Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:44 AM GMT

PDB ID	:	3PRE
Title	:	Quinazolines with intra-molecular hydrogen bonding scaffold (iMHBS) as PI3K/mTOR dual inhibitors.
Authors	:	Knighton, D.R.; Greasley, S.E.; Rodgers, C.M.-L.
Deposited on	:	2010-11-29
Resolution	:	2.91 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

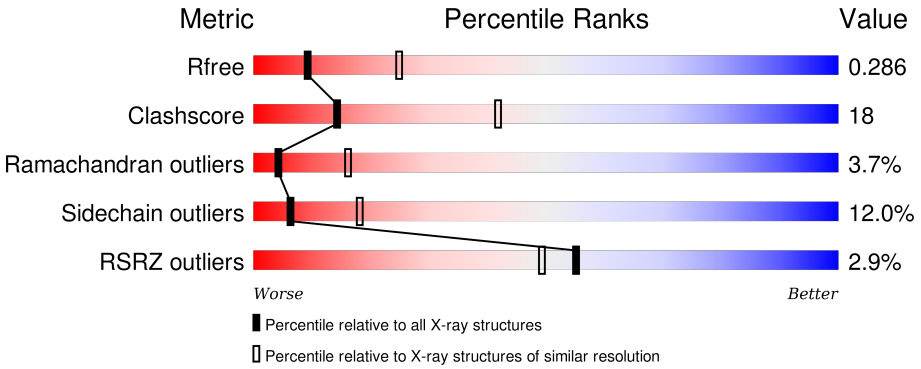
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.91 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	1643 (2.94-2.90)
Clashscore	102246	1871 (2.94-2.90)
Ramachandran outliers	100387	1824 (2.94-2.90)
Sidechain outliers	100360	1826 (2.94-2.90)
RSRZ outliers	91569	1650 (2.94-2.90)

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 <=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	966	2% 49% 31% 7% 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6813 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.

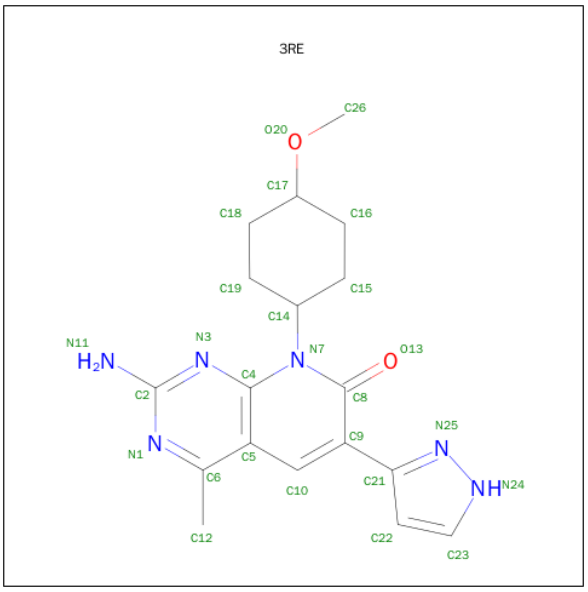
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	839	6787	4364	1154	1234	35	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	INITIATING METHIONINE	UNP P48736
A	1103	HIS	-	EXPRESSION TAG	UNP P48736
A	1104	HIS	-	EXPRESSION TAG	UNP P48736
A	1105	HIS	-	EXPRESSION TAG	UNP P48736
A	1106	HIS	-	EXPRESSION TAG	UNP P48736
A	1107	HIS	-	EXPRESSION TAG	UNP P48736
A	1108	HIS	-	EXPRESSION TAG	UNP P48736

- Molecule 2 is 2-AMINO-8-(TRANS-4-METHOXYCYCLOHEXYL)-4-METHYL-6-(1H-PYRAZOL-3-YL)PYRIDO[2,3-D]PYRIMIDIN-7(8H)-ONE (three-letter code: 3RE) (formula: $C_{18}H_{22}N_6O_2$).



