WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:25 AM GMT

PDB ID : 2QPT
Title : Crystal structure of an EHD ATPase involved in membrane remodelling
Authors : Daumke, O.
Deposited on : 2007-07-25
Resolution : 3.10 Å(reported)

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

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 3.10 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.
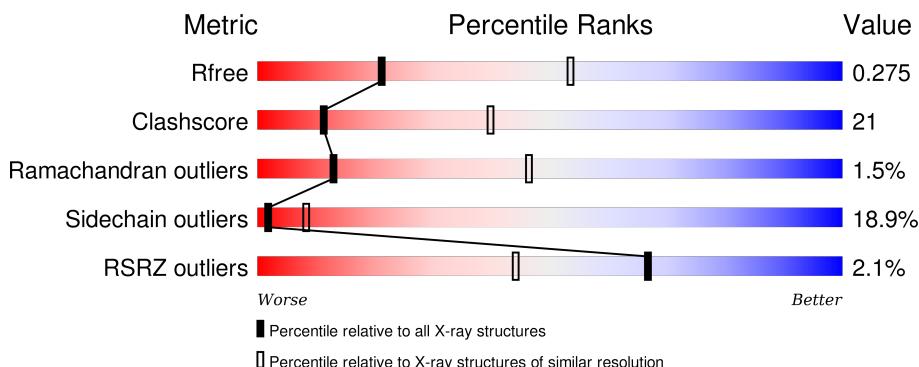
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	550	
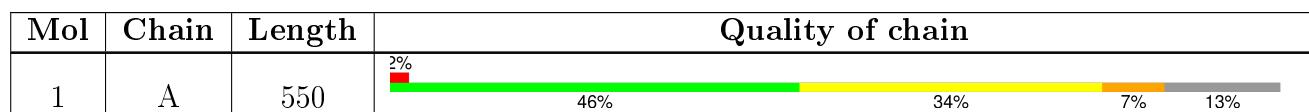
2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3834 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 EH DOMAIN-CONTAINING PROTEIN-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total 3795	C 2437	N 652	O 689	S 17	6	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	EXPRESSION TAG	UNP Q8BH64
A	-5	PRO	-	EXPRESSION TAG	UNP Q8BH64
A	-4	HIS	-	EXPRESSION TAG	UNP Q8BH64
A	-3	MET	-	EXPRESSION TAG	UNP Q8BH64
A	-2	GLY	-	EXPRESSION TAG	UNP Q8BH64
A	-1	GLY	-	EXPRESSION TAG	UNP Q8BH64
A	0	SER	-	EXPRESSION TAG	UNP Q8BH64
A	410	ALA	GLN	ENGINEERED	UNP Q8BH64

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mg 1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Ca 1	0	0

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).
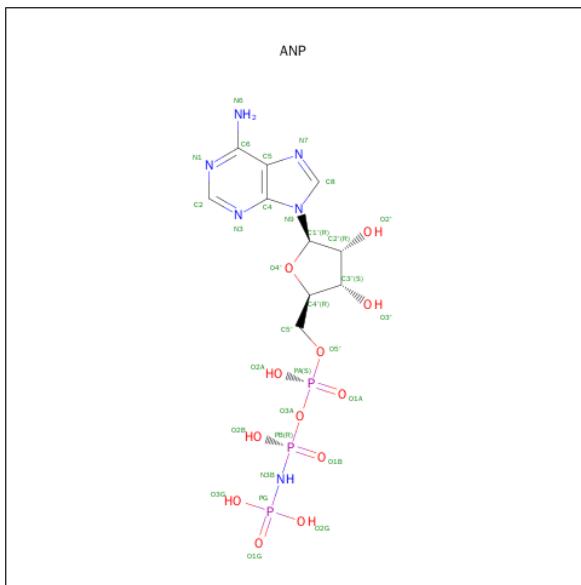
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	O	0	0
			6	6		

