Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:24 AM GMT

PDB ID : 3IBE

Title : Crystal Structure of a Pyrazolopyrimidine Inhibitor Bound to PI3 Kinase Gamma

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Deposited on : 2009-07-15

Resolution : 2.80 Å(reported)

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 2.80 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.
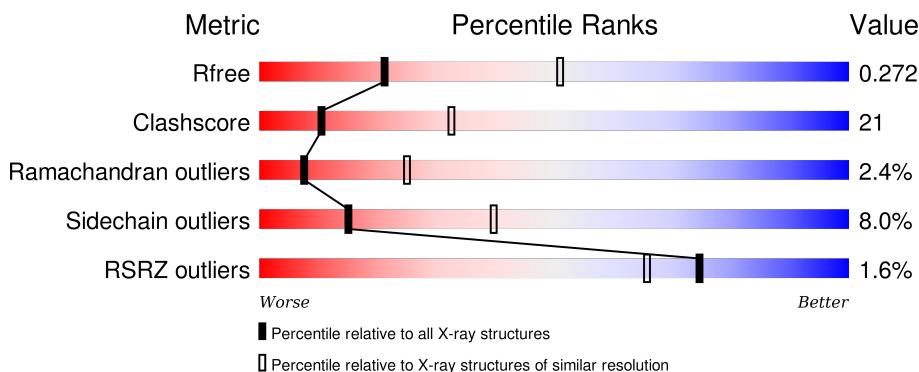
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	51% 34% • 12%
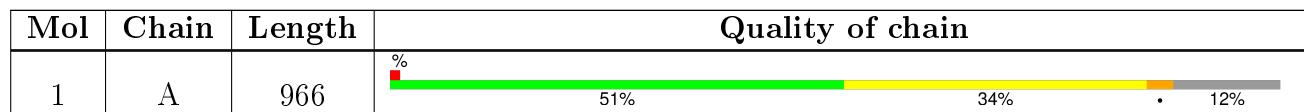
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	L64	A	1109	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6622 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
1	A	850	Total 6530	C 4195	N 1102	O 1199	S 34	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	EXPRESSION TAG	UNP P48736
A	459	ARG	GLN	VARIANT	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 SULFATE ION (three-letter code: SO4) (formula: O_4S).
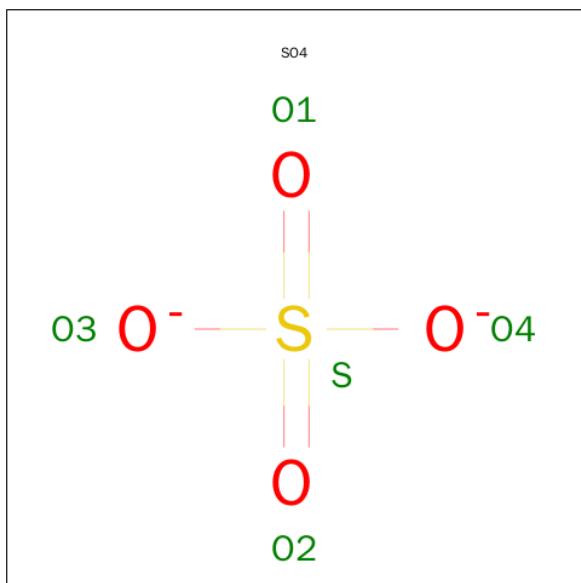
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0

- Molecule 3 is 1-(4-{4-MORPHOLIN-4-YL-1-[1-(PYRIDIN-3-YLCARBONYL)PIPERIDIN-4-YL]-1H-PYRAZOLO[3,4-D]PYRIMIDIN-6-YL}PHENYL)-3-PYRIDIN-4-YLUREA (three-letter code: L64) (formula: $C_{32}H_{32}N_{10}O_3$).
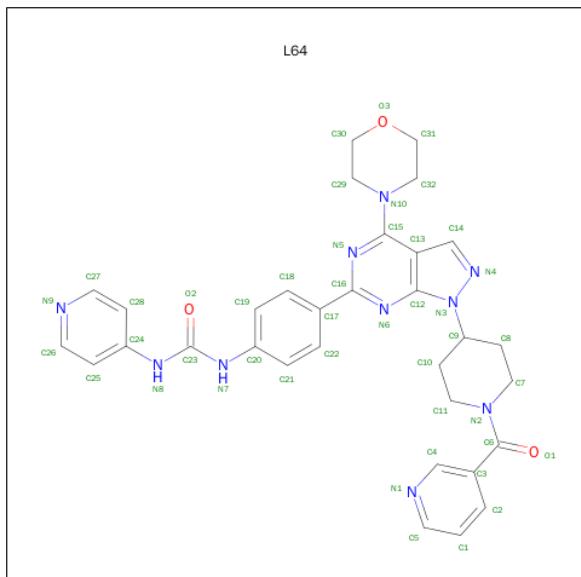
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 45	C 32	N 10	O 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total 42	O 42	0	0

