Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2020 – 10:13 PM BST

PDB ID	:	1R42
Title	:	Native Human Angiotensin Converting Enzyme-Related Carboxypeptidase (ACE2)
Authors	:	Towler, P.; Staker, B.; Prasad, S.G.; Menon, S.; Ryan, D.; Tang, J.; Parsons, T.; Fisher, M.; Williams, D.; Dales, N.A.; Patane, M.A.; Pantoliano, M.W.
Deposited on	:	2003-10-07
Resolution	:	2.20 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 (i) symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.20 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	Percentile Ranks	Value
Rfree		0.284
Clashscore		25
Ramachandran outliers		0.5%
Sidechain outliers		9.5%
RSRZ outliers		6.5%

Worse — *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
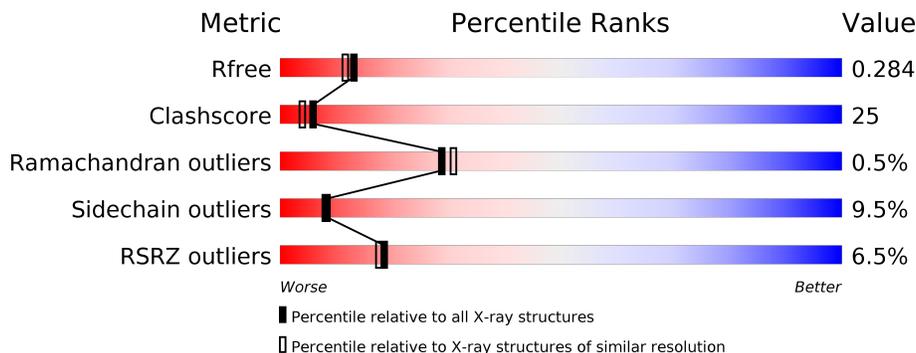
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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	615	6% / 62% / 28% / 6% ·
2	B	6	83% / 17%
3	C	20	50% / 50%
4	D	18	89% / 11%
5	E	14	100%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 5511 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 angiotensin I converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	0	0	0
			4871	3115	806	921	29			

- Molecule 2 is a protein called disordered segment of collectrin homology domain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	6	Total	C	N	O	0	0	0
			31	18	6	7			

- Molecule 3 is a protein called disordered segment of collectrin homology domain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	20	Total	C	N	O	0	0	0
			101	60	20	21			

- Molecule 4 is a protein called disordered segment of collectrin homology domain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	18	Total	C	N	O	0	0	0
			91	54	18	19			

- Molecule 5 is a protein called disordered segment of collectrin homology domain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	14	Total	C	N	O	0	0	0
			71	42	14	15			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
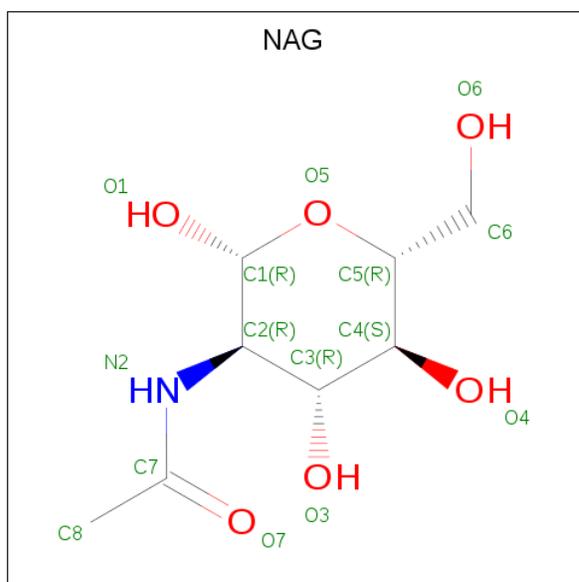
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 14	C 8	N 1	O 5	0	0
6	A	1	Total 14	C 8	N 1	O 5	0	0
6	A	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total 1	Cl 1	0	0

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total 1	Zn 1	0	0

- Molecule 9 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	298	Total 298	O 298	0	0
9	C	1	Total 1	O 1	0	0

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	E	3	Total 3	O 3	0	0

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: angiotensin I converting enzyme 2

Chain A:

6%

62%   28%   6%
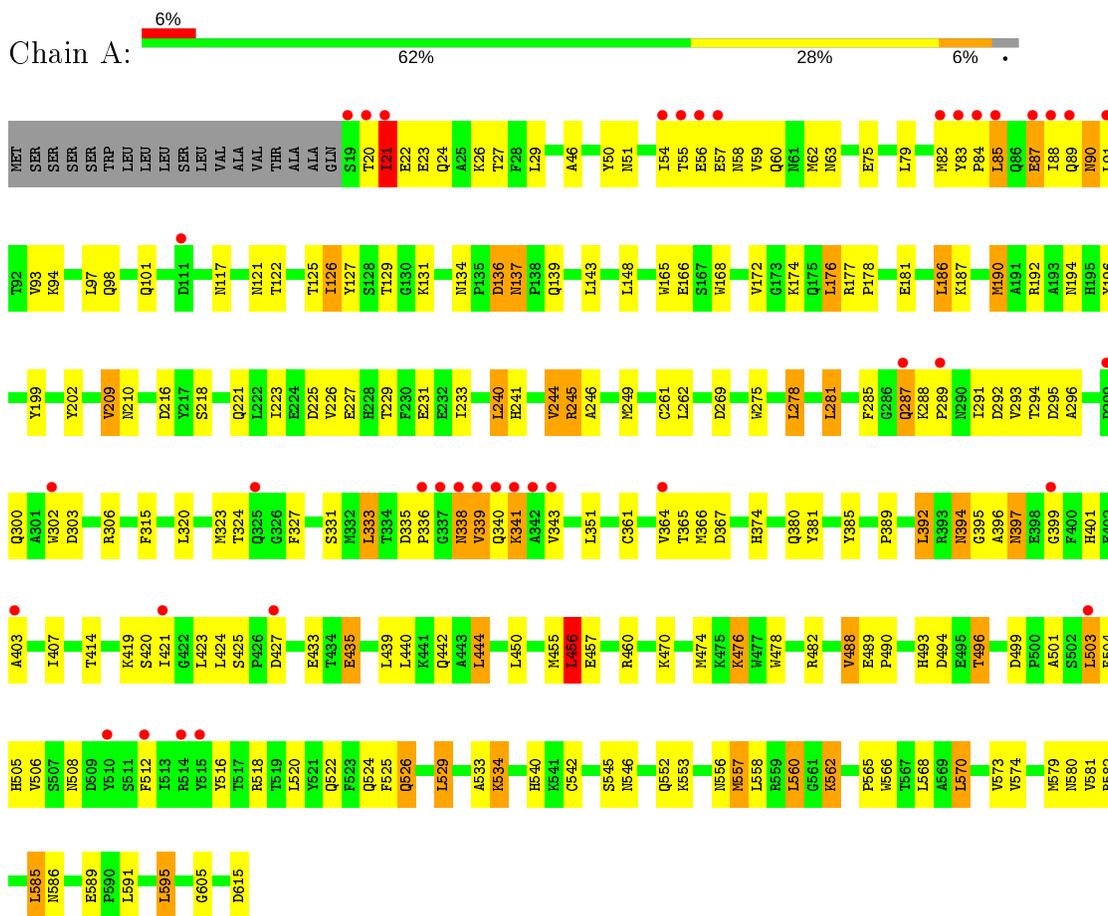
- Molecule 2: disordered segment of collectrin homology domain

Chain B:

83%   17%
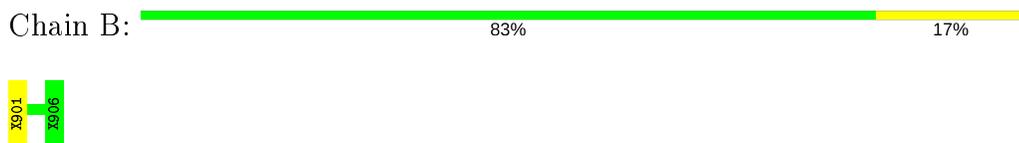
- Molecule 3: disordered segment of collectrin homology domain

Chain C:

50%   50%

`X907` `X910` `X914` `X915` `X916` `X917` `X918` `X919` `X920` `X921` `X922` `X923` `X924` `X925` `X926`

• Molecule 4: disordered segment of collectrin homology domain

Chain D:

89%   11%

`X927` `X940` `X941` `X944`

• Molecule 5: disordered segment of collectrin homology domain

Chain E:

100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	103.64Å 89.48Å 112.40Å 90.00° 109.15° 90.00°	Depositor
Resolution (Å)	46.74 – 2.20 46.74 – 2.09	Depositor EDS
% Data completeness (in resolution range)	96.3 (46.74-2.20) 89.7 (46.74-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$<I/\sigma(I)>$ [1]	1.45 (at 2.10Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.235 , 0.287 0.233 , 0.284	Depositor DCC
R_{free} test set	4798 reflections (9.36%)	wwPDB-VP
Wilson B-factor (Å^2)	50.9	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 59.9	EDS
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5511	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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.