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: EH DOMAIN-CONTAINING PROTEIN-2
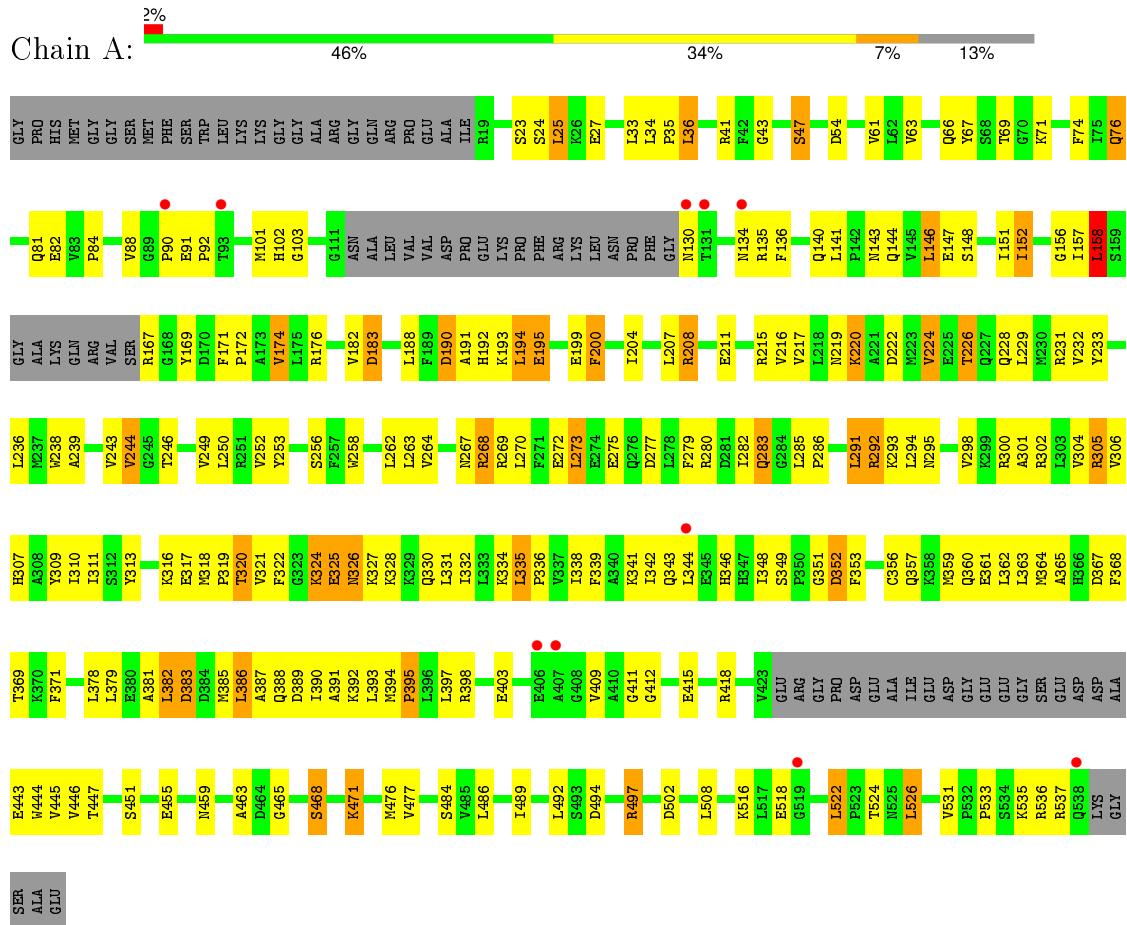
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	99.85Å 134.65Å 56.07Å 90.00° 106.05° 90.00°	Depositor
Resolution (Å)	19.96 – 3.10 19.80 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (19.96-3.10) 98.7 (19.80-3.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	5.40 (at 3.09Å)	Xtriage
Refinement program	REFMAC 5.3.0022	Depositor
R, R_{free}	0.234 , 0.276 0.231 , 0.275	Depositor DCC
R_{free} test set	623 reflections (5.15%)	DCC
Wilson B-factor (Å^2)	77.2	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 55.8	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 12713 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	3834	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 5.52% 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: CA, ANP, MG

