Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:13 PM GMT

PDB ID	:	1JDY
Title	:	RABBIT MUSCLE PHOSPHOGLUCOMUTASE
Authors	:	Ray Junior, W.J.; Baranidharan, S.; Liu, Y.
Deposited on	:	1996-07-11
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

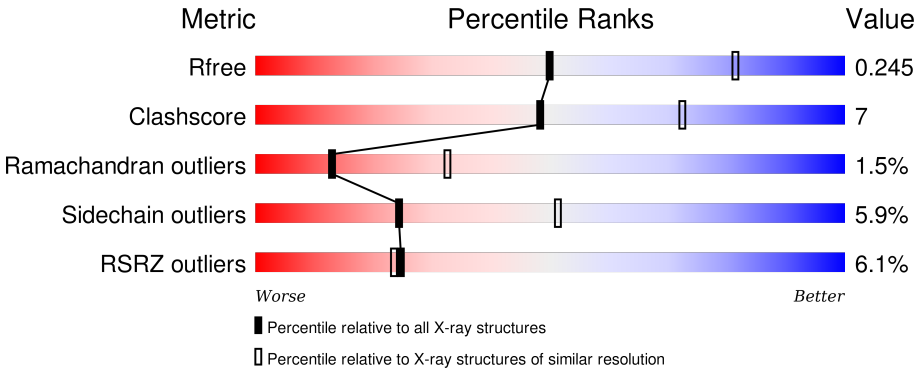
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	561	11% 71% 24%
1	B	561	% 76% 21%

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
2	CD	A	562	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9010 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.

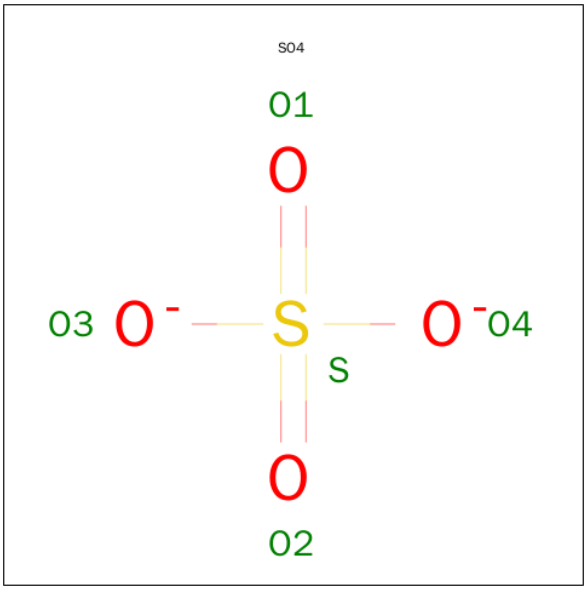
- Molecule 1 is a protein called PHOSPHOGLUCOMUTASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	561	Total	C	N	O	P	S	0	0	0
			4333	2753	743	820	1	16			
1	B	561	Total	C	N	O	P	S	0	0	0
			4333	2753	743	820	1	16			

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cd	0	0
			1	1		
2	A	1	Total	Cd	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

