HE22	1.64	0.62
1:A:612:PRO:HB3	1:A:638:GLN:HB2	1.80	0.62
1:B:608:PRO:HB3	1:B:642:ALA:HB3	1.80	0.61
1:B:484:TYR:OH	1:B:540:SER:HB2	2.01	0.61
1:A:238:GLU:HB3	1:A:244:THR:HA	1.82	0.61
1:A:142:ALA:HB2	1:A:349:ARG:HB2	1.83	0.61
1:A:318:TYR:OH	1:A:350:ARG:NH1	2.34	0.61
1:A:97:ASP:OD1	1:A:98:GLY:N	2.34	0.60
1:A:293:ARG:O	1:A:294:GLU:HB2	2.00	0.60
1:B:132:ILE:HD13	1:B:182:ILE:HB	1.83	0.60
1:B:534:LYS:HB3	1:B:581:TYR:CE1	2.37	0.59
1:B:121:VAL:HG22	1:B:126:PHE:HB2	1.85	0.59
1:A:162:LEU:HD12	1:A:163:THR:H	1.68	0.59
1:B:132:ILE:CD1	1:B:182:ILE:CD1	2.80	0.58
1:A:306:SER:HB3	1:A:309:LEU:HB3	1.85	0.58
1:A:466:PRO:HG2	1:B:466:PRO:HG2	1.85	0.58
1:B:214:LEU:HD12	1:B:215:ASP:H	1.68	0.58
1:B:71:VAL:HB	1:B:90:ARG:HG3	1.86	0.58
1:A:466:PRO:O	1:A:491:GLU:HG3	2.02	0.57
1:A:416:THR:HG22	1:A:426:ILE:HG23	1.87	0.57
1:A:416:THR:HB	1:A:426:ILE:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ARG:NH2	1:B:215:ASP:OD1	2.37	0.56
1:A:456:THR:O	1:A:456:THR:HG22	2.06	0.56
1:A:260:TRP:CE3	1:A:268:ILE:HD13	2.41	0.56
1:B:672:ARG:HG3	1:B:673:ASN:ND2	2.21	0.56
1:A:584:THR:HG22	1:A:587:TRP:HB2	1.88	0.55
1:A:589:THR:HB	1:A:619:LEU:HD12	1.87	0.55
1:A:638:GLN:HB3	1:A:656:SER:HB3	1.88	0.55
1:B:597:TRP:HE1	1:B:640:ARG:NH1	2.05	0.55
1:B:483:LEU:HD12	1:B:528:LEU:HB3	1.87	0.55
1:A:656:SER:HB2	1:A:691:HIS:HB2	1.88	0.55
1:B:193:GLU:CD	1:B:194:LEU:H	2.10	0.55
1:B:465:LEU:HB3	1:B:491:GLU:HB2	1.88	0.55
1:A:82:ILE:HB	1:A:164:VAL:CG2	2.37	0.55
1:A:484:TYR:OH	1:A:540:SER:HB2	2.07	0.55
1:B:368:VAL:O	1:B:413:GLY:HA2	2.07	0.54
1:A:456:THR:HG22	1:A:459:ASP:HB2	1.89	0.54
1:B:132:ILE:HD13	1:B:182:ILE:CD1	2.38	0.54
1:B:639:ASN:HB3	1:B:655:LYS:HD3	1.89	0.54
1:A:91:GLN:OE1	1:A:665:ASN:HB3	2.07	0.54
1:B:246:PRO:HG3	1:B:700:PHE:CD2	2.43	0.54
1:A:120:PRO:HG3	1:A:151:THR:HG21	1.89	0.54
1:A:337:SER:OG	1:A:338:MET:N	2.41	0.54
1:B:463:ASP:OD1	1:B:464:THR:N	2.42	0.53
1:B:132:ILE:HD11	1:B:182:ILE:CD1	2.39	0.53
1:A:422:ARG:HB3	1:A:475:ASP:HB2	1.89	0.53
1:A:555:ARG:NH1	1:A:556:GLU:H	2.04	0.53
1:B:135:ASN:ND2	1:B:186:ARG:HB2	2.23	0.53
1:B:337:SER:OG	1:B:338:MET:N	2.42	0.52
