Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2024 – 03:32 pm GMT

PDB ID	:	5LZQ
Title	:	Crystal structure of Thermotoga maritima sodium pumping membrane integral pyrophosphatase in complex with imidodiphosphate and magnesium, and with bound sodium ion
Authors	:	Wilkinson, C.; Kellosalo, J.; Kajander, T.; Goldman, A.
Deposited on	:	2016-10-01
Resolution	:	3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

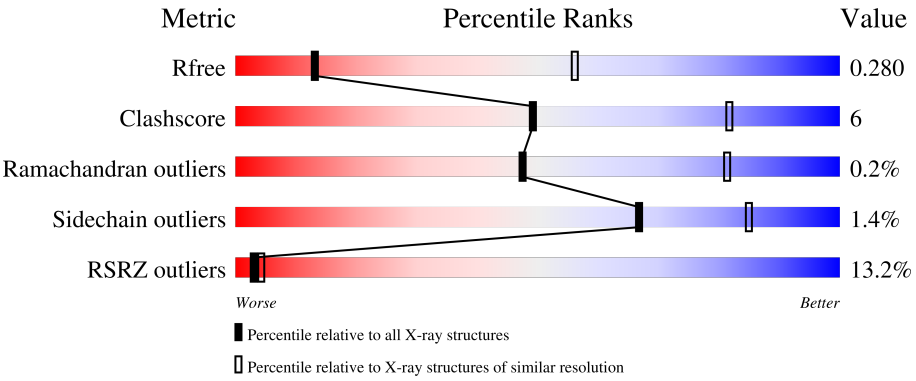
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.50 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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	735	14% 83% 15%
1	B	735	12% 84% 14%

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	2PN	A	809	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10448 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 K(+)-stimulated pyrophosphate-energized sodium pump.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	725	Total	C	N	O	S	0	0	0
			5224	3423	816	958	27			
1	B	725	Total	C	N	O	S	0	0	0
			5170	3387	805	953	25			

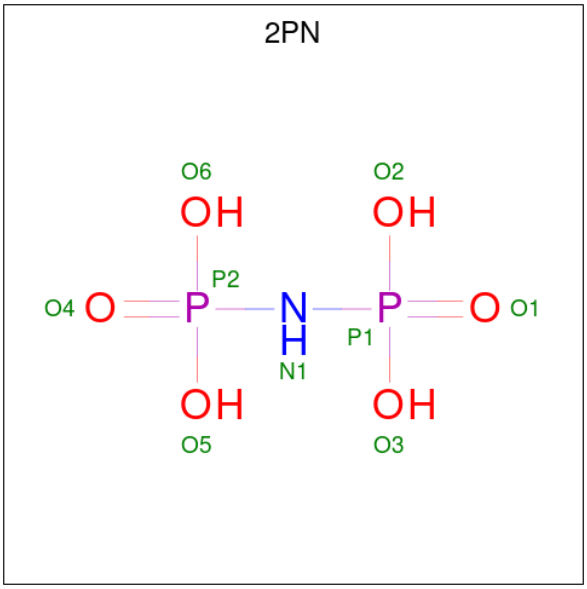
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	initiating methionine	UNP Q9S5X0
A	-7	ARG	-	expression tag	UNP Q9S5X0
A	-6	GLY	-	expression tag	UNP Q9S5X0
A	-5	SER	-	expression tag	UNP Q9S5X0
A	-4	HIS	-	expression tag	UNP Q9S5X0
A	-3	HIS	-	expression tag	UNP Q9S5X0
A	-2	HIS	-	expression tag	UNP Q9S5X0
A	-1	HIS	-	expression tag	UNP Q9S5X0
A	0	HIS	-	expression tag	UNP Q9S5X0
A	1	HIS	-	expression tag	UNP Q9S5X0
A	353	LEU	VAL	engineered mutation	UNP Q9S5X0
A	395	GLY	SER	engineered mutation	UNP Q9S5X0
B	-8	MET	-	initiating methionine	UNP Q9S5X0
B	-7	ARG	-	expression tag	UNP Q9S5X0
B	-6	GLY	-	expression tag	UNP Q9S5X0
B	-5	SER	-	expression tag	UNP Q9S5X0
B	-4	HIS	-	expression tag	UNP Q9S5X0
B	-3	HIS	-	expression tag	UNP Q9S5X0
B	-2	HIS	-	expression tag	UNP Q9S5X0
B	-1	HIS	-	expression tag	UNP Q9S5X0
B	0	HIS	-	expression tag	UNP Q9S5X0
B	1	HIS	-	expression tag	UNP Q9S5X0
B	353	LEU	VAL	engineered mutation	UNP Q9S5X0
B	395	GLY	SER	engineered mutation	UNP Q9S5X0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	5	Total Mg 5 5	0	0
2	B	5	Total Mg 5 5	0	0