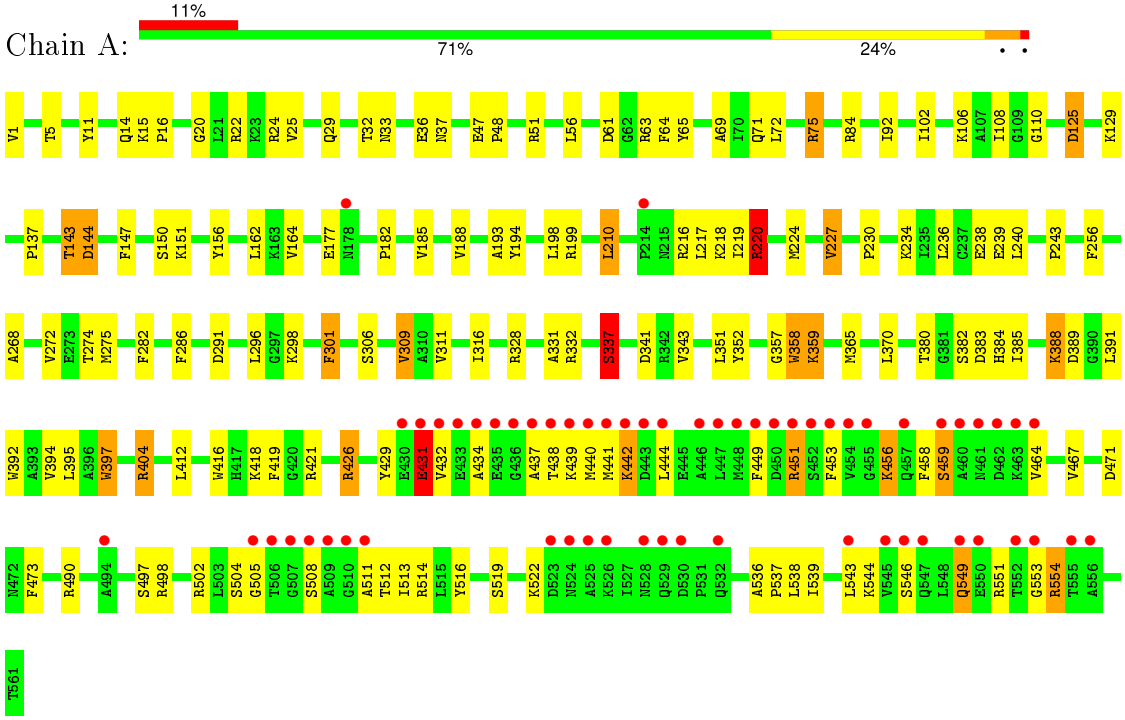
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	136	Total O 136 136	0	0
4	B	196	Total O 196 196	0	0

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.

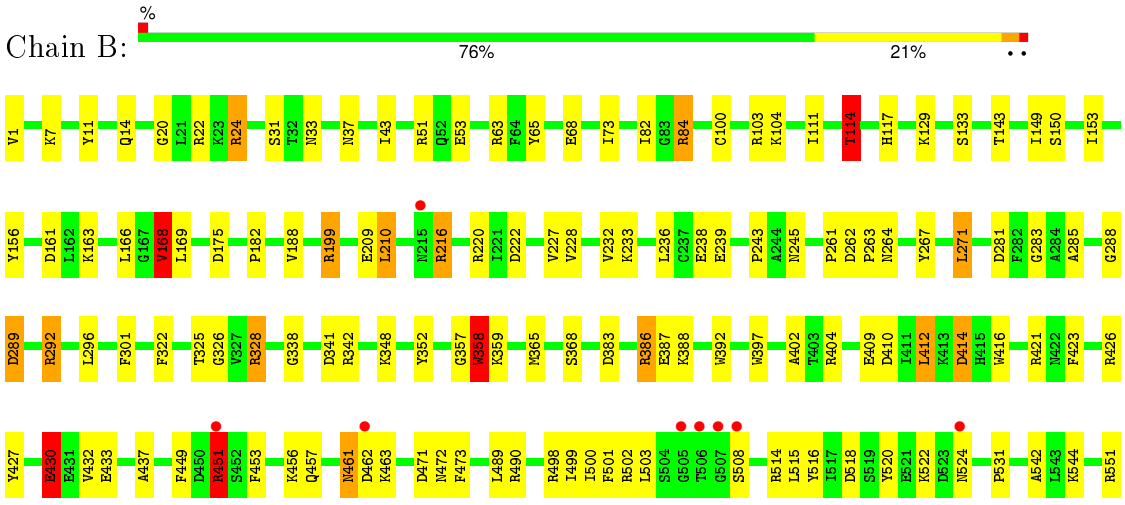
- Molecule 1: PHOSPHOGLUCOMUTASE

Chain A:



- Molecule 1: PHOSPHOGLUCOMUTASE

Chain B:




R554
T561

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	174.42Å 174.42Å 101.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.70 6.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	89.7 (6.00-2.70) 94.9 (6.00-2.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.91 (at 2.69Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.186 , 0.244 0.214 , 0.245	Depositor DCC
R_{free} test set	3800 reflections (11.38%)	DCC
Wilson B-factor (Å^2)	33.7	Xtriage
Anisotropy	0.476	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 88.8	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 37816 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9010	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CD, SO4, SEP

