Full wwPDB X-ray Structure Validation Report (i)

Mar 16, 2016 – 06:49 PM EDT

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PDB ID	:	5EUQ
Title	:	Crystal structure of an engineered construct of phosphatidylinositol 4 kinase III beta with a potent and selective inhibitor in complex with GDP loaded Rab11
Authors	:	Burke, J.E.; Fowler, M.L.
Deposited on	:	2015-11-19
Resolution	:	3.20 Å(reported)

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.20 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.
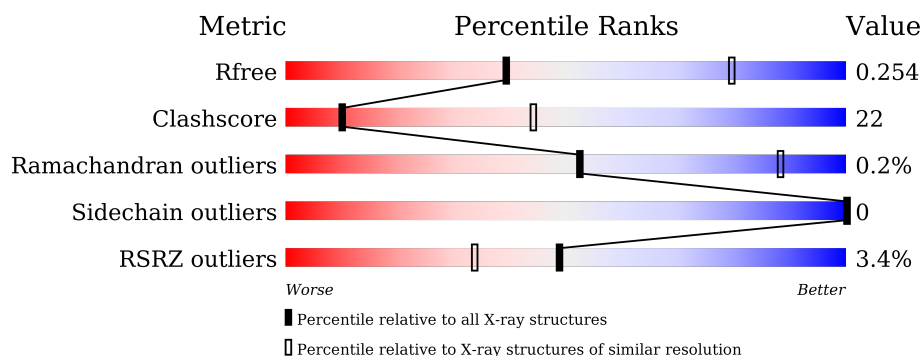
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	B	219	6% / 44% 26% 29%
2	E	529	2% / 52% 35% 12%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5065 atoms, of which 25 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 Ras-related protein Rab-11A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	155	Total 1230	C 781	N 209	O 239	S 1	90	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP P62491
B	-1	SER	-	expression tag	UNP P62491
B	0	HIS	-	expression tag	UNP P62491
B	70	LEU	GLN	conflict	UNP P62491

- Molecule 2 is a protein called Phosphatidylinositol 4-kinase beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	464	Total 3739	C 2402	N 644	O 669	S 24	37	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	117	GLY	-	expression tag	UNP Q9UBF8
E	118	SER	-	expression tag	UNP Q9UBF8
E	119	HIS	-	expression tag	UNP Q9UBF8
E	120	MET	-	expression tag	UNP Q9UBF8
E	294	ALA	SER	engineered mutation	UNP O02810

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).
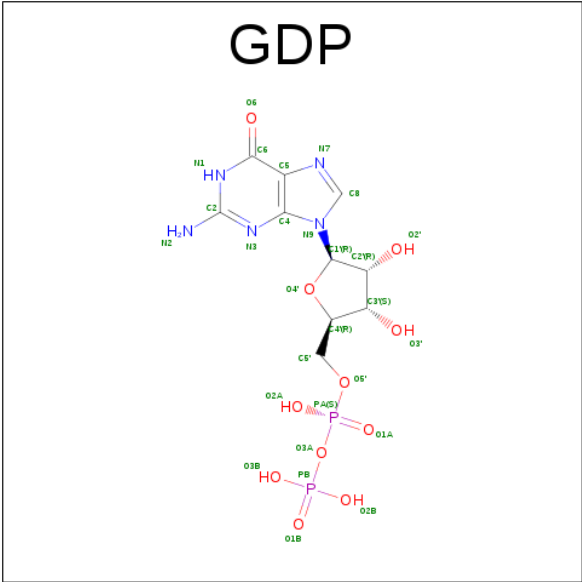
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
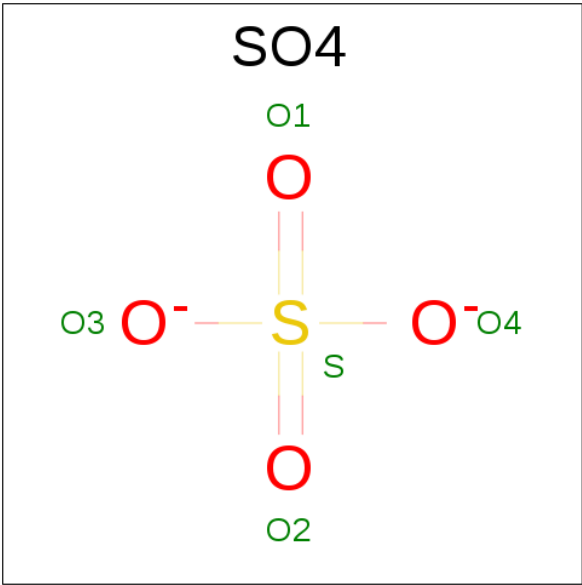
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is {N}-[5-[3-[[(4-hydroxyphenyl)amino]-bis(oxidanyl)-l^{4}-sulfanyl]-4-met