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	0.59	5/3877 (0.1%)	0.60	6/5236 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	455	GLU	CG-CD	25.95	1.90	1.51
1	A	395	PRO	C-O	8.78	1.40	1.23
1	A	395	PRO	C-N	5.98	1.47	1.34
1	A	158	LEU	CB-CG	-5.91	1.35	1.52
1	A	392	LYS	C-O	5.78	1.34	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	455	GLU	CB-CG-CD	-10.10	86.94	114.20
1	A	158	LEU	CB-CG-CD1	8.19	124.92	111.00
1	A	455	GLU	CG-CD-OE1	-6.57	105.17	118.30
1	A	158	LEU	CA-CB-CG	6.36	129.91	115.30
1	A	395	PRO	C-N-CA	-6.16	106.31	121.70
1	A	395	PRO	O-C-N	5.35	131.25	122.70

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	3795	0	3849	158	1
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	31	0	13	3	0
5	A	6	0	0	0	0
All	All	3834	0	3862	158	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 21.

All (158) 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:305:ARG:HH21	1:A:305:ARG:HG2	1.17	1.08
1:A:357:GLN:HA	1:A:360:GLN:HE21	1.16	1.06
1:A:188:LEU:HD22	1:A:217:VAL:HG22	1.47	0.96
1:A:66:GLN:NE2	1:A:195:GLU:O	2.00	0.94
1:A:208:ARG:HG2	1:A:208:ARG:HH11	1.32	0.93
1:A:334:LYS:HG2	1:A:334:LYS:O	1.73	0.87
1:A:357:GLN:HA	1:A:360:GLN:NE2	1.91	0.85
1:A:277:ASP:HA	1:A:280:ARG:HH12	1.41	0.85
1:A:403:GLU:HA	1:A:403:GLU:OE1	1.80	0.82
1:A:277:ASP:HA	1:A:280:ARG:NH1	1.96	0.81
1:A:91:GLU:HG3	1:A:92:PRO:HD2	1.65	0.79
1:A:208:ARG:NH1	1:A:208:ARG:HG2	1.94	0.79
1:A:244:VAL:HG23	1:A:246:THR:HG22	1.65	0.77
1:A:382:LEU:HD13	1:A:386:LEU:HD21	1.67	0.76
1:A:171:PHE:HB3	1:A:172:PRO:HD3	1.67	0.76
1:A:533:PRO:HA	1:A:535:LYS:HE3	1.69	0.75
1:A:194:LEU:HG	1:A:232:VAL:HG13	1.70	0.73
1:A:415:GLU:HG3	1:A:418:ARG:HG3	1.70	0.73
1:A:305:ARG:NH2	1:A:305:ARG:HG2	1.97	0.72
1:A:394:MET:HB2	1:A:395:PRO:HD3	1.72	0.70
1:A:305:ARG:CG	1:A:305:ARG:HH21	2.02	0.69
1:A:200:PHE:HD2	1:A:204:ILE:CD1	2.07	0.68
1:A:268:ARG:O	1:A:272:GLU:HG2	1.94	0.67
1:A:302:ARG:O	1:A:306:VAL:HG23	1.95	0.67
1:A:216:VAL:O	1:A:252:VAL:HA	1.97	0.65