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	0.79	0/4409	1.61	50/5958 (0.8%)
1	B	0.80	1/4409 (0.0%)	1.62	60/5958 (1.0%)
All	All	0.80	1/8818 (0.0%)	1.61	110/11916 (0.9%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	358	TRP	CG-CD2	-5.05	1.35	1.43

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	386	ARG	NE-CZ-NH2	-12.66	113.97	120.30
1	B	421	ARG	NE-CZ-NH2	-10.94	114.83	120.30
1	A	22	ARG	NE-CZ-NH1	10.89	125.75	120.30
1	B	498	ARG	NE-CZ-NH2	-10.42	115.09	120.30
1	B	514	ARG	NE-CZ-NH2	-10.41	115.09	120.30
1	A	51	ARG	NE-CZ-NH2	-10.23	115.19	120.30
1	B	502	ARG	NE-CZ-NH1	10.21	125.41	120.30
1	A	421	ARG	NE-CZ-NH2	-10.03	115.29	120.30
1	A	220	ARG	NE-CZ-NH1	9.19	124.90	120.30
1	A	220	ARG	NE-CZ-NH2	-9.16	115.72	120.30
1	A	392	TRP	CD1-CG-CD2	9.16	113.63	106.30
1	B	416	TRP	CD1-CG-CD2	8.65	113.22	106.30
1	A	392	TRP	CE2-CD2-CG	-8.57	100.44	107.30
1	B	84	ARG	NE-CZ-NH2	-8.55	116.02	120.30
1	A	332	ARG	NE-CZ-NH2	8.51	124.55	120.30
1	B	386	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	A	199	ARG	NE-CZ-NH2	-8.43	116.08	120.30
1	A	397	TRP	CE2-CD2-CG	-8.43	100.55	107.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	498	ARG	NE-CZ-NH2	-8.43	116.09	120.30
1	B	392	TRP	CD1-CG-CD2	8.33	112.96	106.30
1	B	551	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	A	397	TRP	CD1-CG-CD2	7.97	112.68	106.30
1	B	22	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	B	24	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	B	63	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	A	404	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	B	514	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	B	103	ARG	NE-CZ-NH2	7.74	124.17	120.30
1	B	51	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	B	392	TRP	CE2-CD2-CG	-7.47	101.33	107.30
1	B	551	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	B	416	TRP	CE2-CD2-CG	-7.43	101.36	107.30
1	B	397	TRP	CE2-CD2-CG	-7.38	101.39	107.30
1	A	188	VAL	N-CA-CB	-7.26	95.52	111.50
1	A	404	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	B	328	ARG	NE-CZ-NH2	7.23	123.91	120.30
1	B	397	TRP	CD1-CG-CD2	7.15	112.02	106.30
1	B	358	TRP	CE2-CD2-CG	-7.08	101.64	107.30
1	B	502	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	B	342	ARG	NE-CZ-NH2	-6.97	116.82	120.30
1	B	358	TRP	CD1-CG-CD2	6.96	111.87	106.30
1	B	24	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	B	412	LEU	CA-CB-CG	-6.86	99.52	115.30
1	B	289	ASP	CB-CG-OD1	6.84	124.46	118.30
1	A	11	TYR	CB-CG-CD1	-6.74	116.96	121.00
1	A	22	ARG	NH1-CZ-NH2	-6.70	112.04	119.40
1	A	358	TRP	CE2-CD2-CG	-6.68	101.95	107.30
1	B	404	ARG	NE-CZ-NH2	6.66	123.63	120.30
1	A	392	TRP	CG-CD2-CE3	6.64	139.88	133.90
1	B	498	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	A	490	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	B	103	ARG	NE-CZ-NH1	-6.42	117.09	120.30