- Molecule 3 is IMIDODIPHOSPHORIC ACID (three-letter code: 2PN) (formula: $H_5NO_6P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total N O P 9 1 6 2	0	0
3	A	1	Total N O P 9 1 6 2	0	0
3	A	1	Total N O P 9 1 6 2	0	0
3	B	1	Total N O P 9 1 6 2	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	B	1	Total Na 1 1	0	0

- Molecule 5 is water.

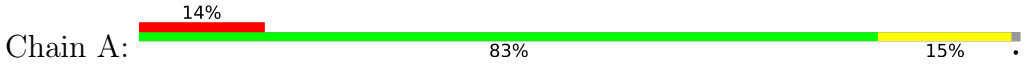
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total O 2 2	0	0
5	B	4	Total O 4 4	0	0

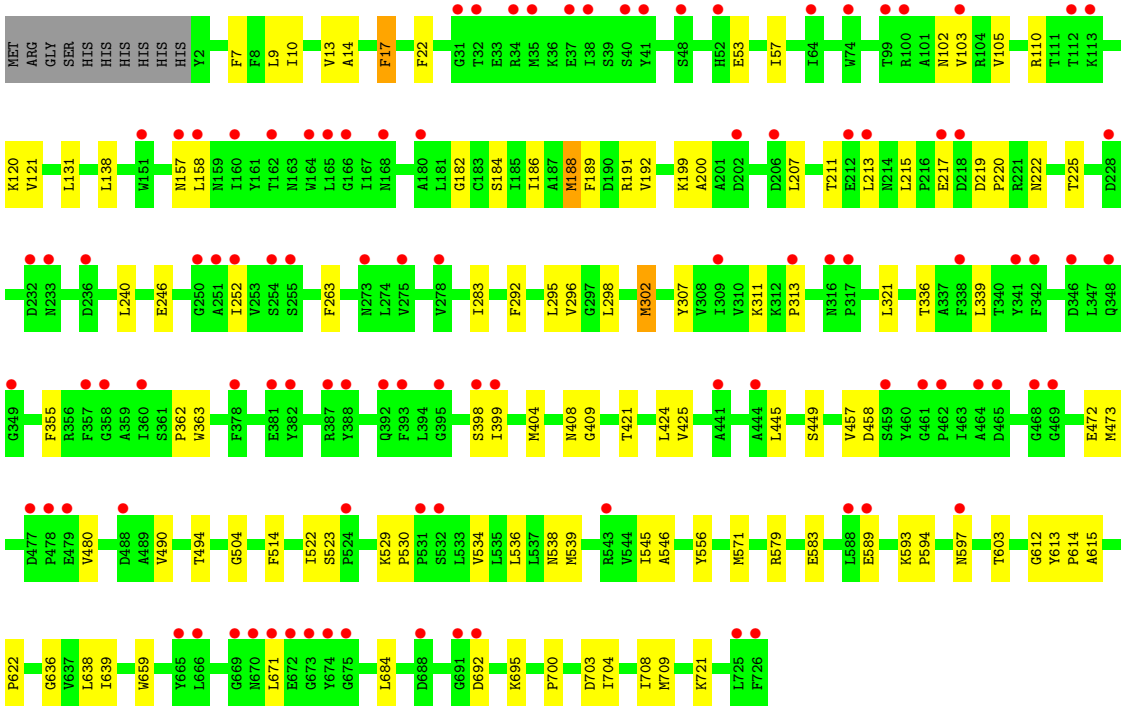
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: K(+)-stimulated pyrophosphate-energized sodium pump

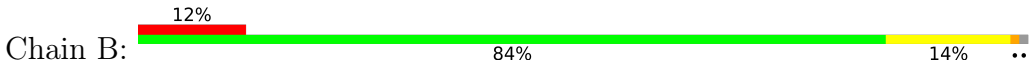
Chain A:

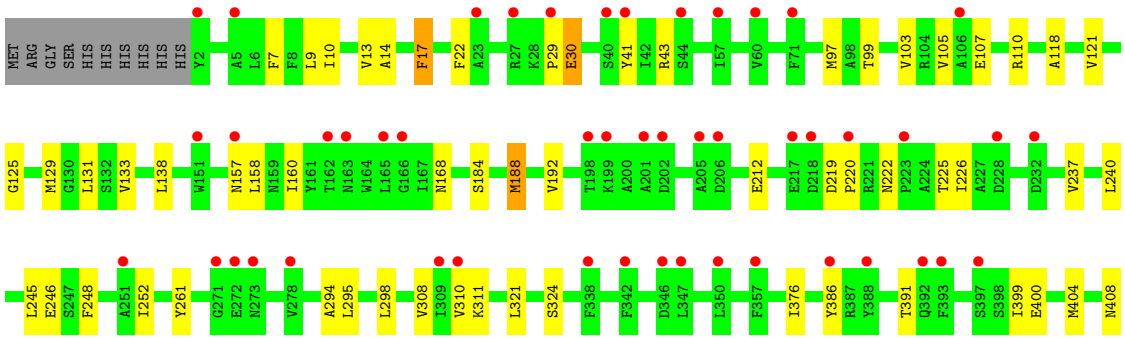


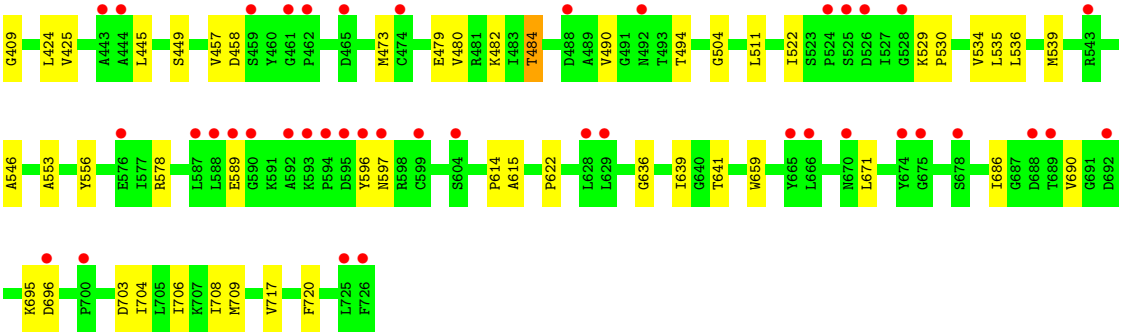


• Molecule 1: K(+)-stimulated pyrophosphate-energized sodium pump

Chain B:






G409
L424
V425
A443
A444
L445
S449
V457
D458
S459
Y460
G461
P462
D465
M473
C474
E479
V480
R481
K482
T483
T484
D488
A489
V490
G491
N492
T493
T494
G504
L511
I522
S523
P524
S525
D526
I527
G528
K529
P530
V534
L535
L536
M539
R543
A546
A553
Y556
E576
I577
R578
L587
L588
E589
G590
K591
A592
K593
P594
D595
Y596
N597
R598
C599
S604
P614
A615
P622
L628
L629
G636
I639
G640
T641
W659
Y665
L666
N670
L671
Y674
G675
S678
I686
G687
D688
T689
V690
G691
D692
K695
D696
P700
D703
I704
L705
I706
K707
I708
M709
V717
F720
L725
F726

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	106.42Å 106.76Å 161.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.75 – 3.50 29.75 – 3.49	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.75-3.50) 99.8 (29.75-3.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 3.47Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.245 , 0.273 0.250 , 0.280	Depositor DCC
R_{free} test set	1196 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	148.7	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 104.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.028 for k,h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10448	wwPDB-VP
Average B, all atoms (Å^2)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.31% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: 2PN, MG, NA

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	0.23	0/5337	0.40	0/7295
1	B	0.23	0/5281	0.40	0/7229
All	All	0.23	0/10618	0.40	0/14524

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

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	5224	0	5166	67	0
1	B	5170	0	5076	63	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	27	0	2	0	0
3	B	9	0	1	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	4	0	0	0	0
All	All	10448	0	10245	121	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 6.