3 Residue-property plots ⓘ

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
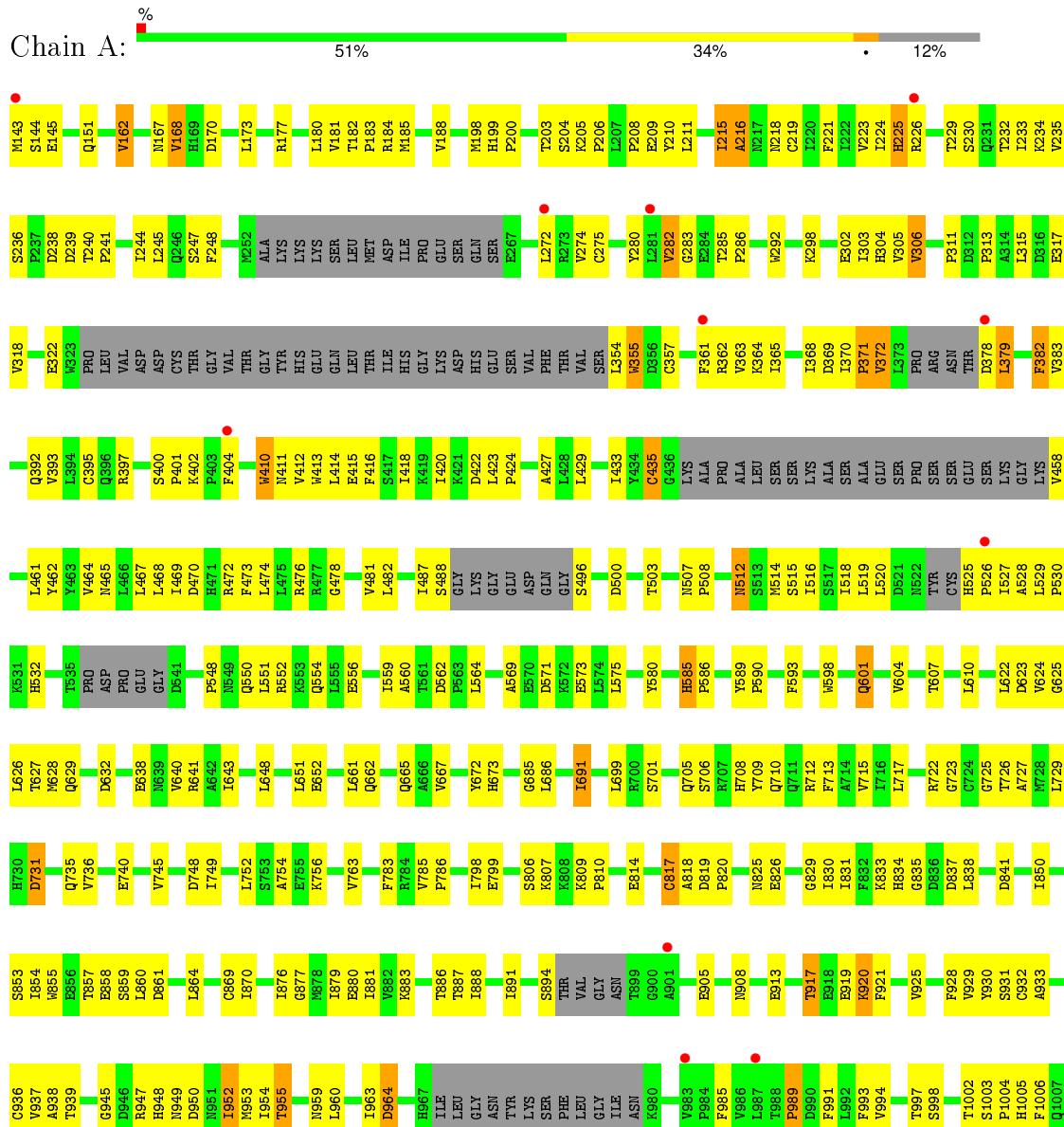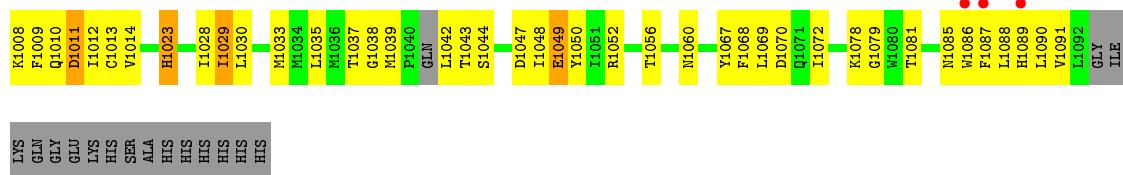
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	145.16Å 68.46Å 106.90Å 90.00° 94.80° 90.00°	Depositor
Resolution (Å)	44.71 – 2.80 44.71 – 2.80	Depositor EDS
% Data completeness (in resolution range)	83.1 (44.71-2.80) 83.2 (44.71-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.56 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.210 , 0.277 0.206 , 0.272	Depositor DCC
R_{free} test set	1117 reflections (5.43%)	DCC
Wilson B-factor (Å^2)	69.4	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 58.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.32$	Xtriage
Outliers	0 of 21699 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6622	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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: L64, SO4

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	0.56	0/6672	0.69	0/9081

There are no bond length outliers.