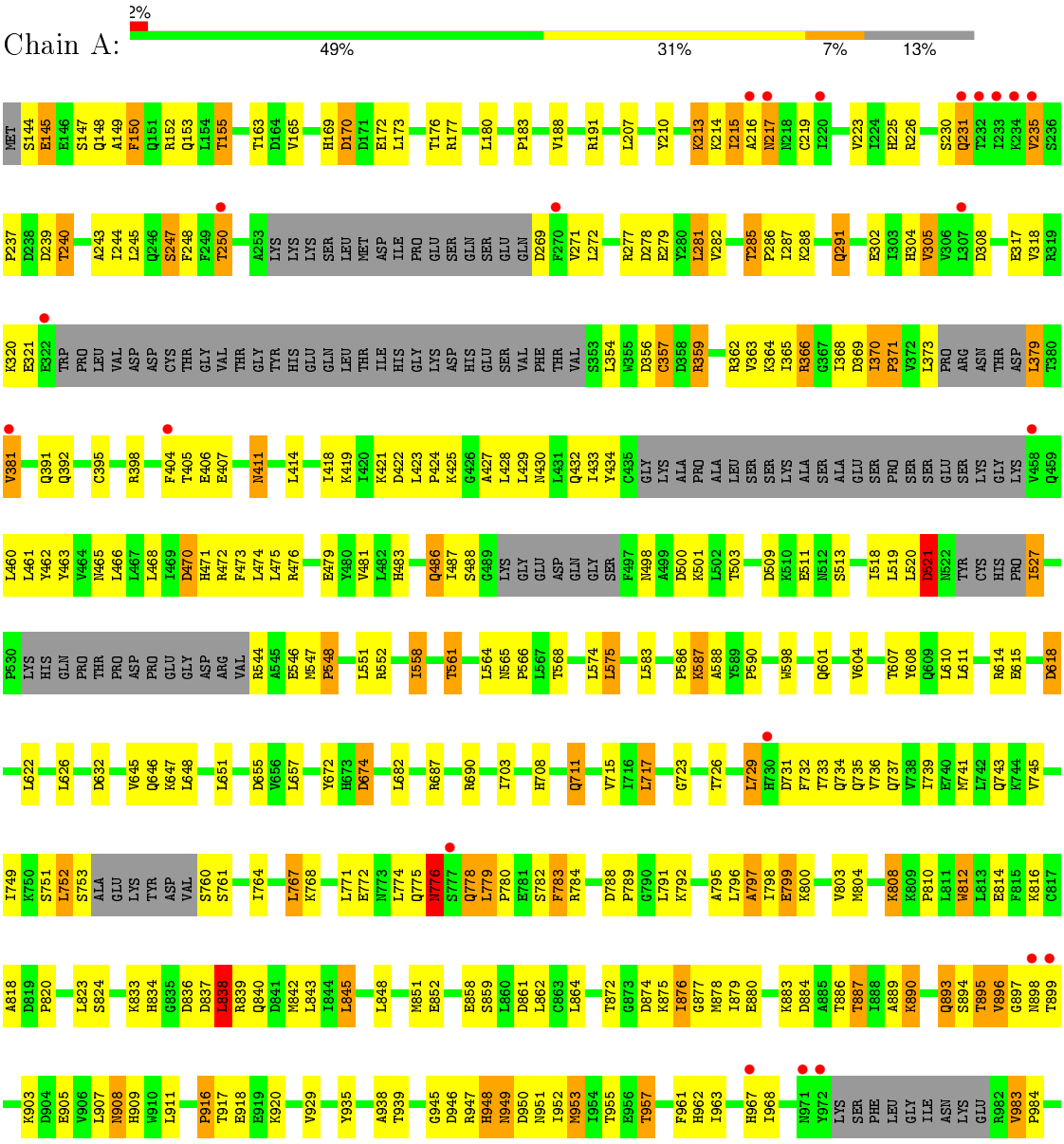
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			26	18	6	2		

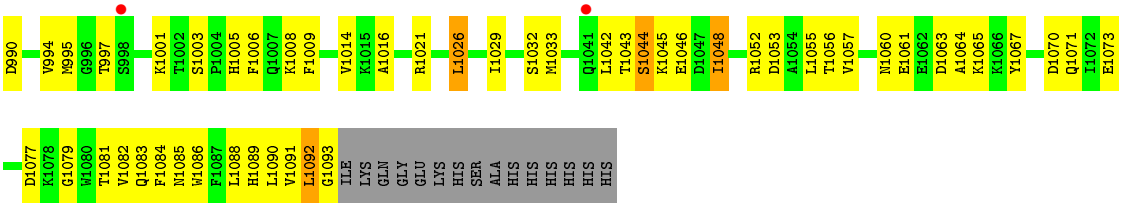
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform

Chain A:




D990
V994
M995
G996
T997
S998
K1001
T1002
S1003
P1004
H1005
F1006
Q1007
K1008
F1009
V1014
K1015
A1016
R1021
L1026
I1029
S1032
M1033
Q1041
L1042
T1043
S1044
K1045
E1046
D1047
I1048
R1052
D1053
A1054
L1055
T1056
V1057
N1060
E1061
E1062
D1063
A1064
K1065
K1066
Y1067
D1070
Q1071
I1072
E1073
D1077
K1078
G1079
W1080
T1081
V1082
Q1083
F1084
N1085
W1086
F1087
L1088
H1089
L1090
V1091
L1092
G1093
ILE
LYS
GLN
GLY
GLU
LYS
HIS
SER
ALA
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	143.54Å 67.28Å 106.53Å 90.00° 95.77° 90.00°	Depositor
Resolution (Å)	50.00 – 2.91 44.76 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.91) 99.3 (44.76-2.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.232 , 0.295 0.223 , 0.286	Depositor DCC
R_{free} test set	1147 reflections (5.40%)	DCC
Wilson B-factor (Å^2)	73.1	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 54.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 22390 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6813	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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, 0.375 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: 3RE