All (121) 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:539:MET:HB2	1:B:539:MET:HE3	1.69	0.74
1:A:636:GLY:HA2	1:A:639:ILE:HD12	1.79	0.65
1:B:424:LEU:HD21	1:B:504:GLY:HA2	1.79	0.65
1:A:546:ALA:HB1	1:B:425:VAL:HG13	1.80	0.64
1:A:14:ALA:HB2	1:A:298:LEU:HD21	1.80	0.62
1:A:425:VAL:HG13	1:B:546:ALA:HB1	1.82	0.62
1:A:424:LEU:HD21	1:A:504:GLY:HA2	1.82	0.62
1:B:695:LYS:NZ	1:B:696:ASP:OD2	2.33	0.59
1:B:7:PHE:HB3	1:B:295:LEU:HD13	1.85	0.57
1:A:188:MET:HB2	1:A:704:ILE:HG21	1.86	0.57
1:A:579:ARG:NH1	1:A:583:GLU:OE1	2.38	0.56
1:A:184:SER:HA	1:A:246:GLU:HG3	1.86	0.56
1:B:622:PRO:HG3	1:B:709:MET:HG3	1.87	0.56
1:B:184:SER:HA	1:B:246:GLU:HG3	1.88	0.55
1:A:222:ASN:HB3	1:A:225:THR:HG23	1.88	0.55
1:B:212:GLU:OE2	1:B:578:ARG:NH2	2.37	0.55
1:B:105:VAL:HG13	1:B:118:ALA:HB1	1.88	0.55
1:A:321:LEU:HD22	1:A:457:VAL:HG13	1.88	0.55
1:A:53:GLU:HG2	1:A:57:ILE:HD11	1.89	0.54
1:B:480:VAL:O	1:B:484:THR:OG1	2.18	0.54
1:B:30:GLU:HG3	1:B:103:VAL:HG11	1.88	0.53
1:A:200:ALA:HB3	1:A:603:THR:HG22	1.89	0.53
1:B:14:ALA:HB2	1:B:298:LEU:HD21	1.91	0.53
1:B:222:ASN:HB3	1:B:225:THR:HG23	1.91	0.53
1:A:105:VAL:HG22	1:A:121:VAL:HG13	1.91	0.53
1:B:321:LEU:HD22	1:B:457:VAL:HG13	1.91	0.53
1:A:538:ASN:ND2	1:B:535:LEU:O	2.39	0.52
1:B:110:ARG:HA	1:B:480:VAL:HG22	1.91	0.52
1:A:192:VAL:HG11	1:A:614:PRO:HG3	1.91	0.51
1:A:404:MET:O	1:A:408:ASN:ND2	2.38	0.51
1:B:107:GLU:HG3	1:B:110:ARG:HH21	1.76	0.51
1:B:399:ILE:HD11	1:B:671:LEU:HD21	1.93	0.51
1:B:43:ARG:HG2	1:B:99:THR:HB	1.92	0.51
1:A:240:LEU:HD21	1:A:458:ASP:HB3	1.93	0.51
1:B:240:LEU:HD21	1:B:458:ASP:HB3	1.93	0.51
1:B:522:ILE:HD11	1:B:534:VAL:HG21	1.94	0.50
1:A:10:ILE:HG22	1:A:298:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:SER:HB2	1:A:708:ILE:HB	1.93	0.50
1:A:7:PHE:HB3	1:A:295:LEU:HD13	1.94	0.50
1:A:399:ILE:HD11	1:A:671:LEU:HD21	1.92	0.50
1:B:192:VAL:HG11	1:B:614:PRO:HG3	1.93	0.50
1:A:556:TYR:OH	1:B:556:TYR:OH	2.16	0.49
1:B:188:MET:HB2	1:B:704:ILE:HG21	1.93	0.49
1:A:252:ILE:HG12	1:A:445:LEU:HD13	1.92	0.49
1:B:252:ILE:HG12	1:B:445:LEU:HD13	1.95	0.49
1:A:571:MET:HG2	1:B:400:GLU:HG3	1.95	0.49
1:B:479:GLU:HA	1:B:482:LYS:HG2	1.93	0.49
1:B:404:MET:O	1:B:408:ASN:ND2	2.45	0.49
1:A:536:LEU:HD11	1:B:536:LEU:HD11	1.95	0.48
1:A:263:PHE:HB2	1:A:283:ILE:HG13	1.95	0.48
1:A:523:SER:OG	1:A:721:LYS:NZ	2.31	0.48
1:A:622:PRO:HG3	1:A:709:MET:HG3	1.96	0.48
1:B:160:ILE:HD11	1:B:168:ASN:HB3	1.96	0.47
1:A:17:PHE:HB3	1:A:131:LEU:HD13	1.96	0.47
1:A:217:GLU:O	1:A:472:GLU:HG2	2.15	0.46
1:B:10:ILE:HG22	1:B:298:LEU:HD22	1.98	0.46
1:B:445:LEU:O	1:B:449:SER:N	2.49	0.46
1:B:105:VAL:HG22	1:B:121:VAL:HG13	1.97	0.46
1:A:490:VAL:O	1:A:494:THR:HG23	2.16	0.46
1:B:17:PHE:HB3	1:B:131:LEU:HD13	1.98	0.46
1:B:220:PRO:HD3	1:B:473:MET:HA	1.97	0.46
1:A:188:MET:HG2	1:A:615:ALA:HB2	1.97	0.45
1:B:138:LEU:HD13	1:B:295:LEU:HD23	1.98	0.45