There are no bond angle outliers.

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	6530	0	6206	272	0
2	A	5	0	0	0	0
3	A	45	0	32	7	0
4	A	42	0	0	1	0
All	All	6622	0	6238	274	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 21.

All (274) 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:180:LEU:O	1:A:183:PRO:HD2	1.83	0.79
1:A:953:MET:O	1:A:960:LEU:HD12	1.85	0.76
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.70	0.72
1:A:274:VAL:HG21	1:A:292:TRP:CD1	2.26	0.70
1:A:181:VAL:O	1:A:185:MET:HG3	1.94	0.68
1:A:627:THR:HG21	1:A:648:LEU:HD21	1.76	0.68
1:A:685:GLY:HA2	1:A:691:ILE:HG22	1.77	0.67
1:A:219:CYS:SG	1:A:234:LYS:HG2	2.35	0.66
1:A:397:ARG:HD2	1:A:415:GLU:O	1.95	0.66
1:A:731:ASP:O	1:A:735:GLN:HG3	1.95	0.66
1:A:936:CYS:SG	1:A:985:PHE:CD1	2.89	0.65
1:A:925:VAL:O	1:A:929:VAL:HG23	1.96	0.65
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.31	0.65
1:A:564:LEU:HD21	1:A:1048:ILE:HG22	1.77	0.65
1:A:514:MET:HG3	1:A:515:SER:N	2.11	0.65
1:A:833:LYS:O	1:A:876:ILE:HG13	1.96	0.65
1:A:370:ILE:HG12	1:A:371:PRO:O	1.97	0.65
1:A:571:ASP:O	1:A:575:LEU:HD13	1.97	0.64
1:A:378:ASP:O	1:A:379:LEU:HG	1.97	0.64
1:A:355:TRP:CE3	1:A:530:PRO:HG2	2.33	0.64
1:A:627:THR:HG21	1:A:648:LEU:CD2	2.29	0.63
1:A:467:LEU:HD13	1:A:672:TYR:CE2	2.33	0.63
1:A:435:CYS:O	1:A:458:VAL:HA	1.98	0.63
1:A:933:ALA:O	1:A:937:VAL:HG23	1.98	0.62
1:A:368:ILE:HD13	1:A:514:MET:HE1	1.80	0.62
1:A:507:ASN:OD1	1:A:508:PRO:CD	2.48	0.62
1:A:354:LEU:O	1:A:527:ILE:HD11	1.99	0.62
1:A:224:ILE:O	1:A:230:SER:HA	1.99	0.62
1:A:888:ILE:O	1:A:891:ILE:HB	2.00	0.61
1:A:709:TYR:HB3	1:A:713:PHE:CE1	2.35	0.61
1:A:357:CYS:HB2	1:A:527:ILE:CD1	2.30	0.61
1:A:413:TRP:CH2	1:A:519:LEU:HD23	2.35	0.61
1:A:640:VAL:O	1:A:643:ILE:HG12	2.00	0.61
1:A:921:PHE:O	1:A:925:VAL:HG23	2.01	0.61
1:A:1081:THR:O	1:A:1085:ASN:OD1	2.18	0.61
1:A:629:GLN:HG2	1:A:1029:ILE:HG13	1.83	0.60
1:A:173:LEU:HD23	1:A:673:HIS:CD2	2.37	0.60
1:A:464:VAL:HG22	1:A:465:ASN:H	1.65	0.60
1:A:1003:SER:HB2	1:A:1004:PRO:CD	2.31	0.60
1:A:955:THR:OG1	1:A:959:ASN:HB3	2.02	0.60
1:A:469:ILE:N	1:A:469:ILE:HD12	2.17	0.59
1:A:1048:ILE:C	1:A:1050:TYR:N	2.55	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:930:TYR:CE2	1:A:1012:ILE:HD13	2.37	0.59
1:A:461:LEU:C	1:A:462:TYR:CD2	2.75	0.59
1:A:500:ASP:HB3	1:A:708:HIS:CD2	2.36	0.59
1:A:726:THR:HA	1:A:729:LEU:HD12	1.84	0.59
1:A:952:ILE:HG22	1:A:953:MET:N	2.17	0.59
1:A:662:GLN:HG2	1:A:1030:LEU:CD2	2.32	0.58