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	0.62	0/6931	0.74	4/9375 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	474	LEU	CA-CB-CG	7.08	131.59	115.30
1	A	767	LEU	CA-CB-CG	5.22	127.31	115.30
1	A	674	ASP	CB-CG-OD1	5.05	122.84	118.30
1	A	281	LEU	CA-CB-CG	5.02	126.86	115.30

There are no chirality outliers.

There are no planarity outliers.

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	6787	0	6826	245	0
2	A	26	0	22	3	0
All	All	6813	0	6848	247	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (247) 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:939:THR:CG2	1:A:945:GLY:HA2	1.72	1.19
1:A:149:ALA:HA	1:A:152:ARG:NH1	1.77	0.97
1:A:558:ILE:O	1:A:561:THR:HG22	1.72	0.88
1:A:476:ARG:O	1:A:520:LEU:HD23	1.73	0.88
1:A:149:ALA:HA	1:A:152:ARG:HH11	1.35	0.87
1:A:359:ARG:HH11	1:A:359:ARG:HB2	1.43	0.83
1:A:939:THR:HG23	1:A:945:GLY:HA2	1.60	0.83
1:A:949:ASN:OD1	1:A:1083:GLN:NE2	2.13	0.81
1:A:939:THR:CG2	1:A:945:GLY:CA	2.57	0.81
1:A:887:THR:HG22	1:A:890:LYS:H	1.46	0.81
1:A:223:VAL:HB	1:A:304:HIS:HD2	1.47	0.78
1:A:812:TRP:NE1	1:A:814:GLU:OE2	2.16	0.77
1:A:173:LEU:O	1:A:177:ARG:HG3	1.84	0.77
1:A:172:GLU:HG3	1:A:471:HIS:ND1	1.99	0.77
1:A:1088:LEU:O	1:A:1093:GLY:N	2.20	0.74
1:A:428:LEU:HD22	1:A:465:ASN:HB3	1.70	0.74
1:A:851:MET:HE1	1:A:938:ALA:HB1	1.68	0.73
1:A:948:HIS:CE1	1:A:950:ASP:HB2	2.22	0.73
1:A:893:GLN:HA	1:A:896:VAL:O	1.87	0.73
1:A:546:GLU:HG3	1:A:547:MET:H	1.53	0.72
1:A:939:THR:HG22	1:A:945:GLY:HA2	1.71	0.72
1:A:726:THR:HA	1:A:729:LEU:HB2	1.71	0.72
1:A:558:ILE:O	1:A:561:THR:CG2	2.37	0.71
1:A:776:ASN:HD22	1:A:778:GLN:HE22	1.36	0.71
1:A:983:VAL:HG22	1:A:984:PRO:HD2	1.74	0.70
1:A:939:THR:HG21	1:A:945:GLY:HA2	1.70	0.70
1:A:357:CYS:SG	1:A:359:ARG:NH1	2.64	0.69
1:A:732:PHE:O	1:A:736:VAL:HG23	1.94	0.68
1:A:362:ARG:HE	1:A:521:ASP:HB3	1.57	0.68
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.75	0.67
1:A:1055:LEU:O	1:A:1056:THR:HG22	1.95	0.67
1:A:657:LEU:HD11	1:A:690:ARG:HG2	1.77	0.66
1:A:947:ARG:NH2	1:A:963:ILE:O	2.28	0.66
1:A:546:GLU:CG	1:A:547:MET:H	2.08	0.66
1:A:271:VAL:HG12	1:A:308:ASP:O	1.96	0.66
1:A:1056:THR:HG23	1:A:1056:THR:O	1.96	0.66
1:A:223:VAL:HB	1:A:304:HIS:CD2	2.30	0.66
1:A:177:ARG:HG2	1:A:715:VAL:HG13	1.76	0.66
1:A:804:MET:HB2	1:A:810:PRO:HD2	1.77	0.66