1:B:386:TYR:HA	1:B:391:THR:HB	1.97	0.45
1:B:490:VAL:O	1:B:494:THR:HG23	2.16	0.45
1:A:593:LYS:HA	1:A:594:PRO:HD3	1.85	0.45
1:A:213:LEU:HB3	1:A:215:LEU:HD13	1.98	0.45
1:A:157:ASN:OD1	1:A:158:LEU:N	2.40	0.45
1:A:191:ARG:HH21	1:A:240:LEU:HA	1.81	0.45
1:A:692:ASP:OD1	1:A:695:LYS:NZ	2.49	0.45
1:B:188:MET:HG2	1:B:615:ALA:HB2	1.98	0.45
1:B:157:ASN:OD1	1:B:158:LEU:N	2.39	0.45
1:A:14:ALA:HA	1:A:302:MET:SD	2.58	0.44
1:A:589:GLU:OE1	1:A:589:GLU:N	2.50	0.44
1:A:191:ARG:HD3	1:A:700:PRO:HB2	1.99	0.44
1:B:9:LEU:O	1:B:13:VAL:HG23	2.18	0.44
1:A:189:PHE:HE1	1:A:612:GLY:HA2	1.82	0.44
1:B:184:SER:HB2	1:B:708:ILE:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:589:GLU:N	1:B:589:GLU:OE1	2.50	0.44
1:B:184:SER:CA	1:B:246:GLU:HG3	2.48	0.43
1:A:9:LEU:O	1:A:13:VAL:HG23	2.19	0.43
1:B:226:ILE:HD12	1:B:596:TYR:CG	2.53	0.43
1:B:308:VAL:HG21	1:B:324:SER:HB2	1.99	0.43
1:B:409:GLY:HA3	1:B:659:TRP:CZ2	2.53	0.43
1:A:296:VAL:HG21	1:A:339:LEU:HD22	2.00	0.43
1:A:307:TYR:O	1:A:311:LYS:HB2	2.19	0.43
1:A:421:THR:HG21	1:B:553:ALA:HB2	1.99	0.43
1:B:717:VAL:HA	1:B:720:PHE:CZ	2.54	0.43
1:A:409:GLY:HA3	1:A:659:TRP:CZ2	2.54	0.43
1:A:336:THR:HG22	1:A:363:TRP:HD1	1.83	0.43
1:B:376:ILE:HD11	1:B:424:LEU:HD11	2.00	0.43
1:A:207:LEU:O	1:A:211:THR:HG22	2.18	0.42
1:B:129:MET:HE3	1:B:237:VAL:HG12	2.00	0.42
1:A:184:SER:CA	1:A:246:GLU:HG3	2.49	0.42
1:A:398:SER:HB3	1:A:684:LEU:HG	2.01	0.42
1:A:220:PRO:HD3	1:A:473:MET:HA	2.01	0.42
1:A:445:LEU:O	1:A:449:SER:N	2.52	0.42
1:A:514:PHE:HE1	1:A:638:LEU:HB3	1.84	0.42
1:B:133:VAL:HG13	1:B:245:LEU:HB2	2.00	0.42
1:B:636:GLY:HA2	1:B:639:ILE:HD12	2.02	0.42
1:A:138:LEU:HD13	1:A:295:LEU:HD23	2.02	0.42
1:A:292:PHE:HA	1:A:295:LEU:HD12	2.02	0.42
1:B:479:GLU:HA	1:B:482:LYS:HE3	2.02	0.42
1:B:529:LYS:HA	1:B:530:PRO:HD3	1.89	0.42
1:A:182:GLY:O	1:A:186:ILE:HG12	2.20	0.41
1:A:545:ILE:HD13	1:B:511:LEU:HG	2.02	0.41
1:B:641:THR:HG22	1:B:706:ILE:HG12	2.02	0.41
1:B:219:ASP:OD1	1:B:220:PRO:HD2	2.20	0.41
1:A:613:TYR:N	1:A:614:PRO:HD2	2.36	0.41
1:A:199:LYS:HD2	1:A:692:ASP:O	2.21	0.41
1:A:219:ASP:OD1	1:A:220:PRO:HD2	2.20	0.41
1:A:529:LYS:HA	1:A:530:PRO:HD3	1.90	0.41
1:A:110:ARG:HA	1:A:480:VAL:HG22	2.02	0.41
1:A:355:PHE:CE2	1:A:362:PRO:HD3	2.56	0.41
1:B:686:ILE:O	1:B:690:VAL:HG23	2.21	0.41
1:A:102:ASN:OD1	1:A:103:VAL:N	2.54	0.40
1:B:97:MET:HE2	1:B:125:GLY:HA2	2.03	0.40
1:B:29:PRO:HG2	1:B:107:GLU:OE1	2.21	0.40
1:A:120:LYS:HD2	1:A:313:PRO:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:ILE:HD11	1:A:534:VAL:HG21	2.03	0.40
1:B:248:PHE:CZ	1:B:294:ALA:HB1	2.57	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	723/735 (98%)	696 (96%)	27 (4%)	0	100 100
1	B	723/735 (98%)	692 (96%)	28 (4%)	3 (0%)	34 72
All	All	1446/1470 (98%)	1388 (96%)	55 (4%)	3 (0%)	47 81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	310	VAL
1	B	30	GLU
1	B	311	LYS