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5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NAG, CL

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	0.43	0/5008	0.67	2/6803 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	456	LEU	CA-CB-CG	6.66	130.63	115.30
1	A	269	ASP	CB-CG-OD2	5.40	123.16	118.30

There are no chirality outliers.

There are no planarity outliers.

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	4871	0	4640	242	1
2	B	31	0	9	2	0
3	C	101	0	31	7	0
4	D	91	0	21	1	0
5	E	71	0	17	0	0
6	A	42	0	39	4	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
9	A	298	0	0	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	1	0	0	1	0
9	E	3	0	0	0	0
All	All	5511	0	4757	250	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 25.

All (250) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:VAL:HG11	1:A:423:LEU:HB3	1.40	1.02
1:A:54:ILE:HB	1:A:341:LYS:HG3	1.49	0.93
1:A:293:VAL:HG13	1:A:296:ALA:HB3	1.54	0.89
1:A:97:LEU:HG	1:A:101:GLN:HE21	1.39	0.86
1:A:246:ALA:HA	1:A:249:MET:CE	2.06	0.85
1:A:246:ALA:HA	1:A:249:MET:HE2	1.59	0.85
1:A:493:HIS:HD2	1:A:499:ASP:OD1	1.59	0.85
1:A:285:PHE:HB3	1:A:287:GLN:HE22	1.44	0.83
1:A:21:ILE:HD13	1:A:21:ILE:H	1.47	0.80
1:A:60:GLN:HA	1:A:63:ASN:HD21	1.47	0.79
1:A:125:THR:O	1:A:129:THR:HG22	1.83	0.78
1:A:552:GLN:HE21	1:A:556:ASN:HD21	1.32	0.77
1:A:336:PRO:HB2	1:A:340:GLN:HB3	1.65	0.77
1:A:474:MET:HE1	1:A:499:ASP:HB2	1.66	0.77
1:A:229:THR:HG23	1:A:516:TYR:OH	1.85	0.77
1:A:91:LEU:H	1:A:91:LEU:HD12	1.49	0.76
1:A:320:LEU:HD13	1:A:380:GLN:HG2	1.67	0.76
1:A:221:GLN:HG3	9:A:917:HOH:O	1.85	0.75
1:A:407:ILE:HD11	1:A:522:GLN:O	1.87	0.74
1:A:84:PRO:HB2	1:A:87:GLU:HB2	1.67	0.74
1:A:292:ASP:OD2	1:A:294:THR:HG22	1.87	0.74
1:A:546:ASN:OD1	6:A:802:NAG:H2	1.88	0.73
1:A:394:ASN:HD22	1:A:395:GLY:H	1.35	0.73
1:A:90:ASN:O	1:A:93:VAL:HG22	1.88	0.73
1:A:117:ASN:HB3	9:A:865:HOH:O	1.88	0.73
1:A:23:GLU:O	1:A:27:THR:HG23	1.89	0.72
1:A:397:ASN:C	1:A:397:ASN:HD22	1.93	0.72
1:A:424:LEU:HD12	9:A:934:HOH:O	1.91	0.71
1:A:287:GLN:NE2	1:A:287:GLN:H	1.89	0.70
3:C:916:UNK:O	3:C:918:UNK:N	2.25	0.69
1:A:55:THR:HB	1:A:58:ASN:HB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:GLN:HE21	1:A:556:ASN:ND2	1.90	0.69
1:A:293:VAL:CG1	1:A:296:ALA:HB3	2.24	0.68
1:A:293:VAL:O	1:A:293:VAL:HG12	1.92	0.67