1:A:953:MET:SD	1:A:963:ILE:HD13	2.43	0.58
1:A:548:PRO:HG2	1:A:551:LEU:HD12	1.84	0.58
1:A:936:CYS:HB3	1:A:985:PHE:CE1	2.39	0.58
1:A:302:GLU:O	1:A:304:HIS:CD2	2.55	0.58
1:A:952:ILE:CG2	1:A:960:LEU:HD11	2.33	0.58
1:A:424:PRO:HD2	1:A:427:ALA:HB2	1.85	0.58
1:A:1069:LEU:HA	1:A:1072:ILE:HG13	1.85	0.58
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.85	0.57
1:A:1048:ILE:C	1:A:1050:TYR:H	2.07	0.57
1:A:424:PRO:HG3	1:A:598:TRP:O	2.04	0.57
1:A:143:MET:C	1:A:145:GLU:H	2.07	0.57
1:A:1044:SER:HB3	1:A:1047:ASP:OD2	2.04	0.57
1:A:215:ILE:O	1:A:216:ALA:HB3	2.05	0.56
1:A:585:HIS:ND1	1:A:585:HIS:N	2.53	0.56
1:A:928:PHE:HZ	1:A:991:PHE:CD1	2.22	0.56
1:A:282:VAL:CG2	1:A:283:GLY:N	2.69	0.56
1:A:928:PHE:O	1:A:932:CYS:HB3	2.06	0.56
1:A:275:CYS:SG	1:A:306:VAL:HG12	2.46	0.56
1:A:357:CYS:HB2	1:A:527:ILE:HD12	1.87	0.56
1:A:624:VAL:O	1:A:628:MET:HG2	2.05	0.55
1:A:745:VAL:O	1:A:749:ILE:HG12	2.05	0.55
1:A:1035:LEU:O	1:A:1042:LEU:CB	2.53	0.55
1:A:225:HIS:N	1:A:225:HIS:CD2	2.74	0.55
1:A:625:GLY:O	1:A:629:GLN:HG3	2.06	0.55
1:A:236:SER:HB3	1:A:239:ASP:OD1	2.07	0.55
1:A:422:ASP:OD1	1:A:601:GLN:HB3	2.07	0.55
1:A:1003:SER:HB2	1:A:1004:PRO:HD2	1.88	0.55
1:A:413:TRP:CZ2	1:A:519:LEU:HD23	2.41	0.55
1:A:831:ILE:O	1:A:831:ILE:HG22	2.05	0.54
1:A:952:ILE:HG21	1:A:960:LEU:HD11	1.90	0.54
1:A:685:GLY:HA2	1:A:691:ILE:CG2	2.38	0.54
1:A:831:ILE:HG13	1:A:881:ILE:HG13	1.90	0.54
1:A:853:SER:O	1:A:857:THR:HG23	2.07	0.54
1:A:913:GLU:O	1:A:913:GLU:HG2	2.08	0.54
1:A:280:TYR:HB3	1:A:282:VAL:HG12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:ILE:O	1:A:1050:TYR:N	2.40	0.53
1:A:887:THR:HA	1:A:953:MET:HG2	1.89	0.53
1:A:1006:PHE:CE2	1:A:1010:GLN:CD	2.82	0.53
1:A:317:GLU:HG2	1:A:318:VAL:N	2.24	0.53
1:A:837:ASP:O	3:A:1109:L64:C28	2.57	0.53
1:A:180:LEU:C	1:A:183:PRO:HD2	2.30	0.52
1:A:482:LEU:HB2	1:A:516:ILE:HG22	1.92	0.52
1:A:478:GLY:H	1:A:520:LEU:HB2	1.75	0.52
1:A:837:ASP:O	3:A:1109:L64:C27	2.57	0.52
1:A:838:LEU:HD12	1:A:877:GLY:CA	2.39	0.52
1:A:208:PRO:HD2	1:A:211:LEU:HB2	1.90	0.52
1:A:1035:LEU:HB3	1:A:1042:LEU:HA	1.90	0.52
1:A:948:HIS:CD2	1:A:1086:TRP:HB2	2.45	0.52
1:A:507:ASN:OD1	1:A:508:PRO:HD2	2.10	0.52
1:A:151:GLN:OE1	1:A:722:ARG:NH2	2.43	0.51
1:A:274:VAL:HG21	1:A:292:TRP:NE1	2.26	0.51
1:A:496:SER:HB3	1:A:1043:THR:HB	1.93	0.51
1:A:879:ILE:HG22	1:A:880:GLU:N	2.25	0.51
1:A:361:PHE:HD2	1:A:416:PHE:HD1	1.58	0.51
1:A:876:ILE:O	1:A:876:ILE:HG23	2.10	0.51
1:A:365:ILE:O	1:A:365:ILE:HG22	2.09	0.50
1:A:274:VAL:CG2	1:A:292:TRP:CD1	2.94	0.50