1:A:948:HIS:NE2	1:A:950:ASP:HB2	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.76	0.65
1:A:169:HIS:O	1:A:170:ASP:HB3	1.97	0.65
1:A:734:GLN:HE21	1:A:780:PRO:HB2	1.63	0.64
1:A:359:ARG:HB2	1:A:359:ARG:NH1	2.12	0.63
1:A:165:VAL:O	1:A:165:VAL:HG12	1.98	0.62
1:A:564:LEU:HB2	1:A:1052:ARG:HD2	1.81	0.62
1:A:939:THR:HG22	1:A:945:GLY:CA	2.26	0.62
1:A:782:SER:O	1:A:783:PHE:HB3	1.99	0.62
1:A:470:ASP:HB2	1:A:476:ARG:NH2	2.14	0.61
1:A:368:ILE:HG21	1:A:433:ILE:HD11	1.80	0.61
1:A:1091:VAL:HG12	1:A:1092:LEU:HD23	1.82	0.61
1:A:291:GLN:HA	1:A:291:GLN:HE21	1.65	0.61
1:A:277:ARG:NH2	1:A:791:LEU:HG	2.16	0.60
1:A:808:LYS:O	1:A:810:PRO:HD3	2.01	0.60
1:A:172:GLU:HG3	1:A:471:HIS:HD1	1.64	0.60
1:A:935:TYR:O	1:A:939:THR:HB	2.02	0.60
1:A:737:GLN:O	1:A:741:MET:HG3	2.01	0.60
1:A:743:GLN:HE21	1:A:876:ILE:HG12	1.67	0.59
1:A:948:HIS:O	1:A:950:ASP:N	2.36	0.59
1:A:461:LEU:HB2	1:A:462:TYR:CD2	2.38	0.59
1:A:519:LEU:HD12	1:A:520:LEU:H	1.68	0.59
1:A:519:LEU:HD12	1:A:520:LEU:N	2.18	0.59
1:A:405:THR:O	1:A:407:GLU:N	2.36	0.58
1:A:851:MET:CE	1:A:938:ALA:HB1	2.33	0.58
1:A:645:VAL:HA	1:A:648:LEU:HD12	1.86	0.58
1:A:207:LEU:HD12	1:A:288:LYS:HB2	1.84	0.58
1:A:1021:ARG:HE	1:A:1056:THR:HG22	1.68	0.57
1:A:487:ILE:HG22	1:A:488:SER:N	2.19	0.57
1:A:207:LEU:HD12	1:A:288:LYS:HD2	1.86	0.57
1:A:878:MET:C	1:A:879:ILE:HD12	2.25	0.57
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.85	0.57
1:A:837:ASP:HB3	1:A:840:GLN:NE2	2.20	0.56
1:A:487:ILE:CG2	1:A:488:SER:N	2.68	0.56
1:A:235:VAL:HG11	1:A:244:ILE:HG12	1.86	0.56
1:A:424:PRO:HD2	1:A:427:ALA:HB2	1.88	0.55
1:A:188:VAL:HG11	1:A:318:VAL:HG21	1.88	0.55
1:A:240:THR:HG23	1:A:243:ALA:CB	2.36	0.55
1:A:547:MET:HB3	1:A:552:ARG:HH12	1.73	0.54
1:A:818:ALA:O	1:A:820:PRO:HD3	2.07	0.54
1:A:905:GLU:HG2	1:A:909:HIS:CE1	2.43	0.54
1:A:997:THR:HG23	1:A:1001:LYS:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ARG:HH21	1:A:791:LEU:HG	1.74	0.53
1:A:509:ASP:O	1:A:513:SER:HB3	2.08	0.53
1:A:365:ILE:HD13	1:A:518:ILE:HG22	1.89	0.53
1:A:607:THR:O	1:A:610:LEU:HB2	2.08	0.53
1:A:837:ASP:HB3	1:A:840:GLN:HE21	1.72	0.53
1:A:608:TYR:HD2	1:A:608:TYR:N	2.05	0.53
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.09	0.53
1:A:285:THR:HG22	1:A:286:PRO:HD2	1.90	0.53
1:A:767:LEU:HG	1:A:803:VAL:HG23	1.91	0.53
1:A:240:THR:HG23	1:A:243:ALA:HB2	1.92	0.52