1	B	472	ASN	N-CA-C	-6.37	93.79	111.00
1	B	156	TYR	CB-CG-CD2	-6.36	117.19	121.00
1	A	554	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	B	430	GLU	N-CA-C	6.35	128.15	111.00
1	A	416	TRP	CD1-CG-CD2	6.30	111.34	106.30
1	B	210	LEU	CA-CB-CG	6.30	129.78	115.30
1	A	514	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	B	65	TYR	CB-CG-CD1	-6.27	117.24	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	352	TYR	CB-CG-CD1	-6.26	117.24	121.00
1	A	337	SER	CB-CA-C	-6.19	98.34	110.10
1	A	392	TRP	CB-CG-CD1	-6.12	119.05	127.00
1	B	199	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	B	554	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	A	309	VAL	CB-CA-C	-5.99	100.02	111.40
1	B	358	TRP	N-CA-C	5.95	127.05	111.00
1	B	228	VAL	CA-CB-CG2	-5.90	102.05	110.90
1	A	426	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	B	518	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	75	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	B	22	ARG	NH1-CZ-NH2	-5.79	113.03	119.40
1	A	328	ARG	NE-CZ-NH1	-5.79	117.40	120.30
1	B	168	VAL	CA-CB-CG2	-5.78	102.23	110.90
1	B	188	VAL	N-CA-CB	-5.75	98.85	111.50
1	B	392	TRP	CB-CG-CD1	-5.75	119.53	127.00
1	B	114	THR	CB-CA-C	-5.73	96.12	111.60
1	A	397	TRP	CG-CD2-CE3	5.72	139.05	133.90
1	A	84	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	A	426	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	451	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	B	228	VAL	CG1-CB-CG2	-5.59	101.96	110.90
1	A	32	THR	CA-CB-CG2	5.58	120.22	112.40
1	B	292	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	5	THR	CA-CB-CG2	5.55	120.17	112.40
1	A	416	TRP	CE2-CD2-CG	-5.51	102.89	107.30
1	A	65	TYR	CB-CG-CD1	-5.47	117.72	121.00
1	B	421	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	391	LEU	CA-CB-CG	5.42	127.76	115.30
1	B	63	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	177	GLU	CA-CB-CG	5.37	125.22	113.40
1	B	357	GLY	N-CA-C	5.32	126.40	113.10
1	B	451	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	A	25	VAL	CG1-CB-CG2	-5.30	102.42	110.90
1	A	392	TRP	CG-CD1-NE1	-5.30	104.80	110.10
1	A	331	ALA	CB-CA-C	-5.28	102.18	110.10
1	A	332	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	A	194	TYR	CB-CG-CD1	-5.27	117.84	121.00
1	B	414	ASP	N-CA-CB	-5.26	101.14	110.60
1	B	365	MET	CG-SD-CE	-5.25	91.81	100.20
1	B	397	TRP	CG-CD2-CE3	5.17	138.56	133.90
1	A	51	ARG	NE-CZ-NH1	5.17	122.88	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	358	TRP	CA-CB-CG	-5.17	103.88	113.70
1	A	358	TRP	CD1-CG-CD2	5.17	110.43	106.30
1	B	188	VAL	CA-CB-CG2	-5.14	103.19	110.90
1	A	502	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	B	433	GLU	CA-CB-CG	5.08	124.57	113.40
1	A	383	ASP	CB-CG-OD1	5.05	122.85	118.30
1	A	238	GLU	CA-CB-CG	-5.04	102.31	113.40
1	B	416	TRP	CG-CD1-NE1	-5.00	105.09	110.10