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	517/575 (90%)	511 (99%)	6 (1%)	71 87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	507/575 (88%)	499 (98%)	8 (2%)	62 83
All	All	1024/1150 (89%)	1010 (99%)	14 (1%)	67 85

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	PHE
1	A	22	PHE
1	A	188	MET
1	A	302	MET
1	A	597	ASN
1	A	703	ASP
1	B	17	PHE
1	B	22	PHE
1	B	41	TYR
1	B	188	MET
1	B	261	TYR
1	B	484	THR
1	B	597	ASN
1	B	703	ASP

Sometimes 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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
3	2PN	A	809	-	8,8,8	2.22	2 (25%)	8,13,13	1.44	0
3	2PN	A	808	-	8,8,8	2.23	2 (25%)	8,13,13	1.40	0
3	2PN	B	806	2	8,8,8	2.22	2 (25%)	8,13,13	1.40	0
3	2PN	A	806	2	8,8,8	2.22	2 (25%)	8,13,13	1.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	2PN	A	809	-	-	0/2/6/6	-
3	2PN	A	808	-	-	2/2/6/6	-
3	2PN	B	806	2	-	1/2/6/6	-
3	2PN	A	806	2	-	1/2/6/6	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	808	2PN	P2-O4	3.39	1.51	1.46
3	A	806	2PN	P2-O4	3.38	1.51	1.46
3	B	806	2PN	P1-O1	3.37	1.51	1.46
3	A	809	2PN	P2-O4	3.37	1.51	1.46
3	A	806	2PN	P1-O1	3.36	1.51	1.46
3	A	808	2PN	P1-O1	3.34	1.51	1.46
3	B	806	2PN	P2-O4	3.33	1.51	1.46
3	A	809	2PN	P1-O1	3.33	1.51	1.46

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	806	2PN	P2-N1-P1-O1
3	A	808	2PN	P2-N1-P1-O1
3	A	808	2PN	P1-N1-P2-O4
3	B	806	2PN	P2-N1-P1-O1

There are no ring outliers.