1:B:120:PRO:HG3	1:B:151:THR:HG21	1.90	0.52
1:A:361:ARG:NH2	1:A:366:LYS:HD2	2.25	0.52
1:A:437:LYS:HG2	1:A:439:TYR:CE2	2.45	0.52
1:A:213:VAL:HG22	1:A:230:ASN:HB2	1.92	0.52
1:B:163:THR:HB	1:B:183:LEU:HB2	1.91	0.52
1:A:642:ALA:O	1:A:652:ASP:HB2	2.10	0.51
1:A:438:ASP:OD1	1:A:440:ARG:HD3	2.10	0.51
1:A:603:ASP:HB2	1:A:605:ARG:HG3	1.92	0.51
1:B:306:SER:OG	1:B:307:ASP:N	2.43	0.51
1:B:534:LYS:HB3	1:B:581:TYR:HE1	1.73	0.51
1:B:103:LYS:HE2	1:B:110:VAL:HG21	1.93	0.51
1:A:192:GLY:O	1:A:221:ARG:HB3	2.11	0.51
1:B:502:PRO:HG3	1:B:552:PHE:CZ	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:GLN:HB3	1:B:471:ARG:NH1	2.26	0.51
1:B:467:SER:HB3	1:B:490:ALA:HA	1.92	0.51
1:A:290:GLN:HB3	1:A:324:ILE:HD12	1.93	0.51
1:A:260:TRP:CE2	1:A:262:PRO:HG3	2.45	0.50
1:B:584:THR:HG22	1:B:586:ASN:H	1.76	0.50
1:B:697:ASP:O	1:B:702:PHE:HB2	2.11	0.50
1:A:387:MET:HG3	1:A:388:MET:N	2.26	0.50
1:B:535:LEU:HD11	1:B:537:ALA:HB2	1.94	0.50
1:B:702:PHE:HD1	1:B:706:GLU:HB3	1.77	0.50
1:B:78:SER:CA	1:B:529:GLN:HE22	2.24	0.50
1:B:491:GLU:OE2	1:B:520:LYS:HD3	2.12	0.50
1:A:290:GLN:CD	1:A:292:LYS:HG3	2.32	0.49
1:B:71:VAL:HB	1:B:90:ARG:HA	1.95	0.49
1:A:584:THR:HG23	1:A:587:TRP:H	1.77	0.49
1:B:404:ALA:HB2	1:B:500:PHE:CZ	2.47	0.49
1:B:148:ASP:HB2	1:B:153:TYR:CE2	2.48	0.49
1:B:125:MET:HB3	1:B:129:ARG:HD3	1.94	0.49
1:A:328:PHE:CE1	1:A:329:ARG:HG3	2.48	0.48
1:A:99:ALA:HA	1:A:102:LEU:HD12	1.94	0.48
1:A:465:LEU:HB3	1:A:491:GLU:HB2	1.95	0.48
1:A:108:PHE:CE1	1:A:122:LEU:HB2	2.47	0.48
1:B:76:GLN:NE2	1:B:529:GLN:OE1	2.45	0.48
1:B:129:ARG:NH2	1:B:519:GLU:OE1	2.46	0.48
1:B:383:SER:OG	1:B:384:LYS:N	2.47	0.48
1:A:584:THR:OG1	1:A:585:GLY:N	2.47	0.48
1:B:479:SER:HB2	1:B:481:THR:CG2	2.43	0.48
1:A:467:SER:OG	1:A:490:ALA:HA	2.14	0.48
1:B:509:SER:O	1:B:510:VAL:HG22	2.13	0.48
1:B:694:LYS:HG3	1:B:695:ALA:N	2.29	0.48
1:A:246:PRO:HB3	1:A:280:ARG:HD2	1.95	0.48
1:A:300:PHE:HB3	1:A:314:ALA:HB3	1.95	0.48
1:A:588:LYS:HG2	1:A:589:THR:N	2.28	0.48
1:B:430:ARG:NH2	1:B:432:ASP:OD1	2.30	0.48
1:A:580:SER:HA	1:A:590:ASP:HB3	1.96	0.48
1:B:101:TYR:CD1	1:B:156:PRO:HG2	2.48	0.47
1:A:236:ASP:OD1	1:A:248:ARG:N	2.47	0.47