1:A:608:TYR:CD2	1:A:608:TYR:N	2.76	0.52
1:A:191:ARG:NH2	1:A:723:GLY:O	2.39	0.52
1:A:144:SER:HB3	1:A:147:SER:HB3	1.91	0.52
1:A:929:VAL:HG22	1:A:995:MET:HG2	1.91	0.52
1:A:583:LEU:HD22	1:A:610:LEU:HD22	1.90	0.52
1:A:784:ARG:HG2	1:A:792:LYS:HE3	1.92	0.51
1:A:317:GLU:O	1:A:726:THR:HG23	2.11	0.51
1:A:862:LEU:HD11	1:A:1016:ALA:HB2	1.92	0.51
1:A:990:ASP:O	1:A:994:VAL:HG23	2.11	0.51
1:A:145:GLU:C	1:A:147:SER:H	2.13	0.51
1:A:897:GLY:C	1:A:899:THR:H	2.14	0.51
1:A:1086:TRP:HE3	1:A:1090:LEU:CD2	2.23	0.51
1:A:379:LEU:N	1:A:404:PHE:HB3	2.26	0.51
1:A:800:LYS:HB2	1:A:814:GLU:HG3	1.92	0.51
1:A:237:PRO:HA	1:A:287:ILE:HD11	1.92	0.51
1:A:144:SER:O	1:A:148:GLN:HG2	2.09	0.51
1:A:461:LEU:O	1:A:487:ILE:HG12	2.11	0.51
1:A:800:LYS:CB	1:A:814:GLU:HG3	2.41	0.50
1:A:1067:TYR:O	1:A:1071:GLN:HG2	2.11	0.50
1:A:845:LEU:HD12	1:A:848:LEU:HD22	1.92	0.50
1:A:889:ALA:HA	1:A:949:ASN:HD22	1.76	0.50
1:A:462:TYR:CE1	1:A:486:GLN:HG3	2.45	0.50
1:A:731:ASP:O	1:A:735:GLN:HG3	2.11	0.50
1:A:834:HIS:HA	1:A:875:LYS:O	2.11	0.50
1:A:419:LYS:O	1:A:422:ASP:N	2.42	0.50
1:A:734:GLN:NE2	1:A:780:PRO:HB2	2.25	0.50
1:A:796:LEU:O	1:A:798:ILE:HG13	2.11	0.50
1:A:463:TYR:CE1	1:A:501:LYS:HA	2.47	0.49
1:A:430:ASN:OD1	1:A:432:GLN:NE2	2.46	0.49
1:A:1014:VAL:CG1	1:A:1065:LYS:HG3	2.44	0.48
1:A:564:LEU:CB	1:A:1052:ARG:HD2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:VAL:HG13	1:A:191:ARG:NH2	2.28	0.48
1:A:953:MET:HB2	1:A:961:PHE:CZ	2.48	0.48
1:A:1052:ARG:O	1:A:1057:VAL:HG23	2.14	0.48
1:A:739:ILE:O	1:A:743:GLN:HG3	2.14	0.48
1:A:604:VAL:O	1:A:607:THR:HB	2.14	0.48
1:A:622:LEU:HD13	1:A:647:LYS:O	2.13	0.48
1:A:879:ILE:HD12	1:A:879:ILE:N	2.29	0.47
1:A:432:GLN:HB3	1:A:460:LEU:CD1	2.44	0.47
1:A:1043:THR:O	1:A:1044:SER:C	2.52	0.47
1:A:1014:VAL:HG11	1:A:1065:LYS:HG3	1.96	0.47
1:A:180:LEU:O	1:A:183:PRO:HD2	2.14	0.47
1:A:476:ARG:C	1:A:520:LEU:HD23	2.35	0.47
1:A:225:HIS:HE1	1:A:304:HIS:CD2	2.32	0.47
1:A:1070:ASP:O	1:A:1073:GLU:HB2	2.15	0.47
1:A:703:ILE:HD12	1:A:717:LEU:HD12	1.97	0.47
1:A:916:PRO:HG2	1:A:920:LYS:HD3	1.96	0.47
1:A:149:ALA:HA	1:A:152:ARG:HH12	1.72	0.47
1:A:861:ASP:C	1:A:861:ASP:OD1	2.54	0.47
1:A:291:GLN:NE2	1:A:291:GLN:HA	2.29	0.46
1:A:1089:HIS:CD2	1:A:1090:LEU:HD22	2.51	0.46
1:A:155:THR:O	1:A:155:THR:HG22	2.14	0.46
1:A:1084:PHE:O	1:A:1088:LEU:HG	2.15	0.46