hoxy-phenyl]-4-methyl-1,3-thiazol-2-yl]cyclopentanecarboxamide (three-letter code: 5S8) (formula: $C_{23}H_{27}N_3O_5S_2$).
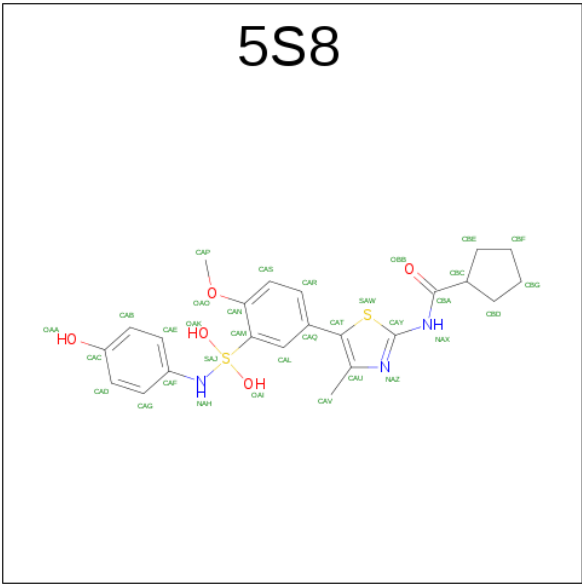
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
5	E	1	58	23	25	3	5	2	0	0