1:A:208:ARG:CG	1:A:208:ARG:HH11	2.07	0.65
1:A:363:LEU:HD12	1:A:368:PHE:CZ	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:LEU:O	1:A:390:ILE:HB	1.98	0.63
1:A:200:PHE:CD2	1:A:204:ILE:HD11	2.33	0.63
1:A:388:GLN:O	1:A:391:ALA:HB3	1.99	0.63
1:A:200:PHE:HD2	1:A:204:ILE:HD12	1.64	0.63
1:A:76:GLN:NE2	1:A:82:GLU:HA	2.14	0.63
1:A:200:PHE:CD2	1:A:204:ILE:CD1	2.82	0.63
1:A:275:GLU:HG2	1:A:279:PHE:CE2	2.35	0.62
1:A:318:MET:HG3	1:A:368:PHE:HB3	1.81	0.61
1:A:361:GLU:O	1:A:364:MET:HB3	2.00	0.61
1:A:233:TYR:CE2	1:A:252:VAL:HG21	2.37	0.60
1:A:190:ASP:OD2	1:A:220:LYS:HE2	2.02	0.59
1:A:27:GLU:OE1	1:A:27:GLU:HA	2.01	0.59
1:A:220:LYS:HB3	4:A:600:ANP:N1	2.19	0.58
1:A:341:LYS:O	1:A:344:LEU:HB2	2.04	0.57
1:A:220:LYS:HA	1:A:256:SER:HB3	1.87	0.57
1:A:71:LYS:HE3	4:A:600:ANP:O1B	2.03	0.57
1:A:152:ILE:O	1:A:152:ILE:HG13	2.04	0.57
1:A:394:MET:O	1:A:397:LEU:HB3	2.04	0.56
1:A:47:SER:HB3	1:A:300:ARG:NH1	2.20	0.56
1:A:171:PHE:O	1:A:174:VAL:HG13	2.06	0.56
1:A:216:VAL:CG1	1:A:252:VAL:HG12	2.35	0.56
1:A:395:PRO:HA	1:A:398:ARG:HD3	1.87	0.56
1:A:102:HIS:CG	1:A:103:GLY:H	2.23	0.56
1:A:327:LYS:O	1:A:331:LEU:HB2	2.06	0.56
1:A:494:ASP:CG	1:A:497:ARG:HA	2.26	0.55
1:A:307:HIS:CE1	1:A:311:ILE:HD13	2.41	0.55
1:A:148:SER:HB2	1:A:409:VAL:HG13	1.88	0.55
1:A:188:LEU:CD2	1:A:217:VAL:HG22	2.29	0.55
1:A:91:GLU:CG	1:A:92:PRO:HD2	2.37	0.54
1:A:215:ARG:HD2	1:A:253:TYR:HE1	1.73	0.53
1:A:135:ARG:NH2	1:A:169:TYR:HB3	2.23	0.53
1:A:334:LYS:CG	1:A:334:LYS:O	2.49	0.53
1:A:219:ASN:C	1:A:220:LYS:HG2	2.28	0.53
1:A:334:LYS:O	1:A:338:ILE:HG12	2.07	0.53
1:A:291:LEU:HG	1:A:397:LEU:HD21	1.91	0.53
1:A:465:GLY:O	1:A:502:ASP:HA	2.09	0.53
1:A:239:ALA:O	1:A:243:VAL:HG23	2.09	0.53
1:A:102:HIS:CG	1:A:103:GLY:N	2.77	0.52
1:A:313:TYR:O	1:A:316:LYS:HG2	2.10	0.52
1:A:335:LEU:HD12	1:A:360:GLN:HG3	1.92	0.51
1:A:25:LEU:HD11	1:A:294:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:LEU:O	1:A:365:ALA:N	2.43	0.51
1:A:382:LEU:HD13	1:A:386:LEU:CD2	2.40	0.51