1:A:335:ASP:HB2	1:A:361:CYS:HB3	1.74	0.67
1:A:225:ASP:O	1:A:229:THR:HG22	1.95	0.67
1:A:287:GLN:CD	1:A:287:GLN:H	1.96	0.66
1:A:552:GLN:NE2	1:A:556:ASN:HD21	1.94	0.66
1:A:51:ASN:HD22	1:A:343:VAL:HG21	1.59	0.66
1:A:240:LEU:O	1:A:244:VAL:HG13	1.96	0.66
1:A:97:LEU:HG	1:A:101:GLN:NE2	2.08	0.66
1:A:166:GLU:OE1	1:A:493:HIS:HE1	1.78	0.66
1:A:494:ASP:OD2	1:A:496:THR:HB	1.95	0.66
1:A:60:GLN:HA	1:A:63:ASN:ND2	2.09	0.66
1:A:389:PRO:HG2	1:A:392:LEU:HD22	1.78	0.65
1:A:261:CYS:HB2	1:A:488:VAL:HG22	1.78	0.64
1:A:336:PRO:HB2	1:A:340:GLN:CB	2.27	0.64
1:A:545:SER:O	1:A:546:ASN:HB2	1.96	0.64
1:A:557:MET:HG2	1:A:573:VAL:HG21	1.80	0.64
1:A:306:ARG:HG2	1:A:306:ARG:HH11	1.63	0.63
3:C:923:UNK:O	3:C:924:UNK:C	2.46	0.63
1:A:209:VAL:C	1:A:210:ASN:HD22	2.01	0.63
1:A:223:ILE:O	1:A:227:GLU:HG3	1.97	0.63
1:A:457:GLU:HG2	1:A:512:PHE:HB3	1.79	0.63
1:A:285:PHE:CE1	1:A:433:GLU:HG2	2.33	0.63
1:A:526:GLN:HE21	1:A:526:GLN:HA	1.64	0.63
1:A:177:ARG:HB3	1:A:178:PRO:HD3	1.82	0.62
1:A:21:ILE:H	1:A:21:ILE:CD1	2.13	0.62
1:A:397:ASN:ND2	1:A:399:GLY:H	1.98	0.62
1:A:56:GLU:O	1:A:59:VAL:HG12	2.00	0.62
1:A:21:ILE:HD13	1:A:21:ILE:N	2.13	0.62
1:A:397:ASN:HD22	1:A:399:GLY:H	1.48	0.62
1:A:456:LEU:HD21	1:A:503:LEU:HD12	1.82	0.62
1:A:562:LYS:HG2	9:A:1093:HOH:O	1.99	0.61
1:A:55:THR:HG22	1:A:57:GLU:H	1.63	0.61
1:A:365:THR:HG22	1:A:366:MET:N	2.15	0.61
1:A:557:MET:HA	1:A:560:LEU:HD22	1.82	0.61
1:A:331:SER:HB3	1:A:333:LEU:HD13	1.81	0.61
1:A:245:ARG:HB2	1:A:262:LEU:HD21	1.83	0.61
1:A:338:ASN:HD22	1:A:338:ASN:N	1.97	0.61
1:A:246:ALA:HA	1:A:249:MET:HE3	1.83	0.61
1:A:296:ALA:O	1:A:300:GLN:HG3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:ASN:ND2	1:A:395:GLY:H	1.99	0.60
1:A:570:LEU:HD22	1:A:574:VAL:HG22	1.82	0.60
2:B:901:UNK:HA	3:C:910:UNK:O	2.01	0.60
1:A:21:ILE:HA	1:A:24:GLN:HE21	1.65	0.60
1:A:97:LEU:O	1:A:101:GLN:HG2	2.02	0.59
1:A:209:VAL:HG21	1:A:565:PRO:HB3	1.84	0.59
1:A:91:LEU:CD1	1:A:91:LEU:H	2.15	0.59
1:A:91:LEU:HD12	1:A:91:LEU:N	2.18	0.58
3:C:920:UNK:HA	9:C:288:HOH:O	2.03	0.58
1:A:82:MET:O	1:A:84:PRO:HD3	2.03	0.58
1:A:403:ALA:O	1:A:407:ILE:HG12	2.04	0.57
1:A:85:LEU:N	1:A:85:LEU:HD23	2.20	0.57
1:A:122:THR:O	1:A:126:ILE:HG23	2.05	0.56
1:A:365:THR:HG22	1:A:367:ASP:H	1.71	0.56
1:A:420:SER:OG	6:A:802:NAG:H83	2.05	0.56
1:A:166:GLU:OE1	1:A:493:HIS:CE1	2.58	0.56
1:A:285:PHE:CZ	1:A:433:GLU:HG2	2.41	0.56