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	4333	0	4331	73	0
1	B	4333	0	4331	54	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	136	0	0	8	0
4	B	196	0	0	6	0
All	All	9010	0	8662	126	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 7.

All (126) 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:B:114:THR:HG21	1:B:289:ASP:HB3	1.46	0.94
1:A:14:GLN:HE21	1:A:150:SER:HB2	1.52	0.73
1:A:505:GLY:HA2	1:A:511:ALA:HA	1.71	0.73
1:B:33:ASN:HB3	1:B:37:ASN:ND2	2.03	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:GLY:HA3	1:A:359:LYS:HE3	1.78	0.66
1:B:68:GLU:HB2	4:B:715:HOH:O	1.98	0.63
1:B:271:LEU:HD13	1:B:296:LEU:HD12	1.80	0.63
1:A:519:SER:HB3	1:A:538:LEU:HD12	1.80	0.62
1:A:301:PHE:HE2	1:A:412:LEU:HD12	1.66	0.61
1:A:426:ARG:HG3	1:A:516:TYR:CD1	2.35	0.61
1:B:473:PHE:HB2	1:B:490:ARG:HD2	1.82	0.60
1:B:368:SER:HA	4:B:653:HOH:O	2.00	0.60
1:A:440:MET:O	1:A:444:LEU:HB2	2.03	0.59
1:A:164:VAL:HG21	1:A:185:VAL:HG11	1.84	0.58
1:A:449:PHE:HE1	1:A:471:ASP:HA	1.69	0.58
1:B:426:ARG:HG3	1:B:516:TYR:CD1	2.38	0.58
1:A:453:PHE:HA	1:A:456:LYS:NZ	2.17	0.58
1:A:63:ARG:HB3	1:A:256:PHE:CE1	2.40	0.57
1:A:193:ALA:HB2	4:A:682:HOH:O	2.03	0.57
1:A:453:PHE:HA	1:A:456:LYS:HZ1	1.69	0.56
1:B:264:ASN:HD21	1:B:267:TYR:HD2	1.53	0.56
1:B:114:THR:CG2	1:B:289:ASP:HB3	2.30	0.56
1:A:218:LYS:NZ	1:A:218:LYS:HB2	2.21	0.56
1:A:210:LEU:HD22	1:A:217:LEU:HB2	1.87	0.55
1:B:359:LYS:H	1:B:359:LYS:HD3	1.72	0.55
1:B:243:PRO:HB2	1:B:245:ASN:OD1	2.07	0.55
1:B:423:PHE:HD2	1:B:531:PRO:HB3	1.72	0.55
1:A:268:ALA:O	1:A:272:VAL:HG23	2.07	0.54
1:A:459:SER:OG	1:A:464:VAL:HA	2.07	0.54
1:A:306:SER:HB3	1:A:337:SER:HB2	1.87	0.54
1:A:219:ILE:HG22	1:A:282:PHE:HB3	1.88	0.54
1:A:382:SER:OG	1:A:384:HIS:HD2	1.91	0.54
1:A:311:VAL:HG11	1:A:397:TRP:CH2	2.44	0.53
1:B:43:ILE:HG23	1:B:82:ILE:HD11	1.91	0.52
1:A:432:VAL:HG22	1:A:511:ALA:O	2.09	0.52
1:A:220:ARG:NH1	1:A:274:THR:HG21	2.25	0.52
1:A:1:VAL:HG11	1:A:162:LEU:HD12	1.91	0.52
1:A:437:ALA:O	1:A:441:MET:HG2	2.10	0.51
1:B:33:ASN:HB3	1:B:37:ASN:HD22	1.76	0.51
1:B:451:ARG:H	1:B:451:ARG:HD3	1.75	0.51
1:A:497:SER:HB3	1:A:538:LEU:HD11	1.91	0.51
1:A:61:ASP:HA	1:A:227:VAL:HB	1.94	0.50
1:B:14:GLN:HE21	1:B:150:SER:HB2	1.77	0.50
1:A:16:PRO:HB2	1:A:143:THR:HG22	1.93	0.50
1:B:210:LEU:HG	1:B:402:ALA:HB2	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:LYS:HG2	4:A:566:HOH:O	2.11	0.49
1:A:182:PRO:HA	4:A:652:HOH:O	2.12	0.49
1:A:239:GLU:HB2	1:B:168:VAL:HG21	1.94	0.49
1:A:69:ALA:O	1:A:72:LEU:HB2	2.12	0.49
1:A:365:MET:HG3	1:A:370:LEU:HD23	1.95	0.49
1:A:301:PHE:CE2	1:A:412:LEU:HD12	2.48	0.49
1:B:220:ARG:O	1:B:283:GLY:HA2	2.13	0.49
1:B:129:LYS:NZ	1:B:387:GLU:OE1	2.46	0.49
1:A:14:GLN:NE2	1:A:150:SER:HB2	2.23	0.49
1:A:384:HIS:CE1	1:A:385:ILE:HG12	2.47	0.49
1:A:549:GLN:O	1:A:553:GLY:HA2	2.13	0.49
1:B:232:VAL:HG13	1:B:236:LEU:HD12	1.95	0.48
1:A:404:ARG:NH2	4:A:659:HOH:O	2.47	0.48
1:A:388:LYS:NZ	4:A:579:HOH:O	2.47	0.48
1:A:24:ARG:HA	1:A:125:ASP:HA	1.96	0.48
1:B:216:ARG:NH2	1:B:243:PRO:HG3	2.29	0.47