1:A:237:TYR:CZ	1:A:245:VAL:HG11	2.49	0.47
1:B:443:LEU:HD12	1:B:454:ASN:HA	1.96	0.47
1:B:175:PRO:HB3	1:B:432:ASP:OD1	2.15	0.47
1:A:475:ASP:OD1	1:A:482:THR:HG23	2.15	0.47
1:A:456:THR:OG1	1:A:511:ASN:ND2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:MET:HG2	1:A:597:TRP:CE3	2.50	0.46
1:B:162:LEU:HG	1:B:184:PHE:CE1	2.51	0.46
1:B:220:ASN:OD1	1:B:220:ASN:N	2.46	0.46
1:B:71:VAL:O	1:B:91:GLN:N	2.45	0.46
1:B:649:VAL:O	1:B:694:LYS:HE3	2.15	0.46
1:B:672:ARG:HG3	1:B:673:ASN:CG	2.35	0.46
1:B:417:TRP:CE2	1:B:419:ALA:HB2	2.50	0.46
1:B:494:PRO:HB2	1:B:499:LEU:HG	1.96	0.46
1:A:671:THR:HG23	1:A:673:ASN:H	1.81	0.46
1:A:164:VAL:HG12	1:A:182:ILE:HG12	1.98	0.46
1:A:555:ARG:NH1	1:A:556:GLU:HB2	2.31	0.46
1:B:616:ARG:HE	1:B:633:ARG:CD	2.28	0.46
1:A:76:GLN:NE2	1:A:80:LEU:H	2.13	0.46
1:A:501:SER:N	1:A:502:PRO:HD2	2.31	0.46
1:B:140:LEU:HA	1:B:140:LEU:HD23	1.65	0.46
1:A:443:LEU:HG	1:A:454:ASN:HB2	1.97	0.45
1:A:121:VAL:HG21	1:A:692:LEU:HD13	1.97	0.45
1:A:203:LEU:HD12	1:A:718:LYS:HB2	1.98	0.45
1:B:108:PHE:CZ	1:B:122:LEU:HD13	2.52	0.45
1:B:674:VAL:HG22	1:B:721:PHE:HD1	1.81	0.45
1:A:87:LYS:HE3	1:A:157:GLU:O	2.16	0.45
1:B:68:PRO:HB2	1:B:667:ALA:HB1	1.99	0.45
1:B:671:THR:OG1	1:B:672:ARG:N	2.49	0.45
1:B:372:ASP:OD2	1:B:430:ARG:NH2	2.45	0.45
1:B:592:SER:O	1:B:615:ALA:HA	2.15	0.45
1:A:238:GLU:OE1	1:A:244:THR:HG22	2.16	0.45
1:A:246:PRO:HG2	1:A:700:PHE:CD2	2.51	0.45
1:B:80:LEU:HD12	1:B:166:LYS:HB2	1.98	0.45
1:A:162:LEU:HD12	1:A:163:THR:N	2.30	0.45
1:B:497:TRP:O	1:B:502:PRO:HD3	2.17	0.45
1:A:101:TYR:OH	1:A:157:GLU:HG2	2.17	0.45
1:B:305:VAL:HG23	1:B:309:LEU:HG	1.98	0.45
1:B:402:LYS:O	1:B:404:ALA:N	2.50	0.45
1:A:214:LEU:HD12	1:A:215:ASP:N	2.32	0.45
1:A:586:ASN:HB3	1:A:621:TYR:CE1	2.52	0.45
1:B:69:SER:O	1:B:70:VAL:HG23	2.16	0.45
1:B:607:LEU:HA	1:B:607:LEU:HD23	1.75	0.45
1:B:478:ASP:OD1	1:B:478:ASP:N	2.50	0.44
1:A:614:GLU:OE1	1:A:633:ARG:NH2	2.43	0.44
1:B:675:LYS:HE3	1:B:675:LYS:HB3	1.80	0.44
1:A:74:VAL:HG11	1:A:84:THR:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:GLU:HG3	1:A:186:ARG:N	2.33	0.44
1:B:535:LEU:HD12	1:B:536:GLN:N	2.32	0.44
1:B:309:LEU:HB2	1:B:360:TRP:CZ3	2.52	0.44