1:A:190:ASP:OD2	1:A:192:HIS:HB3	2.10	0.51
1:A:144:GLN:O	1:A:147:GLU:HB2	2.11	0.51
1:A:403:GLU:CA	1:A:403:GLU:OE1	2.54	0.51
1:A:335:LEU:N	1:A:336:PRO:HD2	2.26	0.50
1:A:103:GLY:HA3	1:A:140:GLN:HB3	1.92	0.50
1:A:342:ILE:O	1:A:346:HIS:HB2	2.11	0.50
1:A:102:HIS:HB2	1:A:146:LEU:O	2.12	0.50
1:A:224:VAL:HG22	1:A:228:GLN:HG2	1.94	0.50
1:A:171:PHE:HB3	1:A:172:PRO:CD	2.41	0.50
1:A:226:THR:HB	1:A:267:ASN:HD21	1.77	0.50
1:A:306:VAL:HG21	1:A:352:ASP:HB3	1.93	0.49
1:A:386:LEU:HA	1:A:390:ILE:HD12	1.92	0.49
1:A:148:SER:OG	1:A:409:VAL:HA	2.12	0.49
1:A:244:VAL:CG2	1:A:246:THR:HG22	2.37	0.49
1:A:101:MET:O	1:A:140:GLN:HA	2.12	0.49
1:A:200:PHE:CE2	1:A:204:ILE:HD11	2.47	0.48
1:A:489:ILE:CG1	1:A:522:LEU:HD21	2.43	0.48
1:A:357:GLN:O	1:A:360:GLN:HB2	2.13	0.48
1:A:298:VAL:HG22	1:A:390:ILE:HD13	1.96	0.48
1:A:63:VAL:HG12	1:A:71:LYS:HG2	1.95	0.48
1:A:84:PRO:HD3	1:A:141:LEU:HD13	1.96	0.48
1:A:378:LEU:O	1:A:381:ALA:HB3	2.14	0.47
1:A:157:ILE:HG12	1:A:171:PHE:CE2	2.49	0.47
1:A:305:ARG:HD2	1:A:309:TYR:HE1	1.80	0.47
1:A:359:MET:O	1:A:363:LEU:HB2	2.15	0.47
1:A:25:LEU:HD13	1:A:393:LEU:HD13	1.96	0.47
1:A:343:GLN:HG3	1:A:353:PHE:CE2	2.50	0.47
1:A:359:MET:HG3	1:A:363:LEU:HD23	1.96	0.46
1:A:182:VAL:CG1	1:A:183:ASP:N	2.78	0.46
1:A:497:ARG:CG	1:A:497:ARG:O	2.63	0.46
1:A:285:LEU:HB2	1:A:286:PRO:HD3	1.97	0.46
1:A:69:THR:HG21	1:A:188:LEU:C	2.36	0.46
1:A:382:LEU:O	1:A:386:LEU:HD23	2.16	0.46
1:A:204:ILE:HG21	1:A:244:VAL:HG12	1.97	0.46
1:A:385:MET:O	1:A:389:ASP:HB2	2.15	0.46
1:A:135:ARG:CZ	1:A:169:TYR:HB3	2.46	0.45
1:A:320:THR:OG1	1:A:321:VAL:N	2.50	0.45
1:A:325:GLU:O	1:A:328:LYS:HB3	2.17	0.45
1:A:326:ASN:O	1:A:330:GLN:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:ASP:OD2	1:A:497:ARG:HA	2.16	0.45
1:A:157:ILE:HG23	1:A:199:GLU:HG2	1.99	0.45
1:A:292:ARG:HG3	1:A:293:LYS:N	2.32	0.44
1:A:43:GLY:HA2	1:A:47:SER:O	2.17	0.44
1:A:368:PHE:HA	1:A:371:PHE:CD1	2.53	0.44
1:A:394:MET:CB	1:A:395:PRO:HD3	2.47	0.43