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: Ras-related protein Rab-11A
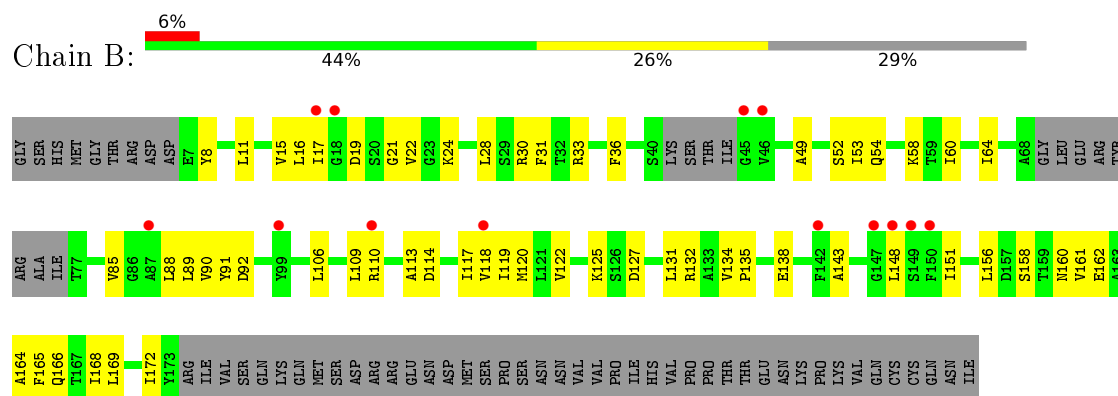
• Molecule 2: Phosphatidylinositol 4-kinase beta
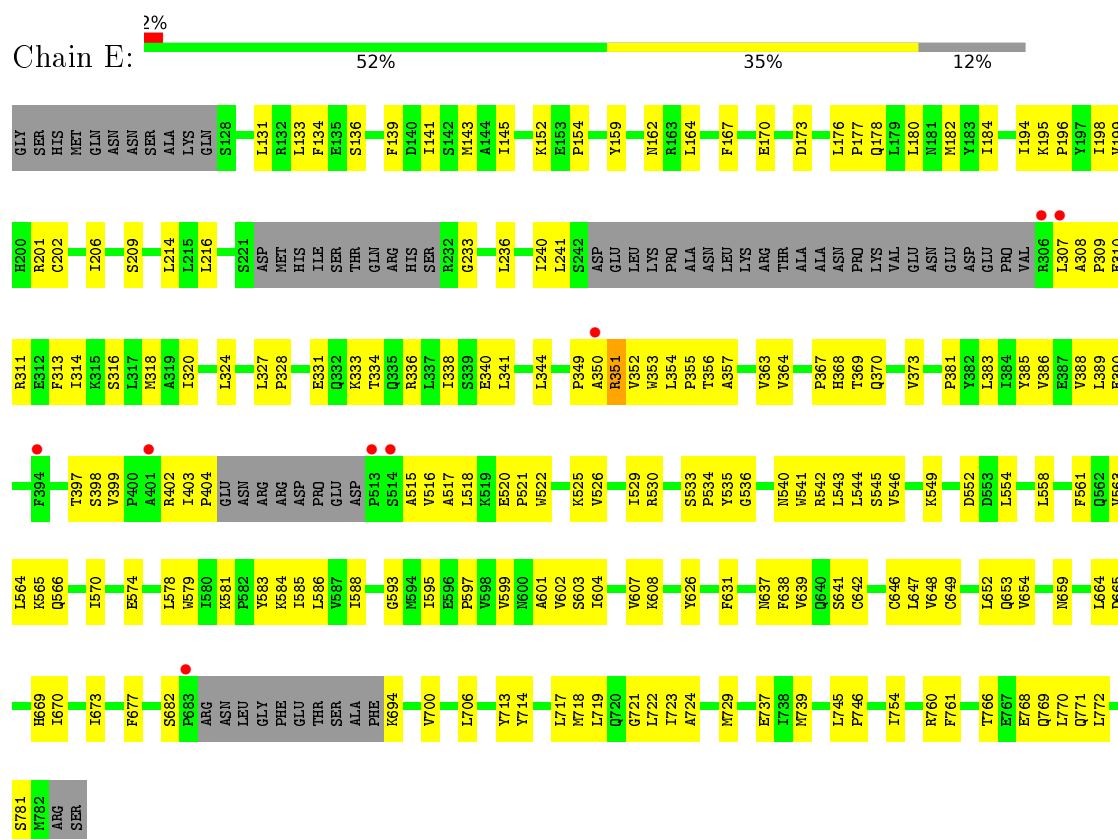
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	48.90Å 103.49Å 188.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.34 – 3.20 47.34 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.4 (47.34-3.20) 98.6 (47.34-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.12 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.233 , 0.266 0.235 , 0.254	Depositor DCC
R_{free} test set	1397 reflections (4.94%)	DCC
Wilson B-factor (Å^2)	81.1	Xtriage
Anisotropy	0.795	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 79.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.46, <L^2> = 0.29$	Xtriage
Outliers	1 of 16316 reflections (0.006%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5065	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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: GDP, SO4, 5S8

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	B	0.24	0/1249	0.39	0/1688
2	E	0.24	0/3817	0.39	0/5155
All	All	0.24	0/5066	0.39	0/6843

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	B	1230	0	1213	64	0
2	E	3739	0	3797	153	0
3	B	28	0	12	5	0
4	E	10	0	0	2	0
5	E	33	25	0	0	0
All	All	5040	25	5022	214	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 22.