1:A:248:PHE:C	1:A:250:THR:H	2.18	0.46
1:A:188:VAL:HG13	1:A:191:ARG:HH21	1.81	0.46
1:A:398:ARG:O	1:A:414:LEU:HD21	2.15	0.46
1:A:1060:ASN:ND2	1:A:1063:ASP:HB2	2.31	0.46
1:A:947:ARG:NH1	1:A:951:ASN:OD1	2.49	0.46
1:A:741:MET:O	1:A:745:VAL:HG23	2.15	0.46
1:A:434:TYR:CE1	1:A:460:LEU:HB2	2.51	0.45
1:A:291:GLN:CA	1:A:291:GLN:HE21	2.25	0.45
1:A:425:LYS:HE2	1:A:672:TYR:CE1	2.51	0.45
1:A:611:LEU:O	1:A:614:ARG:HB2	2.17	0.45
1:A:764:ILE:O	1:A:768:LYS:HG2	2.16	0.45
1:A:768:LYS:O	1:A:772:GLU:HG2	2.17	0.45
1:A:711:GLN:HE21	1:A:711:GLN:HB3	1.50	0.45
1:A:1005:HIS:O	1:A:1008:LYS:HB3	2.16	0.45
1:A:363:VAL:O	1:A:363:VAL:HG13	2.16	0.45
1:A:213:LYS:C	1:A:215:ILE:H	2.20	0.45
1:A:955:THR:C	1:A:957:THR:H	2.18	0.45
1:A:546:GLU:CG	1:A:547:MET:N	2.77	0.45
1:A:239:ASP:O	1:A:287:ILE:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:ASP:CB	1:A:476:ARG:NH2	2.80	0.45
1:A:887:THR:HG22	1:A:890:LYS:N	2.23	0.45
1:A:1053:ASP:O	1:A:1056:THR:N	2.48	0.45
1:A:833:LYS:HE3	1:A:836:ASP:HB2	1.99	0.44
1:A:1026:LEU:O	1:A:1029:ILE:HG22	2.17	0.44
1:A:896:VAL:HG21	1:A:899:THR:HB	2.00	0.44
1:A:1056:THR:CG2	1:A:1056:THR:O	2.64	0.44
1:A:1086:TRP:HE3	1:A:1090:LEU:HD23	1.82	0.44
1:A:895:THR:O	1:A:896:VAL:HB	2.17	0.44
1:A:774:LEU:O	1:A:779:LEU:HB2	2.18	0.44
1:A:548:PRO:HG2	1:A:551:LEU:HD12	1.98	0.44
1:A:558:ILE:HG21	1:A:575:LEU:HD21	2.00	0.44
1:A:423:LEU:HA	1:A:424:PRO:HD3	1.86	0.44
1:A:839:ARG:O	1:A:842:MET:HB2	2.18	0.44
1:A:272:LEU:HD22	1:A:305:VAL:HG11	1.99	0.44
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.65	0.44
1:A:395:CYS:HB2	1:A:418:ILE:HG13	2.00	0.44
1:A:797:ALA:HA	1:A:816:LYS:HE2	1.98	0.44
1:A:734:GLN:NE2	1:A:782:SER:O	2.50	0.44
1:A:302:GLU:HB2	1:A:304:HIS:CE1	2.52	0.43
1:A:880:GLU:O	2:A:101:3RE:H12A	2.18	0.43
1:A:795:ALA:O	1:A:816:LYS:HE3	2.18	0.43
1:A:245:LEU:C	1:A:247:SER:H	2.21	0.43
1:A:565:ASN:HA	1:A:566:PRO:HD3	1.77	0.43
1:A:472:ARG:O	1:A:473:PHE:HB2	2.18	0.43
1:A:392:GLN:NE2	1:A:598:TRP:HD1	2.16	0.43
1:A:364:LYS:HE3	1:A:411:ASN:O	2.18	0.43
2:A:101:3RE:H12	2:A:101:3RE:H10	1.73	0.43
1:A:586:PRO:O	1:A:588:ALA:N	2.51	0.43
1:A:354:LEU:O	1:A:421:LYS:HB3	2.19	0.43
1:A:851:MET:CE	1:A:938:ALA:CB	2.97	0.43
1:A:210:TYR:CE2	1:A:859:SER:HA	2.53	0.43
1:A:687:ARG:HG2	1:A:687:ARG:O	2.19	0.43
1:A:216:ALA:O	1:A:217:ASN:HB3	2.18	0.42