1:A:29:GLN:HE22	1:A:64:PHE:HE2	1.62	0.47
1:B:544:LYS:HE2	4:B:677:HOH:O	2.15	0.46
1:B:432:VAL:CG1	1:B:437:ALA:HB2	2.45	0.46
1:B:261:PRO:HB2	1:B:288:GLY:N	2.31	0.46
1:A:36:GLU:HG2	1:A:156:TYR:CZ	2.51	0.46
1:A:536:ALA:HB3	1:A:537:PRO:HD3	1.97	0.46
1:B:456:LYS:NZ	1:B:457:GLN:O	2.49	0.46
1:B:73:ILE:HD13	1:B:111:ILE:HG21	1.97	0.46
1:A:438:THR:O	1:A:442:LYS:HG2	2.16	0.46
1:A:236:LEU:HD23	1:A:240:LEU:HD12	1.97	0.46
1:A:71:GLN:HB3	1:A:75:ARG:HH12	1.79	0.45
1:B:338:GLY:HA2	1:B:341:ASP:OD1	2.16	0.45
1:A:439:LYS:HB2	1:A:439:LYS:HE3	1.78	0.45
1:A:351:LEU:HG	1:A:352:TYR:N	2.31	0.45
1:A:298:LYS:HG3	4:A:606:HOH:O	2.16	0.45
1:B:149:ILE:O	1:B:153:ILE:HB	2.16	0.45
1:A:147:PHE:CZ	1:A:151:LYS:HD2	2.50	0.45
1:B:501:PHE:CE1	1:B:515:LEU:HD13	2.51	0.45
1:A:473:PHE:HA	4:A:697:HOH:O	2.16	0.45
1:A:539:ILE:O	1:A:543:LEU:HD23	2.15	0.45
1:A:14:GLN:O	1:A:16:PRO:HD3	2.16	0.45
1:A:431:GLU:O	1:A:554:ARG:NH2	2.50	0.45
1:B:383:ASP:O	1:B:386:ARG:NH2	2.50	0.45
1:A:275:MET:HG3	1:A:296:LEU:HD13	1.97	0.45
1:B:348:LYS:HA	4:B:647:HOH:O	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:ILE:HD13	1:B:542:ALA:HB2	1.98	0.44
1:A:440:MET:HG3	1:A:546:SER:O	2.18	0.44
1:B:426:ARG:HG3	1:B:516:TYR:CE1	2.52	0.44
1:A:504:SER:HB2	1:A:512:THR:HB	2.00	0.44
1:A:15:LYS:HA	1:A:16:PRO:HD3	1.83	0.44
1:B:520:TYR:OH	1:B:522:LYS:HD3	2.17	0.44
1:B:262:ASP:HA	1:B:263:PRO:HD2	1.91	0.43
1:A:343:VAL:HA	1:A:419:PHE:CE1	2.53	0.43
1:B:449:PHE:HE1	1:B:471:ASP:HA	1.82	0.43
1:B:453:PHE:O	1:B:456:LYS:HB3	2.19	0.43
1:A:33:ASN:HB3	1:A:37:ASN:HD22	1.82	0.43
1:A:198:LEU:HD13	1:A:395:LEU:HD12	2.01	0.43
1:A:286:PHE:CZ	1:A:394:VAL:HG21	2.54	0.43
1:A:71:GLN:HB3	1:A:75:ARG:NH1	2.34	0.42
1:B:463:LYS:HE3	4:B:678:HOH:O	2.18	0.42
1:A:20:GLY:HA3	1:A:129:LYS:HA	2.00	0.42
1:B:117:HIS:HB3	1:B:292:ARG:NH2	2.34	0.42
1:B:322:PHE:HA	1:B:325:THR:HG22	2.01	0.42
1:A:384:HIS:HE1	1:A:389:ASP:OD2	2.02	0.42
1:B:20:GLY:HA3	1:B:129:LYS:HA	2.02	0.42
1:A:144:ASP:O	1:A:147:PHE:HB3	2.19	0.42
1:B:222:ASP:O	1:B:285:ALA:HA	2.19	0.42
1:A:56:LEU:HD23	1:A:108:ILE:HG22	2.00	0.42
1:A:129:LYS:HZ1	1:A:137:PRO:HG3	1.85	0.41
1:B:1:VAL:N	1:B:175:ASP:O	2.52	0.41
1:A:102:ILE:HD11	1:A:110:GLY:HA3	2.01	0.41
1:B:358:TRP:CD1	1:B:388:LYS:HG3	2.54	0.41
1:A:546:SER:O	1:A:551:ARG:NH1	2.53	0.41
1:B:325:THR:HG23	1:B:326:GLY:O	2.20	0.41
1:A:429:TYR:HB2	1:A:513:ILE:HB	2.02	0.41
1:B:489:LEU:O	1:B:500:ILE:HA	2.20	0.41
1:B:104:LYS:HD2	4:B:575:HOH:O	2.21	0.41
1:B:410:ASP:O	1:B:414:ASP:HB3	2.20	0.41
1:A:106:LYS:NZ	4:A:689:HOH:O	2.49	0.41
1:B:11:TYR:OH	1:B:31:SER:HB3	2.21	0.41
1:B:84:ARG:HD2	1:B:84:ARG:HH11	1.74	0.41
1:A:418:LYS:HB2	1:A:418:LYS:HE3	1.57	0.40
1:B:503:LEU:HA	1:B:503:LEU:HD12	1.90	0.40
1:B:427:TYR:HB2	1:B:515:LEU:HB3	2.02	0.40
1:B:199:ARG:NH1	1:B:239:GLU:OE1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	558/561 (100%)	505 (90%)	44 (8%)	9 (2%)	12	30
1	B	558/561 (100%)	530 (95%)	20 (4%)	8 (1%)	14	35
All	All	1116/1122 (100%)	1035 (93%)	64 (6%)	17 (2%)	13	32