All (214) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:549:LYS:HD3	2:E:552:ASP:HB2	1.40	1.01
2:E:549:LYS:HD2	2:E:554:LEU:HD21	1.47	0.95
1:B:24:LYS:HG2	3:B:301:GDP:O1B	1.75	0.85
1:B:165:PHE:HA	1:B:168:ILE:HG22	1.59	0.84
1:B:135:PRO:HG2	1:B:138:GLU:HB2	1.59	0.82
2:E:700:VAL:HG11	2:E:706:LEU:HD12	1.61	0.82
2:E:308:ALA:HB3	2:E:309:PRO:HD3	1.61	0.81
2:E:766:THR:HG23	2:E:769:GLN:H	1.45	0.81
1:B:113:ALA:HB1	1:B:117:ILE:HD13	1.65	0.79
2:E:564:LEU:HD21	2:E:648:VAL:HG11	1.66	0.78
1:B:168:ILE:O	1:B:172:ILE:HG12	1.86	0.75
2:E:574:GLU:HG3	2:E:724:ALA:HB1	1.66	0.75
2:E:139:PHE:HA	2:E:143:MET:HE3	1.69	0.74
2:E:333:LYS:HB3	2:E:373:VAL:HG21	1.70	0.73
2:E:206:ILE:HD11	2:E:307:LEU:HG	1.72	0.71
2:E:554:LEU:HD12	2:E:593:GLY:HA3	1.71	0.71
2:E:520:GLU:HG3	2:E:525:LYS:HG3	1.73	0.71
1:B:88:LEU:HD21	1:B:120:MET:CE	2.21	0.70
2:E:351:ARG:HG3	2:E:399:VAL:HG13	1.73	0.69
2:E:351:ARG:HG3	2:E:399:VAL:CG1	2.23	0.69
1:B:125:LYS:HG2	3:B:301:GDP:C5	2.29	0.68
2:E:381:PRO:HB3	2:E:549:LYS:HB3	1.75	0.68
2:E:642:CYS:HA	2:E:670:ILE:HD11	1.75	0.68
2:E:578:LEU:HD21	2:E:717:LEU:HB3	1.76	0.67
1:B:91:TYR:CE1	1:B:134:VAL:HG11	2.30	0.66
2:E:530:ARG:HD2	2:E:541:TRP:CE3	2.32	0.65
1:B:156:LEU:HD21	2:E:131:LEU:HD11	1.78	0.65
2:E:214:LEU:HD22	2:E:588:ILE:HA	1.79	0.64
2:E:180:LEU:HD22	2:E:216:LEU:HD21	1.79	0.64
2:E:722:LEU:HD23	2:E:770:LEU:HD11	1.79	0.64
2:E:390:GLU:N	2:E:540:ASN:OD1	2.30	0.64
2:E:139:PHE:HA	2:E:143:MET:CE	2.28	0.63
2:E:403:ILE:HG13	2:E:534:PRO:HB2	1.79	0.63
2:E:649:CYS:HA	2:E:654:VAL:HG23	1.80	0.62
2:E:722:LEU:CD2	2:E:770:LEU:HD11	2.29	0.62
1:B:21:GLY:N	3:B:301:GDP:O2B	2.18	0.62
2:E:554:LEU:CD1	2:E:593:GLY:HA3	2.30	0.62
2:E:603:SER:O	2:E:607:VAL:HG23	2.00	0.62
2:E:313:PHE:CG	2:E:352:VAL:HG11	2.34	0.61
2:E:530:ARG:HB2	2:E:541:TRP:CH2	2.35	0.61
2:E:355:PRO:HB2	2:E:586:LEU:HD12	1.81	0.61
1:B:88:LEU:HD21	1:B:120:MET:HE2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:VAL:HG13	1:B:92:ASP:HB2	1.84	0.59
2:E:195:LYS:N	2:E:196:PRO:HD2	2.17	0.59
2:E:604:ILE:HB	2:E:659:ASN:HB3	1.83	0.59
2:E:564:LEU:HD21	2:E:648:VAL:CG1	2.31	0.59
1:B:114:ASP:HB3	1:B:117:ILE:HG23	1.85	0.59
1:B:151:ILE:HD11	1:B:160:ASN:HB3	1.84	0.58
2:E:236:LEU:O	2:E:240:ILE:HG12	2.02	0.58
2:E:583:TYR:CE2	2:E:673:ILE:HG22	2.38	0.58
2:E:236:LEU:HD11	2:E:240:ILE:HD11	1.85	0.58
2:E:516:VAL:HG12	2:E:518:LEU:CD1	2.34	0.58
2:E:729:MET:HE3	2:E:761:PHE:HB2	1.85	0.57