1:A:324:LYS:HE3	1:A:369:THR:HG21	2.00	0.43
1:A:273:LEU:HD13	1:A:273:LEU:HA	1.73	0.43
1:A:385:MET:HA	1:A:389:ASP:OD2	2.18	0.43
1:A:193:LYS:HE2	1:A:193:LYS:HB3	1.68	0.43
1:A:531:VAL:O	1:A:535:LYS:HE2	2.18	0.43
1:A:190:ASP:C	1:A:192:HIS:H	2.20	0.43
1:A:222:ASP:O	1:A:264:VAL:HG12	2.19	0.43
1:A:349:SER:C	1:A:351:GLY:N	2.72	0.43
1:A:383:ASP:OD1	1:A:383:ASP:N	2.51	0.43
1:A:194:LEU:HA	1:A:194:LEU:HD23	1.86	0.43
1:A:141:LEU:HD23	1:A:141:LEU:N	2.34	0.43
1:A:282:ILE:O	1:A:285:LEU:HG	2.18	0.43
1:A:526:LEU:HD12	1:A:531:VAL:HG22	2.01	0.42
1:A:226:THR:HB	1:A:267:ASN:ND2	2.33	0.42
1:A:468:SER:HB3	1:A:471:LYS:HG3	2.02	0.42
1:A:283:GLN:HA	1:A:409:VAL:CG2	2.50	0.42
1:A:102:HIS:CA	1:A:146:LEU:HB3	2.50	0.42
1:A:33:LEU:HD21	1:A:301:ALA:HA	2.02	0.42
1:A:191:ALA:HA	1:A:232:VAL:HG11	2.01	0.42
1:A:476:MET:HB3	1:A:486:LEU:HD22	2.01	0.42
1:A:305:ARG:CG	1:A:305:ARG:NH2	2.69	0.41
1:A:215:ARG:HD2	1:A:253:TYR:CE1	2.54	0.41
1:A:317:GLU:HB3	1:A:331:LEU:HD11	2.02	0.41
1:A:47:SER:HB3	1:A:300:ARG:HH12	1.83	0.41
1:A:443:GLU:HG3	1:A:444:TRP:N	2.34	0.41
1:A:394:MET:HB2	1:A:395:PRO:CD	2.47	0.41
1:A:71:LYS:NZ	1:A:156:GLY:HA2	2.35	0.41
1:A:200:PHE:O	1:A:204:ILE:HD12	2.21	0.41
1:A:81:GLN:HE21	1:A:143:ASN:HD22	1.69	0.41
1:A:61:VAL:CG2	1:A:151:ILE:HG23	2.50	0.41
1:A:356:CYS:O	1:A:360:GLN:HG3	2.21	0.41
1:A:319:PRO:HD3	1:A:327:LYS:HG3	2.01	0.41
1:A:61:VAL:HG23	1:A:151:ILE:HG23	2.02	0.41
1:A:256:SER:HB2	4:A:600:ANP:HN62	1.86	0.41
1:A:71:LYS:O	1:A:74:PHE:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:TYR:CE1	1:A:158:LEU:HA	2.56	0.41
1:A:367:ASP:OD2	1:A:367:ASP:C	2.58	0.41
1:A:34:LEU:N	1:A:35:PRO:CD	2.84	0.41
1:A:190:ASP:HB2	1:A:220:LYS:HG3	2.04	0.40
1:A:36:LEU:HD22	1:A:304:VAL:HG12	2.02	0.40
1:A:310:ILE:HD13	1:A:339:PHE:CE1	2.57	0.40
1:A:302:ARG:HB3	1:A:352:ASP:OD1	2.21	0.40
1:A:157:ILE:HG12	1:A:171:PHE:HE2	1.84	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:443:GLU:OE1	1:A:443:GLU:OE1[2_553]	1.56	0.64