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	ARG
1	A	431	GLU
1	B	358	TRP
1	A	224	MET
1	A	301	PHE
1	A	434	ALA
1	A	467	VAL
1	B	133	SER
1	B	238	GLU
1	B	461	ASN
1	B	508	SER
1	A	508	SER
1	B	462	ASP
1	A	337	SER
1	B	430	GLU
1	B	301	PHE
1	A	316	ILE

5.3.2 Protein sidechains

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	461/461 (100%)	433 (94%)	28 (6%)	23 49
1	B	461/461 (100%)	435 (94%)	26 (6%)	26 54
All	All	922/922 (100%)	868 (94%)	54 (6%)	24 51

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

Mol	Chain	Res	Type
1	A	47	GLU
1	A	48	PRO
1	A	92	ILE
1	A	125	ASP
1	A	143	THR
1	A	144	ASP
1	A	210	LEU
1	A	220	ARG
1	A	227	VAL
1	A	230	PRO
1	A	234	LYS
1	A	243	PRO
1	A	291	ASP
1	A	309	VAL
1	A	341	ASP
1	A	358	TRP
1	A	359	LYS
1	A	380	THR
1	A	388	LYS
1	A	431	GLU
1	A	442	LYS
1	A	451	ARG
1	A	456	LYS
1	A	458	PHE
1	A	459	SER
1	A	522	LYS
1	A	544	LYS
1	A	549	GLN
1	B	7	LYS
1	B	24	ARG
1	B	53	GLU
1	B	100	CYS
1	B	114	THR
1	B	143	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	161	ASP
1	B	163	LYS
1	B	166	LEU
1	B	168	VAL
1	B	169	LEU
1	B	182	PRO
1	B	209	GLU
1	B	216	ARG
1	B	227	VAL
1	B	233	LYS
1	B	271	LEU
1	B	281	ASP
1	B	328	ARG
1	B	358	TRP
1	B	409	GLU
1	B	412	LEU
1	B	430	GLU
1	B	451	ARG
1	B	461	ASN
1	B	524	ASN