1:A:487:ILE:CG2	1:A:488:SER:H	2.31	0.42
1:A:952:ILE:HG12	1:A:962:HIS:CD2	2.54	0.42
1:A:848:LEU:HA	1:A:851:MET:HE2	2.02	0.42
1:A:476:ARG:HG2	1:A:520:LEU:HD22	2.02	0.42
1:A:632:ASP:HB3	1:A:1033:MET:CE	2.50	0.42
1:A:858:GLU:O	1:A:859:SER:C	2.58	0.42
1:A:883:LYS:O	1:A:884:ASP:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1006:PHE:O	1:A:1009:PHE:HB3	2.20	0.42
1:A:368:ILE:HD13	1:A:433:ILE:HD13	2.01	0.42
1:A:874:ASP:O	1:A:876:ILE:HG22	2.19	0.42
1:A:366:ARG:NH1	1:A:479:GLU:OE2	2.53	0.42
1:A:897:GLY:O	1:A:899:THR:N	2.53	0.42
1:A:852:GLU:HG3	1:A:864:LEU:HD12	2.02	0.42
1:A:483:HIS:HB3	1:A:513:SER:OG	2.20	0.42
1:A:767:LEU:HD13	1:A:771:LEU:HD12	2.01	0.42
1:A:277:ARG:HH22	1:A:788:ASP:CG	2.23	0.41
1:A:743:GLN:NE2	1:A:876:ILE:HG12	2.32	0.41
1:A:230:SER:OG	1:A:231:GLN:N	2.53	0.41
1:A:466:LEU:HD11	1:A:476:ARG:HD3	2.02	0.41
1:A:248:PHE:C	1:A:250:THR:N	2.73	0.41
1:A:897:GLY:C	1:A:899:THR:N	2.74	0.41
1:A:1086:TRP:CE3	1:A:1090:LEU:HD21	2.55	0.41
1:A:1061:GLU:O	1:A:1064:ALA:HB3	2.19	0.41
1:A:792:LYS:HB3	1:A:818:ALA:HB3	2.02	0.41
1:A:908:ASN:OD1	1:A:994:VAL:HA	2.20	0.41
1:A:476:ARG:HG2	1:A:520:LEU:CD2	2.50	0.41
1:A:1048:ILE:H	1:A:1048:ILE:HG12	1.52	0.41
1:A:432:GLN:HB3	1:A:460:LEU:HD11	2.02	0.41
1:A:180:LEU:O	1:A:183:PRO:CD	2.68	0.41
1:A:475:LEU:HD23	1:A:527:ILE:HD12	2.02	0.41
2:A:101:3RE:H19	2:A:101:3RE:O13	2.20	0.41
1:A:354:LEU:C	1:A:356:ASP:H	2.24	0.41
1:A:752:LEU:O	1:A:753:SER:HB3	2.20	0.41
1:A:799:GLU:H	1:A:799:GLU:CD	2.23	0.41
1:A:150:PHE:O	1:A:153:GLN:N	2.54	0.41
1:A:381:VAL:HG21	1:A:404:PHE:CE1	2.56	0.41
1:A:363:VAL:CG1	1:A:414:LEU:HB2	2.51	0.41
1:A:838:LEU:HD12	1:A:838:LEU:HA	1.90	0.41
1:A:1082:VAL:O	1:A:1085:ASN:HB2	2.20	0.41
1:A:503:THR:O	1:A:503:THR:HG23	2.20	0.41
1:A:500:ASP:HB3	1:A:708:HIS:CD2	2.56	0.41
1:A:729:LEU:O	1:A:733:THR:OG1	2.39	0.41
1:A:618:ASP:OD1	1:A:618:ASP:N	2.51	0.41
1:A:784:ARG:NH1	1:A:789:PRO:O	2.54	0.40
1:A:946:ASP:HB2	1:A:983:VAL:O	2.20	0.40
1:A:163:THR:O	1:A:165:VAL:HG23	2.21	0.40
1:A:929:VAL:HG13	1:A:1009:PHE:HB2	2.04	0.40
1:A:370:ILE:HA	1:A:371:PRO:HD2	1.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:LEU:HD22	1:A:655:ASP:HB3	2.04	0.40
1:A:470:ASP:HB2	1:A:476:ARG:HH21	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	819/966 (85%)	687 (84%)	102 (12%)	30 (4%)	4 16