1:A:555:ARG:HH11	1:A:555:ARG:HG2	1.83	0.44
1:B:436:VAL:HG13	1:B:461:ARG:HG3	1.99	0.44
1:B:530:TYR:O	1:B:536:GLN:HA	2.17	0.44
1:B:320:TYR:CE1	1:B:348:ASP:HB2	2.53	0.44
1:B:671:THR:HG23	1:B:673:ASN:H	1.81	0.44
1:A:263:ASP:N	1:A:263:ASP:OD1	2.50	0.44
1:A:160:ASP:HB2	1:A:186:ARG:HA	1.99	0.44
1:A:302:LYS:O	1:A:311:LYS:HA	2.18	0.44
1:A:101:TYR:CD1	1:A:156:PRO:HG2	2.53	0.43
1:B:659:PHE:HB2	1:B:686:LYS:HD3	2.00	0.43
1:B:680:VAL:HG11	1:B:683:LEU:HD13	2.01	0.43
1:B:81:THR:O	1:B:82:ILE:HG13	2.18	0.43
1:B:633:ARG:NH2	1:B:690:GLU:OE2	2.51	0.43
1:A:524:LEU:HD12	1:A:525:ASP:H	1.83	0.43
1:A:588:LYS:HD2	1:A:620:THR:HB	2.01	0.43
1:B:671:THR:HG22	1:B:674:VAL:HB	2.00	0.43
1:B:100:ASP:HA	1:B:103:LYS:HE3	2.00	0.43
1:B:576:GLU:HA	1:B:593:LEU:O	2.18	0.43
1:A:270:LEU:HD12	1:A:298:LEU:HD13	2.01	0.43
1:B:616:ARG:NE	1:B:633:ARG:HD2	2.29	0.43
1:B:87:LYS:HD3	1:B:157:GLU:O	2.18	0.43
1:A:456:THR:HG21	1:A:513:PHE:HD2	1.73	0.43
1:A:309:LEU:HB2	1:A:360:TRP:CZ3	2.54	0.43
1:A:671:THR:OG1	1:A:672:ARG:N	2.51	0.43
1:A:80:LEU:HD22	1:A:166:LYS:O	2.19	0.42
1:A:535:LEU:HD12	1:A:536:GLN:N	2.33	0.42
1:B:305:VAL:CG2	1:B:309:LEU:HG	2.48	0.42
1:A:533:ASP:N	1:A:533:ASP:OD1	2.52	0.42
1:B:162:LEU:HD23	1:B:163:THR:N	2.33	0.42
1:A:169:GLN:HB3	1:A:471:ARG:NH1	2.34	0.42
1:A:299:ARG:HB3	1:A:315:GLN:HG3	2.02	0.42
1:B:269:GLU:OE1	1:B:299:ARG:NH2	2.52	0.42
1:B:392:TYR:CZ	1:B:394:ASP:HA	2.54	0.42
1:A:134:THR:C	1:A:136:GLY:H	2.23	0.42
1:B:246:PRO:HG2	1:B:282:ALA:CB	2.49	0.42
1:A:162:LEU:HD13	1:A:184:PHE:CE1	2.55	0.42
1:B:209:ARG:HD2	1:B:234:SER:HB2	2.02	0.42
1:A:147:MET:HB3	1:A:281:TYR:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:LYS:HE3	1:A:313:GLU:CD	2.41	0.41
1:B:81:THR:C	1:B:82:ILE:HG13	2.41	0.41
1:B:483:LEU:CD1	1:B:528:LEU:HB3	2.50	0.41
1:B:648:VAL:H	1:B:648:VAL:HG12	1.61	0.41
1:B:289:SER:OG	1:B:326:ASP:OD2	2.34	0.41
1:B:608:PRO:HG2	1:B:646:GLY:HA2	2.02	0.41
1:A:547:GLN:HE21	1:B:433:ARG:HH21	1.69	0.41
1:B:424:ARG:NH2	1:B:475:ASP:OD1	2.53	0.41
1:B:72:THR:HB	1:B:631:LEU:CD1	2.42	0.41
1:B:82:ILE:O	1:B:163:THR:HA	2.21	0.41
1:A:593:LEU:HD11	1:A:613:LEU:HD11	2.01	0.41