1:A:838:LEU:HD12	1:A:877:GLY:HA3	1.93	0.50
1:A:580:TYR:CE2	1:A:610:LEU:CD1	2.94	0.50
1:A:559:ILE:O	1:A:559:ILE:HG22	2.12	0.50
1:A:315:LEU:O	1:A:727:ALA:HB2	2.10	0.50
1:A:1044:SER:HB3	1:A:1047:ASP:CG	2.32	0.50
1:A:205:LYS:HB3	1:A:206:PRO:HD2	1.93	0.50
1:A:182:THR:HB	1:A:183:PRO:HD3	1.93	0.49
1:A:469:ILE:N	1:A:469:ILE:CD1	2.74	0.49
1:A:667:VAL:HG12	1:A:667:VAL:O	2.11	0.49
1:A:1089:HIS:C	1:A:1091:VAL:H	2.15	0.49
1:A:302:GLU:O	1:A:304:HIS:N	2.46	0.49
1:A:1006:PHE:C	1:A:1006:PHE:CD2	2.85	0.49
1:A:954:ILE:HA	1:A:959:ASN:O	2.12	0.49
1:A:238:ASP:HA	1:A:286:PRO:HB3	1.93	0.49
1:A:809:LYS:N	1:A:810:PRO:HD3	2.28	0.49
1:A:736:VAL:O	1:A:740:GLU:HB2	2.13	0.49
1:A:936:CYS:SG	1:A:985:PHE:CE1	3.05	0.49
1:A:952:ILE:N	1:A:952:ILE:CD1	2.75	0.49
1:A:371:PRO:O	1:A:372:VAL:C	2.50	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1056:THR:O	1:A:1056:THR:HG23	2.11	0.49
1:A:952:ILE:CG2	1:A:953:MET:N	2.76	0.48
1:A:1013:CYS:HB3	1:A:1068:PHE:HE2	1.76	0.48
1:A:1035:LEU:CD1	1:A:1048:ILE:HG12	2.42	0.48
1:A:1005:HIS:O	1:A:1008:LYS:HB3	2.12	0.48
1:A:854:ILE:HG22	1:A:854:ILE:O	2.12	0.48
1:A:368:ILE:HD13	1:A:514:MET:SD	2.53	0.48
1:A:948:HIS:ND1	1:A:950:ASP:HB2	2.28	0.48
1:A:465:ASN:HB2	1:A:503:THR:O	2.13	0.48
1:A:837:ASP:O	3:A:1109:L64:H27	2.13	0.48
1:A:363:VAL:O	1:A:363:VAL:HG13	2.14	0.48
1:A:550:GLN:O	1:A:554:GLN:HG3	2.14	0.48
1:A:673:HIS:HA	1:A:712:ARG:HE	1.78	0.48
1:A:754:ALA:C	1:A:756:LYS:N	2.67	0.48
1:A:233:ILE:HD11	1:A:248:PHE:HD1	1.78	0.48
1:A:1023:HIS:N	1:A:1023:HIS:ND1	2.62	0.47
1:A:464:VAL:HG22	1:A:465:ASN:N	2.28	0.47
1:A:1067:TYR:O	1:A:1070:ASP:HB2	2.14	0.47
1:A:274:VAL:CG1	1:A:275:CYS:N	2.76	0.47
1:A:1078:LYS:O	1:A:1079:GLY:C	2.53	0.47
1:A:420:ILE:CG2	1:A:420:ILE:O	2.62	0.47
1:A:224:ILE:C	1:A:225:HIS:CD2	2.88	0.47
1:A:699:LEU:HD13	1:A:717:LEU:HB2	1.97	0.47
1:A:1078:LYS:O	1:A:1081:THR:HG23	2.13	0.47
1:A:361:PHE:HB2	1:A:420:ILE:HG13	1.97	0.47
1:A:184:ARG:HB2	1:A:184:ARG:HH11	1.79	0.47
1:A:725:GLY:O	1:A:729:LEU:HG	2.15	0.47
1:A:917:THR:OG1	1:A:919:GLU:HB3	2.15	0.47
1:A:379:LEU:HD13	1:A:435:CYS:SG	2.55	0.46
1:A:383:VAL:HG22	1:A:433:ILE:HG12	1.98	0.46
1:A:632:ASP:HB3	1:A:1033:MET:HE3	1.97	0.46
1:A:355:TRP:HE3	1:A:530:PRO:HG2	1.78	0.46
1:A:1010:GLN:O	1:A:1014:VAL:HG23	2.15	0.46
1:A:204:SER:HB2	1:A:652:GLU:OE2	2.15	0.46
1:A:604:VAL:O	1:A:607:THR:HB	2.15	0.46
1:A:298:LYS:HE3	1:A:861:ASP:OD2	2.16	0.46
1:A:686:LEU:CD2	1:A:723:GLY:C	2.83	0.46
1:A:414:LEU:HA	1:A:414:LEU:HD23	1.80	0.46