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	GLN
1	A	371	PRO
1	A	406	GLU
1	A	548	PRO
1	A	896	VAL
1	A	949	ASN
1	A	1044	SER
1	A	217	ASN
1	A	411	ASN
1	A	521	ASP
1	A	587	LYS
1	A	783	PHE
1	A	838	LEU
1	A	898	ASN
1	A	917	THR
1	A	1045	LYS
1	A	155	THR
1	A	615	GLU
1	A	761	SER

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Mol	Chain	Res	Type
1	A	797	ALA
1	A	916	PRO
1	A	967	HIS
1	A	214	LYS
1	A	558	ILE
1	A	776	ASN
1	A	1077	ASP
1	A	170	ASP
1	A	226	ARG
1	A	590	PRO
1	A	1079	GLY

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	751/864 (87%)	661 (88%)	90 (12%)	6 18

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	GLU
1	A	150	PHE
1	A	213	LYS
1	A	215	ILE
1	A	219	CYS
1	A	235	VAL
1	A	240	THR
1	A	247	SER
1	A	250	THR
1	A	269	ASP
1	A	278	ASP
1	A	279	GLU
1	A	281	LEU
1	A	282	VAL
1	A	285	THR

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Mol	Chain	Res	Type
1	A	291	GLN
1	A	305	VAL
1	A	320	LYS
1	A	321	GLU
1	A	357	CYS
1	A	359	ARG
1	A	366	ARG
1	A	369	ASP
1	A	370	ILE
1	A	373	LEU
1	A	379	LEU
1	A	381	VAL
1	A	391	GLN
1	A	470	ASP
1	A	481	VAL
1	A	486	GLN
1	A	498	ASN
1	A	511	GLU
1	A	521	ASP
1	A	527	ILE
1	A	544	ARG
1	A	561	THR
1	A	568	THR
1	A	574	LEU
1	A	575	LEU
1	A	587	LYS
1	A	601	GLN
1	A	618	ASP
1	A	626	LEU
1	A	646	GLN
1	A	682	LEU
1	A	711	GLN
1	A	717	LEU
1	A	729	LEU
1	A	749	ILE
1	A	751	SER
1	A	752	LEU
1	A	760	SER
1	A	775	GLN
1	A	776	ASN
1	A	778	GLN
1	A	779	LEU

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Mol	Chain	Res	Type
1	A	799	GLU
1	A	808	LYS
1	A	812	TRP
1	A	823	LEU
1	A	824	SER
1	A	838	LEU
1	A	843	LEU
1	A	845	LEU
1	A	876	ILE
1	A	886	THR
1	A	887	THR
1	A	890	LYS
1	A	893	GLN
1	A	894	SER
1	A	895	THR
1	A	903	LYS
1	A	907	LEU
1	A	908	ASN
1	A	911	LEU
1	A	918	GLU
1	A	948	HIS
1	A	953	MET
1	A	957	THR
1	A	968	ILE
1	A	983	VAL
1	A	1003	SER
1	A	1026	LEU
1	A	1032	SER
1	A	1042	LEU
1	A	1046	GLU
1	A	1048	ILE
1	A	1081	THR
1	A	1092	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	HIS
1	A	225	HIS
1	A	291	GLN
1	A	295	HIS
1	A	304	HIS

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Mol	Chain	Res	Type
1	A	391	GLN
1	A	498	ASN
1	A	550	GLN
1	A	646	GLN
1	A	710	GLN
1	A	711	GLN
1	A	734	GLN
1	A	743	GLN
1	A	778	GLN
1	A	834	HIS
1	A	840	GLN
1	A	893	GLN
1	A	949	ASN
1	A	959	ASN
1	A	971	ASN
1	A	1007	GLN
1	A	1083	GLN
1	A	1085	ASN
1	A	1089	HIS

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)

1 ligand is 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	3RE	A	101	-	26,29,29	1.95	7 (26%)	26,42,42	2.23	7 (26%)

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	3RE	A	101	-	-	0/9/20/20	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	101	3RE	C12-C6	-5.26	1.47	1.50
2	A	101	3RE	C6-C5	-4.42	1.37	1.43
2	A	101	3RE	C5-C4	-3.30	1.37	1.41
2	A	101	3RE	C14-N7	-2.90	1.44	1.49
2	A	101	3RE	C10-C9	-2.43	1.33	1.37
2	A	101	3RE	C8-C9	2.01	1.48	1.44
2	A	101	3RE	C2-N11	2.84	1.39	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	101	3RE	C22-C21-C9	-4.71	124.83	128.74
2	A	101	3RE	C26-O20-C17	-2.90	106.25	113.83
2	A	101	3RE	C22-C21-N25	-2.67	108.32	110.72
2	A	101	3RE	C22-C23-N24	-2.59	105.10	111.38
2	A	101	3RE	C2-N1-C6	-2.50	114.89	117.01
2	A	101	3RE	C9-C21-N25	5.21	126.78	120.77
2	A	101	3RE	C10-C5-C4	5.54	122.18	117.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	101	3RE	3	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, 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	839/966 (86%)	0.13	24 (2%) 55 49	27, 62, 92, 105	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	216	ALA	6.1
1	A	898	ASN	5.8
1	A	899	THR	5.1
1	A	381	VAL	3.1
1	A	234	LYS	3.1
1	A	217	ASN	2.9
1	A	1041	GLN	2.8
1	A	777	SER	2.7
1	A	232	THR	2.7
1	A	307	LEU	2.6
1	A	972	TYR	2.6
1	A	235	VAL	2.6
1	A	220	ILE	2.6
1	A	322	GLU	2.6
1	A	270	PHE	2.5
1	A	231	GLN	2.5
1	A	233	ILE	2.4
1	A	458	VAL	2.3
1	A	967	HIS	2.2
1	A	971	ASN	2.2
1	A	250	THR	2.2
1	A	730	HIS	2.1
1	A	404	PHE	2.0
1	A	998	SER	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, 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	LLDF	B-factors(Å^2)	Q<0.9
2	3RE	A	101	26/26	0.96	0.17	-0.46	38,41,49,49	0

6.5 Other polymers (i)

There are no such residues in this entry.