1:B:132:ILE:HD13	1:B:182:ILE:HD13	1.97	0.41
1:A:172:LEU:HD23	1:A:172:LEU:HA	1.81	0.41
1:B:100:ASP:OD1	1:B:100:ASP:N	2.54	0.41
1:B:83:VAL:HA	1:B:162:LEU:O	2.20	0.41
1:A:148:ASP:N	1:A:148:ASP:OD1	2.49	0.41
1:A:305:VAL:HB	1:A:309:LEU:HD23	2.02	0.41
1:A:607:LEU:HD23	1:A:607:LEU:HA	1.90	0.41
1:B:456:THR:HG22	1:B:511:ASN:ND2	2.36	0.41
1:B:488:GLY:O	1:B:522:THR:HA	2.21	0.41
1:B:593:LEU:HD12	1:B:593:LEU:HA	1.79	0.41
1:B:126:PHE:CD1	1:B:126:PHE:C	2.94	0.41
1:B:551:LEU:HD12	1:B:552:PHE:N	2.36	0.41
1:A:85:ASN:OD1	1:A:87:LYS:HB2	2.21	0.40
1:A:360:TRP:HE1	1:A:369:THR:CG2	2.34	0.40
1:B:614:GLU:HG3	1:B:635:VAL:HG22	2.04	0.40
1:A:197:ARG:NH1	1:A:199:ASN:OD1	2.52	0.40
1:A:91:GLN:O	1:A:91:GLN:NE2	2.54	0.40
1:A:154:ILE:O	1:A:156:PRO:HD3	2.21	0.40
1:B:95:ALA:O	1:B:96:SER:C	2.60	0.40
1:B:484:TYR:O	1:B:526:PHE:HA	2.21	0.40
1:A:627:SER:O	1:A:666:GLY:HA2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:GLU:OE2	1:B:671:THR:OG1[6_545]	1.98	0.22

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	645/723 (89%)	597 (93%)	43 (7%)	5 (1%)	19 46
1	B	642/723 (89%)	577 (90%)	51 (8%)	14 (2%)	6 21
All	All	1287/1446 (89%)	1174 (91%)	94 (7%)	19 (2%)	10 30

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	387	MET
1	A	477	ALA
1	B	510	VAL
1	B	534	LYS
1	B	671	THR
1	A	247	SER
1	B	96	SER
1	B	193	GLU
1	B	390	ASP
1	B	403	ASP
1	B	533	ASP
1	B	95	ALA
1	A	67	ALA
1	B	92	PRO
1	A	96	SER
1	B	86	PRO
1	B	672	ARG
1	B	78	SER
1	B	175	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	521/572 (91%)	490 (94%)	31 (6%)	19	45
1	B	519/572 (91%)	485 (93%)	34 (7%)	16	40
All	All	1040/1144 (91%)	975 (94%)	65 (6%)	18	42

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	LEU
1	A	100	ASP
1	A	126	PHE
1	A	140	LEU
1	A	160	ASP
1	A	191	PHE
1	A	199	ASN
1	A	203	LEU
1	A	233	GLN
1	A	238	GLU
1	A	274	LYS
1	A	284	ARG
1	A	338	MET
1	A	362	TRP
1	A	374	MET
1	A	388	MET
1	A	407	HIS
1	A	463	ASP
1	A	483	LEU
1	A	511	ASN
1	A	540	SER
1	A	555	ARG
1	A	569	ASP
1	A	593	LEU
1	A	613	LEU
1	A	627	SER
1	A	631	LEU
1	A	656	SER
1	A	672	ARG
1	A	717[A]	THR
1	A	717[B]	THR
1	B	90	ARG
1	B	119	ASP