1:A:382:PHE:HD1	1:A:382:PHE:H	1.64	0.46
1:A:472:ARG:O	1:A:473:PHE:HB2	2.16	0.46
1:A:368:ILE:C	1:A:368:ILE:HD12	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:ILE:HD13	1:A:514:MET:CE	2.46	0.46
1:A:748:ASP:O	1:A:752:LEU:HD13	2.16	0.46
1:A:274:VAL:CG2	1:A:292:TRP:NE1	2.79	0.46
1:A:1009:PHE:CD2	1:A:1009:PHE:C	2.89	0.46
1:A:240:THR:O	1:A:244:ILE:HG13	2.15	0.45
1:A:834:HIS:ND1	1:A:835:GLY:N	2.64	0.45
1:A:837:ASP:O	3:A:1109:L64:H28	2.17	0.45
1:A:223:VAL:HG12	1:A:225:HIS:NE2	2.31	0.45
1:A:1008:LYS:O	1:A:1011:ASP:HB2	2.17	0.45
1:A:825:ASN:O	1:A:826:GLU:C	2.53	0.45
1:A:569:ALA:O	1:A:573:GLU:HG3	2.16	0.45
1:A:997:THR:HG22	1:A:998:SER:N	2.31	0.45
1:A:917:THR:HG23	1:A:920:LYS:CD	2.47	0.45
1:A:552:ARG:O	1:A:556:GLU:HG3	2.16	0.45
1:A:306:VAL:O	1:A:306:VAL:HG22	2.17	0.45
1:A:936:CYS:SG	1:A:985:PHE:HD1	2.36	0.45
1:A:834:HIS:HB2	1:A:876:ILE:HD12	1.99	0.45
3:A:1109:L64:H19	3:A:1109:L64:O2	2.16	0.45
1:A:947:ARG:HH21	1:A:947:ARG:HG3	1.82	0.45
1:A:184:ARG:O	1:A:188:VAL:HG23	2.17	0.45
1:A:947:ARG:NH1	1:A:964:ASP:O	2.49	0.44
1:A:838:LEU:HD12	1:A:877:GLY:N	2.32	0.44
1:A:551:LEU:HA	1:A:551:LEU:HD23	1.75	0.44
1:A:686:LEU:HD22	1:A:723:GLY:O	2.17	0.44
1:A:393:VAL:O	1:A:393:VAL:HG23	2.16	0.44
1:A:525:HIS:N	1:A:526:PRO:CD	2.81	0.44
1:A:210:TYR:HE2	1:A:859:SER:HA	1.82	0.44
1:A:209:GLU:HB2	1:A:859:SER:HB3	2.00	0.44
1:A:496:SER:HA	1:A:1043:THR:O	2.17	0.44
1:A:372:VAL:HG12	1:A:372:VAL:O	2.17	0.44
1:A:955:THR:OG1	1:A:959:ASN:CB	2.65	0.44
1:A:210:TYR:HE2	1:A:860:LEU:N	2.16	0.44
1:A:661:LEU:O	1:A:665:GLN:HG2	2.17	0.44
1:A:931:SER:OG	1:A:932:CYS:N	2.50	0.44
1:A:831:ILE:HG13	1:A:881:ILE:CG1	2.48	0.44
1:A:550:GLN:O	1:A:550:GLN:HG3	2.17	0.44
1:A:514:MET:CG	1:A:515:SER:N	2.80	0.43
1:A:167:ASN:C	1:A:168:VAL:CG1	2.85	0.43
1:A:354:LEU:O	1:A:527:ILE:CG1	2.67	0.43
1:A:855:TRP:HZ3	1:A:864:LEU:HD11	1.82	0.43
1:A:210:TYR:CE2	1:A:860:LEU:N	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ASP:O	1:A:379:LEU:CG	2.65	0.43
1:A:799:GLU:H	1:A:799:GLU:CD	2.22	0.43
1:A:931:SER:OG	1:A:960:LEU:HB3	2.19	0.43
1:A:830:ILE:HG22	1:A:831:ILE:N	2.33	0.43
1:A:481:VAL:HA	1:A:516:ILE:O	2.18	0.43
1:A:1088:LEU:O	1:A:1091:VAL:HB	2.19	0.43
1:A:939:THR:HB	1:A:945:GLY:HA2	2.00	0.43
1:A:215:ILE:O	1:A:216:ALA:CB	2.66	0.43
1:A:221:PHE:HD2	1:A:232:THR:CG2	2.32	0.43
1:A:855:TRP:O	1:A:860:LEU:O	2.36	0.43
1:A:170:ASP:C	1:A:170:ASP:OD1	2.57	0.43
1:A:908:ASN:OD1	1:A:994:VAL:HG22	2.17	0.43
1:A:589:TYR:O	1:A:593:PHE:CD1	2.72	0.43