1:B:131:LEU:HD11	2:E:162:ASN:HA	1.87	0.57
2:E:369:THR:HG21	2:E:515:ALA:HB1	1.86	0.57
1:B:113:ALA:HB1	1:B:117:ILE:CD1	2.34	0.57
1:B:156:LEU:HD23	1:B:156:LEU:O	2.05	0.56
1:B:30:ARG:HH21	1:B:36:PHE:HB3	1.70	0.56
2:E:370:GLN:HG3	2:E:529:ILE:HD11	1.86	0.56
1:B:132:ARG:NH1	1:B:134:VAL:O	2.37	0.56
2:E:520:GLU:HB2	2:E:521:PRO:HD2	1.88	0.56
2:E:665:ASP:OD1	2:E:669:HIS:N	2.39	0.56
2:E:677:PHE:HD2	2:E:682:SER:HA	1.69	0.56
2:E:545:SER:O	2:E:597:PRO:HD2	2.06	0.56
2:E:195:LYS:O	2:E:199:VAL:HG23	2.07	0.55
2:E:173:ASP:OD1	2:E:201:ARG:NH1	2.39	0.55
2:E:700:VAL:HG11	2:E:706:LEU:CD1	2.34	0.55
2:E:152:LYS:O	2:E:154:PRO:HD3	2.05	0.55
2:E:729:MET:CE	2:E:761:PHE:HB2	2.36	0.55
2:E:178:GLN:O	2:E:182:MET:HG3	2.07	0.55
2:E:563:VAL:HG11	2:E:652:LEU:HD21	1.88	0.54
1:B:119:ILE:O	1:B:148:LEU:HB2	2.07	0.54
1:B:165:PHE:HA	1:B:168:ILE:CG2	2.34	0.54
1:B:118:VAL:HB	1:B:172:ILE:HD11	1.90	0.54
1:B:8:TYR:HE1	1:B:11:LEU:HB2	1.71	0.54
1:B:8:TYR:OH	1:B:11:LEU:HD12	2.08	0.54
2:E:318:MET:HE3	2:E:588:ILE:HG13	1.90	0.54
2:E:713:TYR:O	2:E:717:LEU:HG	2.08	0.53
2:E:141:ILE:O	2:E:145:ILE:HG13	2.09	0.53
2:E:176:LEU:HB3	2:E:177:PRO:HD3	1.91	0.53
2:E:549:LYS:CD	2:E:554:LEU:HD21	2.30	0.53
2:E:355:PRO:HB2	2:E:586:LEU:CD1	2.40	0.52
2:E:320:ILE:HG12	2:E:340:GLU:CG	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ALA:HB1	1:B:148:LEU:O	2.09	0.52
2:E:367:PRO:HD2	2:E:385:TYR:O	2.10	0.52
2:E:549:LYS:HD3	2:E:552:ASP:CB	2.25	0.52
1:B:17:ILE:CD1	1:B:89:LEU:HA	2.40	0.51
2:E:520:GLU:HG3	2:E:525:LYS:CG	2.39	0.51
2:E:574:GLU:CG	2:E:724:ALA:HB1	2.39	0.51
2:E:637:ASN:HB3	2:E:669:HIS:CD2	2.45	0.51
1:B:31:PHE:CE1	1:B:165:PHE:HB2	2.46	0.51
1:B:64:ILE:H	1:B:64:ILE:HD12	1.76	0.51
2:E:383:LEU:C	2:E:383:LEU:HD23	2.31	0.50
2:E:209:SER:O	2:E:240:ILE:HG21	2.12	0.50
2:E:649:CYS:HA	2:E:654:VAL:CG2	2.41	0.50
2:E:579:TRP:O	2:E:641:SER:HA	2.11	0.50
2:E:370:GLN:HG3	2:E:529:ILE:CD1	2.42	0.50
2:E:522:TRP:CE3	2:E:599:VAL:HG11	2.47	0.50
2:E:639:VAL:HG13	2:E:714:TYR:HB2	1.93	0.50
2:E:164:LEU:HA	2:E:167:PHE:HD2	1.77	0.49
2:E:608:LYS:NZ	4:E:1001:SO4:O4	2.38	0.49
1:B:17:ILE:HD12	1:B:89:LEU:HA	1.93	0.49
2:E:638:PHE:O	2:E:642:CYS:HB2	2.12	0.49
2:E:318:MET:CE	2:E:588:ILE:HG13	2.43	0.49
2:E:363:VAL:HA	2:E:388:VAL:HG12	1.94	0.49
2:E:578:LEU:CD2	2:E:717:LEU:HB3	2.41	0.49
1:B:135:PRO:CG	1:B:138:GLU:HB2	2.36	0.48
1:B:88:LEU:HD22	1:B:122:VAL:HG21	1.93	0.48