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Mol	Chain	Res	Type
1	B	126	PHE
1	B	146	ARG
1	B	190	ARG
1	B	209	ARG
1	B	233	GLN
1	B	248	ARG
1	B	325	MET
1	B	352	LEU
1	B	372	ASP
1	B	383	SER
1	B	403	ASP
1	B	431	LEU
1	B	432	ASP
1	B	478	ASP
1	B	504	ARG
1	B	533	ASP
1	B	540	SER
1	B	555	ARG
1	B	562	SER
1	B	582	GLN
1	B	583	LEU
1	B	592	SER
1	B	622	GLU
1	B	625	ASP
1	B	631	LEU
1	B	652	ASP
1	B	656	SER
1	B	681	ASP
1	B	686	LYS
1	B	717[A]	THR
1	B	717[B]	THR
1	B	723	PHE

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

Mol	Chain	Res	Type
1	B	135	ASN
1	B	564	GLN
1	B	673	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	650/723 (89%)	0.41	29 (4%)	33	28	43, 62, 94, 157	0
1	B	646/723 (89%)	0.43	24 (3%)	41	36	46, 66, 105, 129	0
All	All	1296/1446 (89%)	0.42	53 (4%)	37	31	43, 64, 100, 157	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	388	MET	5.9
1	A	386	ASP	5.4
1	A	703	SER	5.3
1	A	387	MET	5.2
1	A	385	TYR	4.5
1	B	705	ASN	4.4
1	B	703	SER	3.9
1	A	390	ASP	3.9
1	A	389	THR	3.6
1	A	391	TYR	3.6
1	B	77	SER	3.6
1	B	307	ASP	3.5
1	B	338	MET	3.5
1	A	478	ASP	3.5
1	B	333	PRO	3.5
1	A	477	ALA	3.4
1	B	305	VAL	3.4
1	A	421	GLU	3.4
1	A	306	SER	3.3
1	A	393	THR	3.1
1	A	704	ALA	3.1
1	B	72	THR	3.1
1	B	701	GLY	3.1
1	B	390	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	705	ASN	3.0
1	B	362	TRP	3.0
1	B	75	ALA	2.8
1	B	391	TYR	2.8
1	A	338	MET	2.8
1	A	362	TRP	2.8
1	A	696	GLY	2.7
1	A	307	ASP	2.7
1	A	336	SER	2.6
1	B	334	ASP	2.6
1	B	704	ALA	2.4
1	B	336	SER	2.4
1	B	326	ASP	2.4
1	B	613	LEU	2.4
1	B	271	THR	2.4
1	B	700	PHE	2.4
1	B	270	LEU	2.3
1	A	342	PRO	2.3
1	B	395	ALA	2.3
1	A	392	TYR	2.2
1	A	450	HIS	2.2
1	A	335	PRO	2.2
1	A	420	ALA	2.1
1	A	701	GLY	2.1
1	B	504	ARG	2.1
1	A	340	PRO	2.1
1	A	561	SER	2.1
1	B	328	PHE	2.1
1	A	395	ALA	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	AG	B	802	1/1	0.92	0.13	149,149,149,149	0
2	AG	A	802	1/1	0.97	0.05	122,122,122,122	0
2	AG	A	801	1/1	0.97	0.11	88,88,88,88	0
2	AG	B	803	1/1	0.98	0.06	130,130,130,130	0
2	AG	B	801	1/1	0.99	0.09	94,94,94,94	0

6.5 Other polymers (i)

There are no such residues in this entry.