1:A:925:VAL:O	1:A:925:VAL:HG12	2.17	0.43
1:A:401:PRO:O	1:A:402:LYS:HG3	2.19	0.43
1:A:857:THR:C	1:A:858:GLU:HG2	2.38	0.42
1:A:1033:MET:O	1:A:1037:THR:HG23	2.19	0.42
1:A:423:LEU:HA	1:A:424:PRO:HD3	1.82	0.42
1:A:362:ARG:HG3	1:A:413:TRP:CZ3	2.54	0.42
1:A:829:GLY:O	1:A:881:ILE:HB	2.19	0.42
1:A:412:VAL:O	1:A:412:VAL:HG23	2.20	0.42
1:A:474:LEU:HD23	1:A:528:ALA:HB2	2.02	0.42
1:A:512:ASN:OD1	1:A:512:ASN:N	2.53	0.42
1:A:667:VAL:O	1:A:667:VAL:CG1	2.67	0.42
1:A:210:TYR:CE2	1:A:859:SER:HA	2.54	0.42
1:A:218:ASN:O	1:A:218:ASN:ND2	2.53	0.42
1:A:368:ILE:HG23	1:A:410:TRP:HZ3	1.83	0.42
1:A:143:MET:C	1:A:145:GLU:N	2.72	0.42
3:A:1109:L64:H29A	3:A:1109:L64:H14	2.01	0.42
1:A:361:PHE:HD2	1:A:416:PHE:CD1	2.37	0.42
1:A:589:TYR:HB2	1:A:590:PRO:HD3	2.01	0.42
1:A:905:GLU:HG2	1:A:993:PHE:CE1	2.54	0.42
1:A:586:PRO:O	1:A:626:LEU:HD21	2.20	0.42
1:A:470:ASP:CB	1:A:476:ARG:NH1	2.83	0.42
1:A:640:VAL:HG12	1:A:641:ARG:N	2.35	0.41
1:A:241:PRO:O	1:A:245:LEU:HD12	2.20	0.41
1:A:1089:HIS:O	1:A:1091:VAL:N	2.53	0.41
1:A:817:CYS:O	1:A:819:ASP:N	2.53	0.41
1:A:886:THR:HG23	1:A:887:THR:O	2.20	0.41
1:A:706:SER:O	1:A:710:GLN:HB3	2.20	0.41
1:A:478:GLY:N	1:A:520:LEU:HB2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:ILE:CG2	1:A:880:GLU:N	2.83	0.41
1:A:850:ILE:O	1:A:854:ILE:HG13	2.21	0.41
1:A:964:ASP:HA	3:A:1109:L64:C20	2.51	0.41
1:A:798:ILE:HG12	1:A:798:ILE:H	1.65	0.41
1:A:420:ILE:O	1:A:420:ILE:HG22	2.21	0.41
1:A:917:THR:HG23	1:A:920:LYS:HD3	2.03	0.41
1:A:311:PRO:O	1:A:313:PRO:HD3	2.21	0.41
1:A:785:VAL:HA	1:A:786:PRO:HD3	1.91	0.41
1:A:783:PHE:CD2	1:A:783:PHE:C	2.93	0.41
1:A:364:LYS:O	1:A:518:ILE:HA	2.21	0.41
1:A:1042:LEU:O	1:A:1043:THR:C	2.59	0.41
1:A:354:LEU:O	1:A:527:ILE:CD1	2.67	0.41
1:A:199:HIS:O	1:A:200:PRO:C	2.58	0.41
1:A:838:LEU:HD23	1:A:838:LEU:HA	1.88	0.40
1:A:623:ASP:OD1	1:A:623:ASP:C	2.59	0.40
1:A:1089:HIS:C	1:A:1091:VAL:N	2.74	0.40
1:A:817:CYS:SG	1:A:819:ASP:HB3	2.62	0.40
1:A:819:ASP:HA	1:A:820:PRO:HD3	1.90	0.40
1:A:883:LYS:HD3	1:A:883:LYS:HA	1.86	0.40
1:A:198:MET:O	1:A:199:HIS:C	2.60	0.40
1:A:177:ARG:HG2	1:A:715:VAL:HG13	2.02	0.40
1:A:564:LEU:HD13	1:A:1028:ILE:CG2	2.52	0.40
1:A:529:LEU:HA	1:A:530:PRO:HD3	1.85	0.40
1:A:1009:PHE:HE2	1:A:1072:ILE:HD13	1.86	0.40
1:A:1008:LYS:O	1:A:1011:ASP:CB	2.70	0.40
1:A:622:LEU:HD21	1:A:651:LEU:HD21	2.04	0.40
1:A:560:ALA:HB2	4:A:86:HOH:O	2.22	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	828/966 (86%)	714 (86%)	94 (11%)	20 (2%)	7 25