No monomer is involved in short contacts.

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

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	725/735 (98%)	0.61	102 (14%) 2 3	90, 130, 161, 182	0
1	B	725/735 (98%)	0.62	90 (12%) 4 5	94, 141, 180, 204	0
All	All	1450/1470 (98%)	0.62	192 (13%) 3 4	90, 135, 173, 204	0

All (192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	670	ASN	6.6
1	B	594	PRO	6.5
1	A	465	ASP	6.3
1	B	726	PHE	6.2
1	B	202	ASP	6.1
1	B	670	ASN	6.0
1	A	316	ASN	5.9
1	B	228	ASP	5.9
1	A	348	GLN	5.6
1	A	726	PHE	5.5
1	A	218	ASP	5.2
1	B	596	TYR	5.2
1	A	35	MET	5.0
1	A	255	SER	5.0
1	B	272	GLU	4.9
1	B	465	ASP	4.9
1	A	398	SER	4.9
1	A	674	TYR	4.8
1	B	206	ASP	4.7
1	B	218	ASP	4.7
1	B	41	TYR	4.6
1	B	675	GLY	4.5
1	B	590	GLY	4.3
1	B	386	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	671	LEU	4.3
1	B	232	ASP	4.2
1	A	228	ASP	4.2
1	A	236	ASP	4.1
1	B	44	SER	4.1
1	A	395	GLY	4.1
1	B	220	PRO	4.0
1	A	40	SER	4.0
1	A	692	ASP	3.9
1	B	151	TRP	3.9
1	B	696	ASP	3.9
1	A	597	ASN	3.9
1	A	357	PHE	3.8
1	A	232	ASP	3.8
1	A	588	LEU	3.8
1	B	40	SER	3.8
1	A	462	PRO	3.7
1	B	725	LEU	3.7
1	B	692	ASP	3.7
1	A	38	ILE	3.6
1	B	165	LEU	3.6
1	A	313	PRO	3.6
1	B	223	PRO	3.5
1	A	165	LEU	3.5
1	B	587	LEU	3.5
1	A	341	TYR	3.5
1	A	388	TYR	3.5
1	A	393	PHE	3.4
1	B	595	ASP	3.4
1	A	461	GLY	3.4
1	A	459	SER	3.4
1	B	251	ALA	3.4
1	B	388	TYR	3.4
1	A	64	ILE	3.3
1	B	462	PRO	3.3
1	A	100	ARG	3.3
1	B	27	ARG	3.3
1	A	381	GLU	3.3
1	B	525	SER	3.3
1	A	349	GLY	3.3
1	A	675	GLY	3.3
1	A	725	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	163	ASN	3.2
1	A	32	THR	3.2
1	A	52	HIS	3.2
1	A	360	ILE	3.2
1	A	441	ALA	3.2
1	A	202	ASP	3.2
1	B	309	ILE	3.2
1	A	251	ALA	3.2
1	B	392	GLN	3.2
1	B	597	ASN	3.1
1	B	217	GLU	3.1
1	A	688	ASP	3.1
1	A	669	GLY	3.1
1	B	666	LEU	3.1
1	B	166	GLY	3.0
1	A	392	GLN	3.0
1	A	41	TYR	3.0
1	B	592	ALA	3.0
1	A	399	ILE	3.0
1	B	474	CYS	3.0
1	B	60	VAL	3.0
1	A	206	ASP	3.0
1	A	254	SER	3.0
1	A	464	ALA	2.9
1	B	593	LYS	2.9
1	A	166	GLY	2.9
1	A	103	VAL	2.9
1	A	250	GLY	2.9
1	A	31	GLY	2.9
1	A	74	TRP	2.9
1	B	338	PHE	2.9
1	B	201	ALA	2.9
1	B	342	PHE	2.9
1	B	310	VAL	2.9
1	B	162	THR	2.9
1	B	488	ASP	2.8
1	A	48	SER	2.8
1	A	273	ASN	2.8
1	A	665	TYR	2.8
1	B	347	LEU	2.8
1	A	151	TRP	2.8
1	A	160	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	576	GLU	2.7