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	14	GLN
1	A	29	GLN
1	A	71	GLN
1	A	249	ASN
1	A	324	GLN
1	A	345	ASN
1	A	384	HIS
1	A	461	ASN
1	B	14	GLN
1	B	417	HIS
1	B	476	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	SEP	A	116	1,2	8,9,10	1.57	1 (12%)	8,12,14	3.63	2 (25%)
1	SEP	B	116	1,2	8,9,10	1.68	1 (12%)	8,12,14	3.27	2 (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
1	SEP	A	116	1,2	-	0/6/8/10	0/0/0/0
1	SEP	B	116	1,2	-	0/6/8/10	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	116	SEP	P-OG	-3.50	1.48	1.60
1	A	116	SEP	P-OG	-2.80	1.50	1.60

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	116	SEP	O-C-CA	-3.17	117.23	125.49
1	A	116	SEP	O-C-CA	-2.97	117.77	125.49
1	B	116	SEP	OG-CB-CA	8.41	115.45	108.27
1	A	116	SEP	OG-CB-CA	9.63	116.49	108.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	SO4	A	563	-	4,4,4	1.10	0	6,6,6	0.46	0
3	SO4	B	563	-	4,4,4	1.01	0	6,6,6	0.48	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	SO4	A	563	-	-	0/0/0/0	0/0/0/0
3	SO4	B	563	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	560/561 (99%)	0.24	60 (10%) 8 6	0, 34, 88, 98	0
1	B	560/561 (99%)	-0.52	8 (1%) 78 77	3, 25, 58, 89	0
All	All	1120/1122 (99%)	-0.14	68 (6%) 25 23	0, 28, 79, 98	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	443	ASP	8.2
1	A	462	ASP	8.1
1	A	446	ALA	7.8
1	A	461	ASN	7.6
1	A	507	GLY	7.4
1	A	510	GLY	7.1
1	A	452	SER	6.8
1	A	506	THR	6.8
1	A	508	SER	6.8
1	A	436	GLY	6.5
1	B	507	GLY	6.4
1	A	509	ALA	6.2
1	A	464	VAL	5.9
1	A	437	ALA	5.6
1	A	528	ASN	5.5
1	A	463	LYS	5.1
1	A	460	ALA	4.9
1	A	552	THR	4.8
1	A	530	ASP	4.7
1	A	439	LYS	4.6
1	A	450	ASP	4.4
1	A	453	PHE	4.2
1	B	508	SER	4.1
1	A	529	GLN	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	555	THR	3.9
1	A	432	VAL	3.9
1	A	553	GLY	3.7
1	A	511	ALA	3.7
1	A	524	ASN	3.6
1	A	547	GLN	3.6
1	A	532	GLN	3.5
1	A	556	ALA	3.5
1	A	435	GLU	3.5
1	A	434	ALA	3.5
1	A	431	GLU	3.4
1	A	505	GLY	3.3
1	A	545	VAL	3.2
1	A	459	SER	3.2
1	A	549	GLN	3.2
1	A	546	SER	3.2
1	A	438	THR	3.2
1	A	447	LEU	3.1
1	A	457	GLN	2.8
1	A	214	PRO	2.8
1	A	449	PHE	2.8
1	A	523	ASP	2.8
1	B	524	ASN	2.8
1	A	451	ARG	2.8
1	A	178	ASN	2.8
1	B	505	GLY	2.7
1	A	441	MET	2.7
1	B	506	THR	2.7
1	A	455	GLY	2.6
1	A	543	LEU	2.6
1	A	448	MET	2.6
1	A	454	VAL	2.6
1	A	433	GLU	2.6
1	A	550	GLU	2.4
1	B	215	ASN	2.4
1	A	440	MET	2.4
1	A	525	ALA	2.4
1	A	526	LYS	2.4
1	A	444	LEU	2.3
1	A	494	ALA	2.3
1	A	442	LYS	2.3
1	B	451	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	430	GLU	2.2
1	B	462	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	SEP	A	116	10/11	0.93	0.20	-	23,30,44,46	0
1	SEP	B	116	10/11	0.86	0.23	-	19,29,47,49	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CD	A	562	1/1	0.98	0.29	5.68	2,2,2,2	0
2	CD	B	562	1/1	0.99	0.25	-	2,2,2,2	0
3	SO4	A	563	5/5	0.80	0.36	-	95,95,96,96	0
3	SO4	B	563	5/5	0.84	0.43	-	90,90,90,91	0

6.5 Other polymers (i)

There are no such residues in this entry.