1:A:121:ASN:O	1:A:125:THR:HG23	2.05	0.56
1:A:338:ASN:H	1:A:338:ASN:ND2	2.04	0.56
1:A:229:THR:OG1	1:A:581:VAL:HB	2.05	0.55
1:A:20:THR:C	1:A:22:GLU:H	2.08	0.55
1:A:281:LEU:N	1:A:281:LEU:HD12	2.20	0.55
1:A:126:ILE:HG12	1:A:176:LEU:CD1	2.36	0.55
1:A:22:GLU:O	1:A:26:LYS:HG3	2.06	0.55
1:A:51:ASN:HD22	1:A:343:VAL:CG2	2.20	0.55
1:A:75:GLU:O	1:A:79:LEU:HB2	2.07	0.55
1:A:209:VAL:O	1:A:210:ASN:ND2	2.36	0.55
1:A:394:ASN:HD22	1:A:395:GLY:N	2.04	0.55
1:A:568:LEU:HD23	1:A:568:LEU:O	2.08	0.54
1:A:281:LEU:HD12	1:A:281:LEU:H	1.72	0.54
1:A:338:ASN:HD22	1:A:338:ASN:H	1.54	0.54
1:A:85:LEU:H	1:A:85:LEU:CD2	2.20	0.54
1:A:55:THR:HG22	1:A:56:GLU:N	2.21	0.54
1:A:21:ILE:CA	1:A:24:GLN:HE21	2.21	0.54
1:A:380:GLN:NE2	9:A:912:HOH:O	2.40	0.54
1:A:524:GLN:HE22	1:A:579:MET:HA	1.72	0.54
1:A:168:TRP:O	1:A:172:VAL:HG22	2.08	0.53
1:A:55:THR:CG2	1:A:56:GLU:N	2.71	0.53
1:A:524:GLN:NE2	1:A:580:ASN:H	2.06	0.53
1:A:557:MET:HG2	1:A:573:VAL:CG2	2.38	0.53
1:A:199:TYR:O	1:A:202:TYR:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:LEU:HG	1:A:595:LEU:HD22	1.91	0.53
1:A:241:HIS:O	1:A:245:ARG:HB3	2.08	0.53
1:A:174:LYS:HE2	1:A:496:THR:HG22	1.91	0.53
1:A:24:GLN:HG3	1:A:83:TYR:HE2	1.75	0.52
1:A:435:GLU:HG3	1:A:540:HIS:NE2	2.25	0.52
1:A:306:ARG:HG2	1:A:306:ARG:NH1	2.25	0.52
1:A:245:ARG:HG2	1:A:245:ARG:HH21	1.76	0.51
1:A:615:ASP:OXT	2:B:901:UNK:N	2.43	0.51
1:A:419:LYS:HD3	9:A:1073:HOH:O	2.10	0.51
1:A:440:LEU:HD13	1:A:444:LEU:HD22	1.92	0.51
1:A:482:ARG:HG2	1:A:488:VAL:CG1	2.41	0.51
1:A:89:GLN:O	1:A:91:LEU:HD12	2.09	0.51
1:A:505:HIS:CD2	1:A:505:HIS:H	2.27	0.51
1:A:605:GLY:O	9:A:915:HOH:O	2.19	0.51
1:A:190:MET:HE2	1:A:194:ASN:HD22	1.76	0.51
1:A:457:GLU:OE2	1:A:460:ARG:HD3	2.12	0.50
1:A:84:PRO:O	1:A:88:ILE:HG12	2.10	0.50
1:A:165:TRP:CZ3	1:A:490:PRO:HD2	2.47	0.50
1:A:331:SER:HB3	1:A:333:LEU:CD1	2.40	0.50
1:A:21:ILE:HA	1:A:24:GLN:NE2	2.26	0.50
1:A:570:LEU:HD22	1:A:574:VAL:CG2	2.41	0.50
1:A:85:LEU:H	1:A:85:LEU:HD23	1.77	0.50
1:A:229:THR:OG1	1:A:520:LEU:HD21	2.11	0.50
1:A:137:ASN:C	1:A:137:ASN:HD22	2.13	0.50
3:C:920:UNK:O	3:C:921:UNK:C	2.60	0.50
1:A:482:ARG:HG2	1:A:488:VAL:HG13	1.94	0.49
1:A:131:LYS:HE2	1:A:143:LEU:HD12	1.93	0.49
1:A:209:VAL:C	1:A:210:ASN:ND2	2.66	0.49
1:A:137:ASN:ND2	1:A:139:GLN:H	2.11	0.49
1:A:456:LEU:CD1	1:A:460:ARG:HD2	2.43	0.49