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	303	ILE
1	A	371	PRO
1	A	216	ALA
1	A	372	VAL
1	A	638	GLU
1	A	691	ILE
1	A	964	ASP
1	A	1049	GLU
1	A	379	LEU
1	A	532	HIS
1	A	806	SER
1	A	818	ALA
1	A	1090	LEU
1	A	411	ASN
1	A	938	ALA
1	A	144	SER
1	A	162	VAL
1	A	989	PRO
1	A	215	ILE
1	A	1038	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	671/864 (78%)	617 (92%)	54 (8%)	15 40

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	VAL

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Mol	Chain	Res	Type
1	A	168	VAL
1	A	203	THR
1	A	225	HIS
1	A	226	ARG
1	A	229	THR
1	A	235	VAL
1	A	247	SER
1	A	282	VAL
1	A	285	THR
1	A	306	VAL
1	A	322	GLU
1	A	355	TRP
1	A	369	ASP
1	A	382	PHE
1	A	392	GLN
1	A	395	CYS
1	A	400	SER
1	A	404	PHE
1	A	410	TRP
1	A	418	ILE
1	A	435	CYS
1	A	487	ILE
1	A	488	SER
1	A	512	ASN
1	A	562	ASP
1	A	585	HIS
1	A	601	GLN
1	A	701	SER
1	A	705	GLN
1	A	731	ASP
1	A	763	VAL
1	A	807	LYS
1	A	814	GLU
1	A	817	CYS
1	A	841	ASP
1	A	869	CYS
1	A	870	ILE
1	A	894	SER
1	A	917	THR
1	A	920	LYS
1	A	949	ASN
1	A	952	ILE

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Mol	Chain	Res	Type
1	A	955	THR
1	A	989	PRO
1	A	1002	THR
1	A	1011	ASP
1	A	1023	HIS
1	A	1029	ILE
1	A	1039	MET
1	A	1049	GLU
1	A	1052	ARG
1	A	1060	ASN
1	A	1087	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	SO4	A	1	-	4,4,4	0.24	0	6,6,6	0.17	0
3	L64	A	1109	-	49,51,51	0.83	3 (6%)	60,71,71	1.75	15 (25%)

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	SO4	A	1	-	-	0/0/0/0	0/0/0/0
3	L64	A	1109	-	-	0/24/46/46	0/7/7/7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1109	L64	C3-C6	-2.40	1.46	1.50
3	A	1109	L64	C13-C12	-2.02	1.38	1.43
3	A	1109	L64	C15-N5	2.32	1.35	1.32

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1109	L64	C11-C10-C9	-4.60	106.78	110.41
3	A	1109	L64	C3-C6-N2	-4.45	112.82	118.76
3	A	1109	L64	N8-C23-N7	-3.36	107.25	112.53
3	A	1109	L64	C8-C7-N2	-3.17	106.47	111.07
3	A	1109	L64	C10-C11-N2	-2.75	107.08	111.07
3	A	1109	L64	C7-C8-C9	-2.70	108.27	110.41
3	A	1109	L64	C1-C2-C3	-2.49	117.20	120.33
3	A	1109	L64	C14-C13-C12	-2.43	102.95	105.20
3	A	1109	L64	C16-N6-C12	-2.24	111.70	115.00
3	A	1109	L64	C2-C3-C4	2.15	120.19	117.67
3	A	1109	L64	C15-N5-C16	2.27	120.50	116.38
3	A	1109	L64	C24-N8-C23	2.28	131.04	126.65
3	A	1109	L64	C32-N10-C29	2.83	117.54	111.59
3	A	1109	L64	O1-C6-N2	2.85	126.96	122.42
3	A	1109	L64	C8-C9-N3	4.23	116.53	110.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1109	L64	7	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	850/966 (87%)	-0.06	14 (1%)	74　66	34, 68, 115, 148	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	378	ASP	3.5
1	A	404	PHE	3.5
1	A	226	ARG	3.3
1	A	1086	TRP	2.9
1	A	901	ALA	2.9
1	A	361	PHE	2.7
1	A	1089	HIS	2.4
1	A	272	LEU	2.3
1	A	526	PRO	2.3
1	A	983	VAL	2.3
1	A	143	MET	2.2
1	A	281	LEU	2.1
1	A	1087	PHE	2.1
1	A	987	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(Å^2)	Q<0.9
3	L64	A	1109	45/45	0.91	0.28	3.19	52,75,98,110	0
2	SO4	A	1	5/5	0.98	0.08	-2.66	62,75,89,94	0

6.5 Other polymers (i)

There are no such residues in this entry.