1:B:8:TYR:CE1	1:B:11:LEU:HB2	2.48	0.48
1:B:106:LEU:O	1:B:110:ARG:HG2	2.14	0.48
2:E:397:THR:HG22	2:E:398:SER:O	2.13	0.48
1:B:64:ILE:N	1:B:64:ILE:HD12	2.28	0.48
1:B:118:VAL:HB	1:B:172:ILE:CD1	2.43	0.48
2:E:331:GLU:OE1	2:E:331:GLU:N	2.42	0.48
2:E:353:TRP:O	2:E:355:PRO:HD3	2.13	0.48
2:E:542:ARG:HD2	2:E:543:LEU:H	1.79	0.48
2:E:719:LEU:HD13	2:E:771:GLN:HA	1.96	0.48
1:B:54:GLN:HA	1:B:58:LYS:O	2.15	0.47
2:E:350:ALA:O	2:E:352:VAL:N	2.42	0.47
2:E:338:ILE:O	2:E:368:HIS:HB2	2.14	0.47
1:B:28:LEU:HD11	1:B:49:ALA:HB3	1.95	0.47
2:E:677:PHE:CD2	2:E:682:SER:HA	2.49	0.47
2:E:354:LEU:HD13	2:E:546:VAL:CG1	2.45	0.47
2:E:530:ARG:HD2	2:E:541:TRP:CZ3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:517:ALA:C	2:E:518:LEU:HD12	2.35	0.47
2:E:739:MET:HA	2:E:739:MET:HE3	1.96	0.47
2:E:241:LEU:HD13	2:E:311:ARG:NH1	2.30	0.47
2:E:310:GLU:O	2:E:314:ILE:HG12	2.16	0.46
1:B:168:ILE:HG23	1:B:169:LEU:N	2.31	0.46
2:E:170:GLU:O	2:E:173:ASP:HB2	2.14	0.46
1:B:22:VAL:CG1	1:B:90:VAL:HG12	2.45	0.46
2:E:583:TYR:CD1	2:E:585:ILE:HD11	2.50	0.46
1:B:162:GLU:O	1:B:166:GLN:HB2	2.16	0.46
1:B:19:ASP:O	1:B:22:VAL:HG23	2.16	0.46
2:E:561:PHE:CZ	2:E:565:LYS:HD2	2.51	0.46
2:E:729:MET:HE3	2:E:761:PHE:CB	2.45	0.46
2:E:588:ILE:HG12	2:E:593:GLY:HA2	1.97	0.46
2:E:647:LEU:HD11	2:E:718:MET:HA	1.97	0.46
2:E:737:GLU:HA	2:E:754:ILE:HD11	1.97	0.46
1:B:85:VAL:HG11	1:B:172:ILE:HG21	1.97	0.46
2:E:320:ILE:HD13	2:E:341:LEU:HD23	1.98	0.46
2:E:341:LEU:HD22	2:E:344:LEU:HD12	1.97	0.46
2:E:313:PHE:CD2	2:E:352:VAL:HG11	2.50	0.46
2:E:520:GLU:HB2	2:E:521:PRO:CD	2.46	0.46
2:E:522:TRP:O	2:E:526:VAL:HG23	2.15	0.46
2:E:310:GLU:OE1	2:E:352:VAL:HA	2.15	0.46
1:B:52:SER:HA	1:B:60:ILE:O	2.16	0.46
1:B:88:LEU:HD21	1:B:120:MET:HE3	1.97	0.45
2:E:133:LEU:O	2:E:136:SER:HB3	2.17	0.45
2:E:363:VAL:HG13	2:E:386:VAL:CG1	2.47	0.45
2:E:602:VAL:HG23	2:E:607:VAL:CG2	2.46	0.45
1:B:158:SER:HA	1:B:161:VAL:HG21	1.99	0.45
1:B:109:LEU:O	1:B:113:ALA:HB3	2.16	0.45
1:B:30:ARG:HH21	1:B:36:PHE:CB	2.29	0.45
2:E:700:VAL:CG1	2:E:706:LEU:HD12	2.38	0.45
1:B:127:ASP:CG	3:B:301:GDP:HN1	2.19	0.45
2:E:320:ILE:HG12	2:E:340:GLU:HG2	1.98	0.45
2:E:334:THR:O	2:E:338:ILE:HG13	2.17	0.45
2:E:356:THR:O	2:E:584:LYS:HD3	2.17	0.45
2:E:402:ARG:HA	2:E:535:TYR:OH	2.17	0.44
2:E:403:ILE:HG13	2:E:534:PRO:CB	2.47	0.44
2:E:403:ILE:HA	2:E:404:PRO:HD3	1.87	0.44
1:B:85:VAL:CG1	1:B:172:ILE:HG21	2.46	0.44
2:E:333:LYS:HD3	2:E:373:VAL:HG11	1.98	0.44