1:A:562:LYS:NZ	1:A:562:LYS:CB	2.76	0.49
1:A:21:ILE:N	1:A:24:GLN:HE21	2.11	0.48
1:A:442:GLN:NE2	9:A:1086:HOH:O	2.38	0.48
1:A:556:ASN:O	1:A:560:LEU:HD22	2.13	0.48
1:A:315:PHE:HB3	9:A:912:HOH:O	2.14	0.48
1:A:341:LYS:HB2	1:A:341:LYS:NZ	2.28	0.48
1:A:293:VAL:CG1	1:A:293:VAL:O	2.62	0.48
1:A:192:ARG:HA	1:A:196:TYR:O	2.13	0.48
1:A:580:ASN:HD21	1:A:582:ARG:HD3	1.78	0.48
1:A:320:LEU:HD13	1:A:380:GLN:CG	2.42	0.47
1:A:55:THR:HG22	1:A:57:GLU:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:ASN:HB3	9:A:1053:HOH:O	2.13	0.47
1:A:526:GLN:NE2	1:A:526:GLN:HA	2.29	0.47
1:A:94:LYS:O	1:A:98:GLN:HB2	2.14	0.47
1:A:134:ASN:OD1	1:A:136:ASP:N	2.43	0.47
1:A:478:TRP:CD2	1:A:489:GLU:HB3	2.49	0.47
1:A:59:VAL:O	1:A:63:ASN:ND2	2.47	0.47
1:A:339:VAL:O	1:A:339:VAL:HG12	2.14	0.47
1:A:218:SER:HB3	1:A:221:GLN:HB2	1.97	0.47
1:A:126:ILE:HG12	1:A:176:LEU:HD13	1.96	0.47
1:A:85:LEU:N	1:A:85:LEU:CD2	2.78	0.46
1:A:190:MET:HE2	1:A:194:ASN:ND2	2.29	0.46
1:A:365:THR:CG2	1:A:366:MET:N	2.79	0.46
1:A:226:VAL:O	1:A:229:THR:HG22	2.14	0.46
1:A:261:CYS:CB	1:A:488:VAL:HG22	2.43	0.46
1:A:294:THR:OG1	1:A:365:THR:HA	2.15	0.46
1:A:364:VAL:HG12	1:A:364:VAL:O	2.14	0.46
1:A:423:LEU:HA	1:A:423:LEU:HD23	1.72	0.46
1:A:525:PHE:O	1:A:529:LEU:HD22	2.16	0.46
1:A:568:LEU:HD23	1:A:568:LEU:C	2.36	0.46
1:A:24:GLN:HG3	1:A:83:TYR:CE2	2.51	0.46
1:A:245:ARG:HG2	1:A:245:ARG:NH2	2.31	0.46
1:A:351:LEU:HD12	1:A:351:LEU:H	1.81	0.46
1:A:338:ASN:ND2	1:A:338:ASN:N	2.60	0.45
1:A:287:GLN:NE2	1:A:287:GLN:N	2.61	0.45
1:A:414:THR:HG21	1:A:542:CYS:O	2.17	0.45
1:A:456:LEU:HD12	1:A:456:LEU:C	2.37	0.45
1:A:55:THR:HG21	1:A:57:GLU:HG2	1.98	0.45
1:A:302:TRP:NE1	1:A:306:ARG:NH1	2.65	0.45
1:A:57:GLU:OE1	1:A:57:GLU:N	2.49	0.45
1:A:397:ASN:C	1:A:397:ASN:ND2	2.66	0.44
1:A:456:LEU:CD2	1:A:503:LEU:HD12	2.47	0.44
1:A:396:ALA:HB1	1:A:566:TRP:HA	2.00	0.44
1:A:526:GLN:HE21	1:A:526:GLN:CA	2.27	0.44
1:A:323:MET:HB3	1:A:327:PHE:CD1	2.53	0.44
1:A:46:ALA:HB1	1:A:62:MET:HA	1.99	0.44
1:A:221:GLN:HG3	9:A:859:HOH:O	2.17	0.44
1:A:292:ASP:C	1:A:292:ASP:OD2	2.54	0.44
1:A:181:GLU:HB3	1:A:470:LYS:NZ	2.33	0.44
1:A:126:ILE:HG13	1:A:127:TYR:N	2.31	0.44
1:A:552:GLN:NE2	1:A:556:ASN:ND2	2.59	0.44
1:A:395:GLY:O	1:A:562:LYS:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:LYS:NZ	1:A:562:LYS:HB3	2.32	0.44
1:A:501:ALA:HA	1:A:506:VAL:CG1	2.47	0.44