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	468/550 (85%)	404 (86%)	57 (12%)	7 (2%)	13 46

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	387	ALA
1	A	90	PRO
1	A	411	GLY
1	A	463	ALA
1	A	325	GLU
1	A	412	GLY
1	A	320	THR

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	413/468 (88%)	335 (81%)	78 (19%)	2 8

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	SER
1	A	24	SER
1	A	25	LEU
1	A	36	LEU
1	A	41	ARG
1	A	47	SER
1	A	54	ASP
1	A	76	GLN
1	A	88	VAL
1	A	130	ASN
1	A	134	ASN
1	A	136	PHE
1	A	146	LEU
1	A	152	ILE
1	A	158	LEU
1	A	167	ARG
1	A	174	VAL
1	A	176	ARG
1	A	183	ASP
1	A	190	ASP
1	A	194	LEU
1	A	195	GLU
1	A	200	PHE
1	A	207	LEU
1	A	208	ARG
1	A	211	GLU
1	A	220	LYS
1	A	224	VAL
1	A	226	THR
1	A	229	LEU

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Mol	Chain	Res	Type
1	A	231	ARG
1	A	236	LEU
1	A	238	TRP
1	A	244	VAL
1	A	249	VAL
1	A	250	LEU
1	A	258	TRP
1	A	262	LEU
1	A	263	LEU
1	A	268	ARG
1	A	269	ARG
1	A	270	LEU
1	A	273	LEU
1	A	283	GLN
1	A	291	LEU
1	A	292	ARG
1	A	295	ASN
1	A	305	ARG
1	A	322	PHE
1	A	324	LYS
1	A	326	ASN
1	A	332	ILE
1	A	335	LEU
1	A	348	ILE
1	A	352	ASP
1	A	379	LEU
1	A	382	LEU
1	A	383	ASP
1	A	386	LEU
1	A	445	VAL
1	A	446	VAL
1	A	447	THR
1	A	451	SER
1	A	459	ASN
1	A	468	SER
1	A	471	LYS
1	A	477	VAL
1	A	484	SER
1	A	492	LEU
1	A	497	ARG
1	A	508	LEU
1	A	516	LYS

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Mol	Chain	Res	Type
1	A	518	GLU
1	A	522	LEU
1	A	524	THR
1	A	526	LEU
1	A	536	ARG
1	A	537	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	46	HIS
1	A	76	GLN
1	A	81	GLN
1	A	134	ASN
1	A	267	ASN
1	A	276	GLN
1	A	283	GLN
1	A	326	ASN
1	A	357	GLN
1	A	360	GLN

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)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\#|Z| > 2$
4	ANP	A	600	2	27,33,33	2.02	5 (18%)	30,52,52	2.13	6 (20%)

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
4	ANP	A	600	2	-	0/12/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	ANP	C5-C4	2.77	1.46	1.40
4	A	600	ANP	PG-N3B	4.18	1.74	1.63
4	A	600	ANP	PB-N3B	4.26	1.74	1.63
4	A	600	ANP	PB-O1B	4.51	1.51	1.46
4	A	600	ANP	PG-O1G	4.75	1.51	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	600	ANP	N3-C2-N1	-6.90	123.61	128.89
4	A	600	ANP	O1G-PG-N3B	-4.66	104.75	111.90
4	A	600	ANP	PA-O3A-PB	-4.12	118.86	132.67
4	A	600	ANP	C4-C5-N7	-3.04	106.68	109.48
4	A	600	ANP	O3G-PG-O2G	2.03	113.61	107.58
4	A	600	ANP	O2B-PB-O1B	4.05	118.45	110.00

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
4	A	600	ANP	3	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	476/550 (86%)	-0.28	10 (2%) 67	44	51, 59, 66, 70	31 (6%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	406	GLU	4.1
1	A	131	THR	3.8
1	A	538	GLN	3.4
1	A	407	ALA	3.4
1	A	93	THR	3.0
1	A	519	GLY	2.5
1	A	134	ASN	2.4
1	A	344	LEU	2.4
1	A	130	ASN	2.3
1	A	90	PRO	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
4	ANP	A	600	31/31	0.97	0.12	-1.21	51,52,53,53	0
3	CA	A	701	1/1	0.98	0.04	-2.97	48,48,48,48	0
2	MG	A	700	1/1	0.94	0.16	-	48,48,48,48	0

6.5 Other polymers (i)

There are no such residues in this entry.