2:E:324:LEU:HD23	2:E:336:ARG:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:578:LEU:HD11	2:E:721:GLY:HA3	1.98	0.44
2:E:768:GLU:O	2:E:772:LEU:HD13	2.17	0.44
2:E:586:LEU:C	2:E:586:LEU:HD23	2.37	0.44
2:E:646:CYS:SG	2:E:714:TYR:OH	2.66	0.43
2:E:723:ILE:HG12	2:E:770:LEU:HD23	2.00	0.43
1:B:91:TYR:HE1	1:B:134:VAL:HG11	1.80	0.43
2:E:595:ILE:O	2:E:597:PRO:HD3	2.18	0.43
2:E:241:LEU:HD13	2:E:311:ARG:CZ	2.47	0.43
1:B:165:PHE:CA	1:B:168:ILE:HG22	2.39	0.43
2:E:320:ILE:O	2:E:324:LEU:HG	2.19	0.43
2:E:549:LYS:HE2	2:E:549:LYS:HB3	1.80	0.43
1:B:15:VAL:O	1:B:88:LEU:HB2	2.18	0.43
2:E:349:PRO:HB3	2:E:364:VAL:HA	2.01	0.43
2:E:745:LEU:HA	2:E:746:PRO:HD3	1.85	0.43
2:E:194:ILE:O	2:E:198:ILE:HG12	2.19	0.42
2:E:694:LYS:HA	2:E:781:SER:O	2.18	0.42
2:E:327:LEU:HA	2:E:328:PRO:HD3	1.75	0.42
2:E:601:ALA:HA	2:E:664:LEU:O	2.19	0.42
1:B:16:LEU:HD13	1:B:24:LYS:O	2.19	0.42
2:E:530:ARG:HG3	2:E:536:GLY:HA2	2.00	0.42
2:E:558:LEU:O	2:E:561:PHE:HB3	2.20	0.42
2:E:566:GLN:O	2:E:570:ILE:HG13	2.19	0.42
2:E:579:TRP:CH2	2:E:581:LYS:HB2	2.54	0.42
1:B:120:MET:HE1	1:B:164:ALA:O	2.20	0.42
1:B:148:LEU:O	1:B:148:LEU:HD12	2.20	0.42
1:B:131:LEU:HD13	2:E:162:ASN:HB2	2.00	0.42
2:E:180:LEU:O	2:E:184:ILE:HG13	2.20	0.41
1:B:24:LYS:HE2	3:B:301:GDP:O1B	2.20	0.41
1:B:114:ASP:O	1:B:117:ILE:HG12	2.20	0.41
2:E:202:CYS:O	2:E:209:SER:OG	2.38	0.41
2:E:352:VAL:O	2:E:363:VAL:HG23	2.20	0.41
2:E:364:VAL:HG11	2:E:389:LEU:HG	2.02	0.41
2:E:354:LEU:HD22	2:E:546:VAL:HG11	2.01	0.41
2:E:195:LYS:N	2:E:196:PRO:CD	2.82	0.41
1:B:33:ARG:HD3	1:B:33:ARG:HA	1.88	0.41
1:B:16:LEU:HD23	1:B:88:LEU:HB3	2.03	0.41
2:E:338:ILE:HG23	2:E:368:HIS:O	2.21	0.41
2:E:533:SER:HA	2:E:534:PRO:HD3	1.96	0.41
1:B:22:VAL:O	1:B:22:VAL:HG12	2.20	0.40
1:B:131:LEU:HD12	1:B:131:LEU:N	2.36	0.40
1:B:53:ILE:CD1	1:B:169:LEU:HD12	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:310:GLU:OE1	2:E:352:VAL:HG13	2.21	0.40
2:E:233:GLY:HA2	4:E:1002:SO4:O4	2.21	0.40
2:E:134:PHE:HB3	2:E:159:TYR:HE2	1.86	0.40
2:E:626:TYR:HA	2:E:631:PHE:CD2	2.56	0.40
2:E:653:GLN:HG2	2:E:760:ARG:CZ	2.52	0.40
1:B:11:LEU:C	1:B:11:LEU:HD23	2.42	0.40
2:E:316:SER:O	2:E:320:ILE:HG13	2.21	0.40
2:E:357:ALA:HB2	2:E:544:LEU:CD1	2.51	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	B	149/219 (68%)	143 (96%)	6 (4%)	0	100	100
2	E	454/529 (86%)	437 (96%)	16 (4%)	1 (0%)	52	88
All	All	603/748 (81%)	580 (96%)	22 (4%)	1 (0%)	52	88