1:A:420:SER:CB	6:A:802:NAG:H83	2.48	0.43
1:A:231:GLU:HG2	9:A:843:HOH:O	2.17	0.43
1:A:21:ILE:HA	1:A:24:GLN:HG2	2.00	0.43
1:A:209:VAL:HG22	1:A:216:ASP:HA	2.00	0.43
1:A:137:ASN:C	1:A:137:ASN:ND2	2.71	0.43
1:A:55:THR:CG2	1:A:57:GLU:HG2	2.49	0.43
1:A:533:ALA:C	1:A:534:LYS:HG2	2.39	0.43
1:A:291:ILE:HD12	9:A:973:HOH:O	2.18	0.43
1:A:278:LEU:HA	1:A:281:LEU:HD13	2.01	0.43
1:A:414:THR:HA	9:A:989:HOH:O	2.19	0.43
1:A:56:GLU:HA	1:A:56:GLU:OE2	2.19	0.42
4:D:940:UNK:O	4:D:941:UNK:C	2.66	0.42
1:A:210:ASN:ND2	9:A:938:HOH:O	2.51	0.42
1:A:557:MET:HA	1:A:560:LEU:CD2	2.49	0.42
1:A:407:ILE:HD12	1:A:526:GLN:HB2	2.00	0.42
1:A:493:HIS:CD2	1:A:499:ASP:OD1	2.51	0.42
1:A:324:THR:O	1:A:327:PHE:HB3	2.19	0.42
1:A:320:LEU:HB3	1:A:380:GLN:OE1	2.19	0.42
1:A:476:LYS:NZ	9:A:863:HOH:O	2.52	0.42
1:A:553:LYS:HB3	1:A:553:LYS:HE3	1.76	0.42
3:C:914:UNK:O	3:C:915:UNK:CB	2.65	0.42
1:A:50:TYR:CE1	1:A:59:VAL:HG23	2.55	0.42
1:A:425:SER:C	1:A:427:ASP:H	2.22	0.42
1:A:562:LYS:HZ3	1:A:562:LYS:HB3	1.85	0.42
1:A:303:ASP:HB2	9:A:872:HOH:O	2.19	0.42
1:A:294:THR:OG1	1:A:365:THR:HG23	2.19	0.42
1:A:351:LEU:HD12	1:A:351:LEU:N	2.34	0.42
1:A:585:LEU:O	1:A:589:GLU:HG2	2.20	0.41
1:A:137:ASN:HD21	1:A:139:GLN:HB2	1.84	0.41
1:A:240:LEU:HD13	1:A:275:TRP:HZ3	1.84	0.41
1:A:380:GLN:CD	9:A:912:HOH:O	2.59	0.41
1:A:131:LYS:HB3	1:A:131:LYS:HE2	1.75	0.41
1:A:186:LEU:HD12	1:A:186:LEU:HA	1.88	0.41
1:A:85:LEU:HD22	9:A:936:HOH:O	2.19	0.41
1:A:374:HIS:C	1:A:374:HIS:CD2	2.93	0.41
1:A:126:ILE:HG12	1:A:176:LEU:HD11	2.03	0.41
1:A:245:ARG:CB	1:A:262:LEU:HD21	2.48	0.41
1:A:288:LYS:HA	1:A:289:PRO:HD3	1.85	0.41
1:A:504:PHE:O	1:A:508:ASN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ILE:N	1:A:21:ILE:CD1	2.81	0.41
1:A:407:ILE:HA	1:A:407:ILE:HD13	1.76	0.41
1:A:450:LEU:HA	1:A:450:LEU:HD23	1.84	0.41
3:C:917:UNK:O	3:C:918:UNK:C	2.69	0.41
1:A:293:VAL:C	1:A:295:ASP:H	2.22	0.41
1:A:131:LYS:HE2	1:A:143:LEU:CD1	2.51	0.41
1:A:338:ASN:O	1:A:339:VAL:HB	2.21	0.40
1:A:478:TRP:CE3	1:A:489:GLU:HB3	2.56	0.40
1:A:546:ASN:OD1	6:A:802:NAG:C2	2.58	0.40
1:A:343:VAL:O	1:A:343:VAL:CG2	2.69	0.40
1:A:489:GLU:HA	1:A:490:PRO:HD3	1.74	0.40
1:A:341:LYS:CB	1:A:341:LYS:NZ	2.84	0.40
1:A:20:THR:O	1:A:22:GLU:N	2.47	0.40
1:A:302:TRP:CH2	1:A:423:LEU:HD11	2.56	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:89:GLN:OE1	1:A:89:GLN:OE1[2_756]	2.15	0.05