1	B	665	TYR	2.7
1	A	309	ILE	2.7
1	B	2	TYR	2.7
1	B	588	LEU	2.6
1	A	346	ASP	2.6
1	B	526	ASP	2.6
1	B	29	PRO	2.6
1	A	531	PRO	2.6
1	A	168	ASN	2.6
1	B	599	CYS	2.6
1	A	37	GLU	2.6
1	A	275	VAL	2.6
1	A	589	GLU	2.6
1	A	691	GLY	2.6
1	A	358	GLY	2.6
1	B	461	GLY	2.6
1	A	543	ARG	2.5
1	A	99	THR	2.5
1	A	387	ARG	2.5
1	A	278	VAL	2.5
1	A	524	PRO	2.5
1	A	317	PRO	2.5
1	B	57	ILE	2.5
1	A	488	ASP	2.5
1	B	459	SER	2.5
1	A	378	PHE	2.5
1	A	532	SER	2.5
1	B	346	ASP	2.5
1	A	673	GLY	2.5
1	B	198	THR	2.5
1	B	444	ALA	2.4
1	A	672	GLU	2.4
1	B	23	ALA	2.4
1	A	233	ASN	2.4
1	B	205	ALA	2.4
1	A	338	PHE	2.3
1	B	271	GLY	2.3
1	B	273	ASN	2.3
1	B	397	SER	2.3
1	A	158	LEU	2.3
1	A	157	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	357	PHE	2.3
1	A	212	GLU	2.3
1	A	217	GLU	2.3
1	B	157	ASN	2.3
1	B	199	LYS	2.2
1	A	112	THR	2.2
1	B	106	ALA	2.2
1	B	71	PHE	2.2
1	B	278	VAL	2.2
1	A	478	PRO	2.2
1	A	666	LEU	2.2
1	B	629	LEU	2.2
1	B	589	GLU	2.2
1	A	444	ALA	2.2
1	B	393	PHE	2.2
1	A	162	THR	2.2
1	A	164	TRP	2.1
1	A	252	ILE	2.1
1	B	678	SER	2.1
1	A	113	LYS	2.1
1	A	477	ASP	2.1
1	B	543	ARG	2.1
1	B	674	TYR	2.1
1	B	689	THR	2.1
1	A	469	GLY	2.1
1	A	180	ALA	2.1
1	A	479	GLU	2.1
1	A	213	LEU	2.1
1	B	524	PRO	2.1
1	B	528	GLY	2.1
1	A	342	PHE	2.1
1	A	34	ARG	2.1
1	A	382	TYR	2.1
1	B	492	ASN	2.1
1	A	468	GLY	2.1
1	B	688	ASP	2.1
1	B	5	ALA	2.0
1	B	700	PRO	2.0
1	B	443	ALA	2.0
1	B	604	SER	2.0
1	B	350	LEU	2.0
1	B	628	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å^2)	Q<0.9
3	2PN	A	808	9/9	0.67	0.35	182,189,195,202	0
3	2PN	A	809	9/9	0.76	0.52	146,161,184,192	0
4	NA	A	807	1/1	0.80	0.22	115,115,115,115	0
4	NA	B	807	1/1	0.81	0.46	125,125,125,125	0
2	MG	B	802	1/1	0.86	2.12	155,155,155,155	0
2	MG	B	801	1/1	0.87	0.60	136,136,136,136	0
2	MG	B	804	1/1	0.90	0.37	138,138,138,138	0
3	2PN	B	806	9/9	0.90	0.58	153,159,174,179	0
2	MG	A	804	1/1	0.91	0.76	130,130,130,130	0
3	2PN	A	806	9/9	0.92	0.68	142,145,156,164	0
2	MG	B	803	1/1	0.93	0.78	149,149,149,149	0
2	MG	A	803	1/1	0.94	0.58	104,104,104,104	0
2	MG	A	802	1/1	0.94	1.57	126,126,126,126	0
2	MG	B	805	1/1	0.94	0.73	140,140,140,140	0
2	MG	A	801	1/1	0.95	0.68	127,127,127,127	0
2	MG	A	805	1/1	0.97	0.36	130,130,130,130	0

6.5 Other polymers (i)

There are no such residues in this entry.