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	351	ARG

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	B	131/191 (69%)	131 (100%)	0	100	100
2	E	417/475 (88%)	417 (100%)	0	100	100
All	All	548/666 (82%)	548 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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)

4 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	#$|Z| > 2$
3	GDP	B	301	-	24,30,30	1.14	2 (8%)	26,47,47	1.92	4 (15%)
4	SO4	E	1001	-	4,4,4	0.26	0	6,6,6	0.08	0
4	SO4	E	1002	-	4,4,4	0.21	0	6,6,6	0.17	0
5	5S8	E	1003	-	27,36,36	2.85	5 (18%)	30,52,52	1.70	5 (16%)

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
3	GDP	B	301	-	-	0/12/32/32	0/3/3/3
4	SO4	E	1001	-	-	0/0/0/0	0/0/0/0
4	SO4	E	1002	-	-	0/0/0/0	0/0/0/0
5	5S8	E	1003	-	-	2/17/32/32	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	GDP	C5-C4	3.13	1.47	1.40
5	E	1003	5S8	CAT-CAU	3.30	1.47	1.37
3	B	301	GDP	C6-C5	3.50	1.48	1.41
5	E	1003	5S8	CAY-NAX	5.48	1.45	1.36
5	E	1003	5S8	OAO-CAN	6.20	1.46	1.37
5	E	1003	5S8	CBA-NAX	6.29	1.47	1.35
5	E	1003	5S8	CAQ-CAT	9.13	1.57	1.48

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	GDP	C5-C6-N1	-4.28	117.93	123.52
5	E	1003	5S8	OBB-CBA-NAX	-3.62	117.18	123.89
3	B	301	GDP	N3-C2-N1	-3.57	122.70	127.56
3	B	301	GDP	C6-C5-C4	-3.51	116.84	120.86
5	E	1003	5S8	OBB-CBA-CBC	-2.89	118.49	122.20
5	E	1003	5S8	CAM-SAJ-NAH	2.42	110.19	107.23
5	E	1003	5S8	OAO-CAN-CAM	3.00	119.32	116.48
3	B	301	GDP	C6-N1-C2	5.76	122.64	115.88
5	E	1003	5S8	CBC-CBA-NAX	6.23	124.33	115.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	1003	5S8	OBB-CBA-NAX-CAY
5	E	1003	5S8	CBC-CBA-NAX-CAY

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	301	GDP	5	0
4	E	1001	SO4	1	0
4	E	1002	SO4	1	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	B	155/219 (70%)	0.52	13 (8%)	14	7	73, 110, 164, 187	23 (14%)
2	E	464/529 (87%)	0.20	8 (1%)	73	60	49, 88, 136, 190	10 (2%)
All	All	619/748 (82%)	0.28	21 (3%)	49	34	49, 95, 151, 190	33 (5%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	45	GLY	3.4
1	B	18	GLY	3.3
1	B	150	PHE	3.3
1	B	87	ALA	3.1
2	E	350	ALA	2.9
1	B	99	TYR	2.7
2	E	513	PRO	2.7
2	E	306	ARG	2.6
1	B	148	LEU	2.6
2	E	394	PHE	2.6
2	E	683	PRO	2.5
1	B	17	ILE	2.4
2	E	514	SER	2.4
1	B	142	PHE	2.4
1	B	147	GLY	2.3
1	B	46	VAL	2.3
2	E	401	ALA	2.2
1	B	110	ARG	2.2
1	B	149	SER	2.2
1	B	118	VAL	2.1
2	E	307	LEU	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 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
5	5S8	E	1003	33/33	0.88	0.39	1.52	96,121,161,165	0
3	GDP	B	301	28/28	0.92	0.20	-0.60	98,98,98,98	0
4	SO4	E	1002	5/5	0.69	0.24	-0.66	134,134,134,134	0
4	SO4	E	1001	5/5	0.88	0.22	-	124,124,124,124	0

6.5 Other polymers (i)

There are no such residues in this entry.