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	595/615 (97%)	560 (94%)	32 (5%)	3 (0%)	29	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	ILE
1	A	90	ASN

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Mol	Chain	Res	Type
1	A	339	VAL

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	527/542 (97%)	477 (90%)	50 (10%)	8 8

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ILE
1	A	29	LEU
1	A	85	LEU
1	A	87	GLU
1	A	126	ILE
1	A	136	ASP
1	A	137	ASN
1	A	148	LEU
1	A	176	LEU
1	A	186	LEU
1	A	187	LYS
1	A	190	MET
1	A	209	VAL
1	A	233	ILE
1	A	240	LEU
1	A	244	VAL
1	A	245	ARG
1	A	278	LEU
1	A	281	LEU
1	A	287	GLN
1	A	333	LEU
1	A	338	ASN
1	A	341	LYS
1	A	381	TYR
1	A	385	TYR

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Mol	Chain	Res	Type
1	A	392	LEU
1	A	394	ASN
1	A	397	ASN
1	A	401	HIS
1	A	421	ILE
1	A	435	GLU
1	A	439	LEU
1	A	444	LEU
1	A	455	MET
1	A	456	LEU
1	A	476	LYS
1	A	488	VAL
1	A	496	THR
1	A	503	LEU
1	A	518	ARG
1	A	526	GLN
1	A	529	LEU
1	A	534	LYS
1	A	557	MET
1	A	558	LEU
1	A	560	LEU
1	A	562	LYS
1	A	570	LEU
1	A	585	LEU
1	A	595	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	33	ASN
1	A	42	GLN
1	A	49	ASN
1	A	51	ASN
1	A	53	ASN
1	A	58	ASN
1	A	60	GLN
1	A	61	ASN
1	A	64	ASN
1	A	101	GLN
1	A	137	ASN
1	A	149	ASN

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Mol	Chain	Res	Type
1	A	194	ASN
1	A	210	ASN
1	A	277	ASN
1	A	287	GLN
1	A	300	GLN
1	A	338	ASN
1	A	394	ASN
1	A	397	ASN
1	A	429	GLN
1	A	442	GLN
1	A	493	HIS
1	A	505	HIS
1	A	524	GLN
1	A	526	GLN
1	A	531	GLN
1	A	556	ASN
1	A	580	ASN
1	A	586	ASN
1	A	599	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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	$\#|Z| > 2$
6	NAG	A	800	1	14,14,15	0.73	0	17,19,21	0.69	0
6	NAG	A	802	1	14,14,15	0.61	0	17,19,21	0.87	1 (5%)
6	NAG	A	801	1	14,14,15	0.55	0	17,19,21	0.61	0

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
6	NAG	A	800	1	-	4/6/23/26	0/1/1/1
6	NAG	A	802	1	-	4/6/23/26	0/1/1/1
6	NAG	A	801	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	802	NAG	C2-N2-C7	-2.25	119.70	122.90

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	800	NAG	C8-C7-N2-C2
6	A	800	NAG	O7-C7-N2-C2
6	A	802	NAG	C8-C7-N2-C2
6	A	802	NAG	O7-C7-N2-C2
6	A	801	NAG	C8-C7-N2-C2
6	A	801	NAG	O7-C7-N2-C2
6	A	802	NAG	C4-C5-C6-O6
6	A	800	NAG	O5-C5-C6-O6
6	A	801	NAG	O5-C5-C6-O6
6	A	800	NAG	C4-C5-C6-O6
6	A	802	NAG	O5-C5-C6-O6
6	A	801	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	802	NAG	4	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	597/615 (97%)	0.36	39 (6%)	18	17	35, 55, 90, 106	0
2	B	0/6	-	-			-	-
3	C	0/20	-	-			-	-
4	D	0/18	-	-			-	-
5	E	0/14	-	-			-	-
All	All	597/673 (88%)	0.36	39 (6%)	18	17	35, 55, 90, 106	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	339	VAL	6.0
1	A	338	ASN	5.4
1	A	88	ILE	4.9
1	A	341	LYS	4.9
1	A	337	GLY	4.5
1	A	427	ASP	4.2
1	A	84	PRO	4.1
1	A	343	VAL	3.9
1	A	336	PRO	3.8
1	A	21	ILE	3.7
1	A	57	GLU	3.5
1	A	299	ASP	3.5
1	A	83	TYR	3.3
1	A	325	GLN	3.3
1	A	287	GLN	3.2
1	A	19	SER	3.2
1	A	82	MET	3.1
1	A	340	GLN	3.0
1	A	89	GLN	3.0
1	A	364	VAL	2.9
1	A	503	LEU	2.7
1	A	85	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	91	LEU	2.5
1	A	54	ILE	2.5
1	A	20	THR	2.4
1	A	56	GLU	2.4
1	A	111	ASP	2.4
1	A	289	PRO	2.4
1	A	342	ALA	2.2
1	A	514	ARG	2.2
1	A	421	ILE	2.2
1	A	515	TYR	2.2
1	A	87	GLU	2.1
1	A	510	TYR	2.1
1	A	399	GLY	2.1
1	A	302	TRP	2.1
1	A	403	ALA	2.1
1	A	512	PHE	2.1
1	A	55	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	A	800	14/15	0.75	0.20	90,91,95,96	0
6	NAG	A	802	14/15	0.76	0.27	83,87,88,89	0
6	NAG	A	801	14/15	0.86	0.26	88,89,90,91	0
7	CL	A	803	1/1	0.98	0.18	44,44,44,44	0
8	ZN	A	804	1/1	1.00	0.12	53,53,53,53	0

6.5 Other polymers (i)

There are no such residues in this entry.