Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:25 PM GMT

PDB ID	:	1OYY
Title	:	Structure of the RecQ Catalytic Core bound to ATP-gamma-S
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Deposited on	:	2003-04-07
Resolution	:	2.50 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
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:

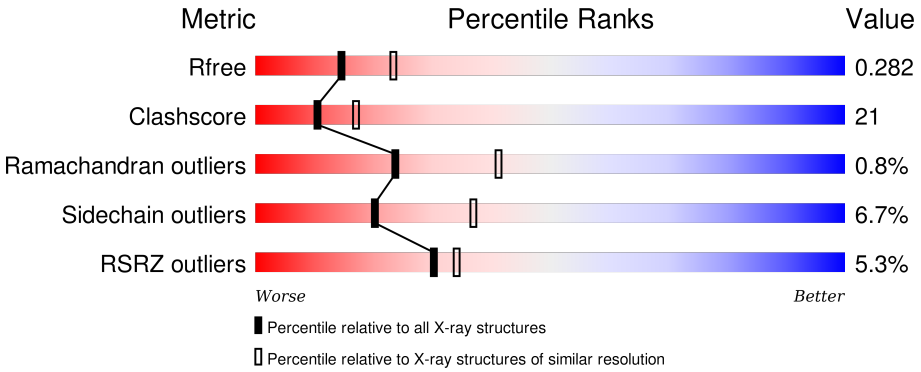
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	523	5% 49% 42% 6%

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
4	AGS	A	527	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4114 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 ATP-dependent DNA helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	512	Total	C	N	O	S	0	0	0
			4037	2529	735	748	25			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING MET	UNP P15043

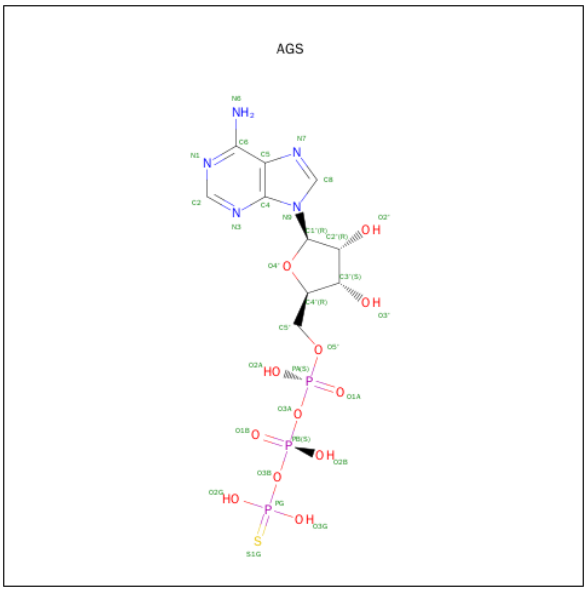
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mn	0	0
			2	2		

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 5 is water.

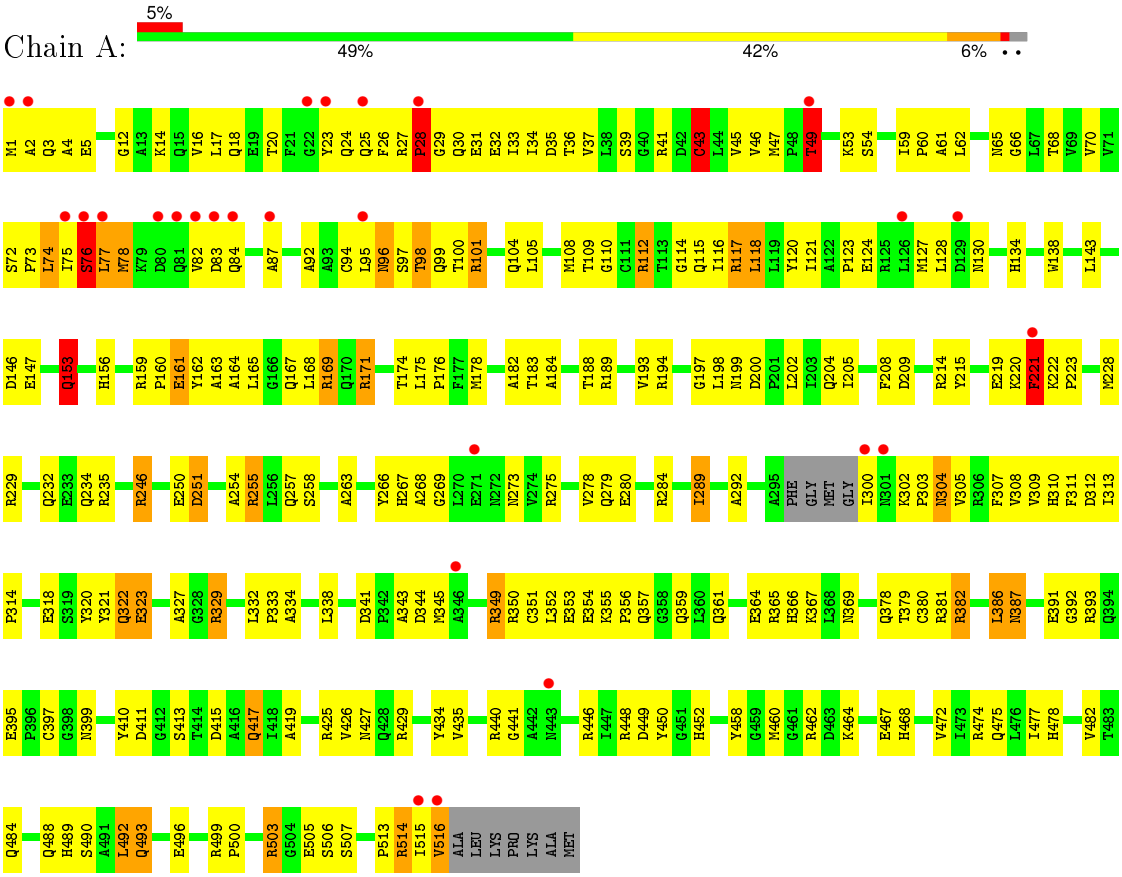
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	43	Total	O	0	0
			43	43		

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: ATP-dependent DNA helicase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.59Å 54.53Å 78.69Å 90.00° 110.78° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.42 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.50) 91.0 (19.42-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	6.84 (at 2.49Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.210 , 0.298 0.198 , 0.282	Depositor DCC
R_{free} test set	826 reflections (5.17%)	DCC
Wilson B-factor (Å^2)	32.3	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 59.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 16814 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4114	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.86% 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: ZN, MN, AGS

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	0.62	0/4108	1.68	62/5559 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	17

There are no bond length outliers.

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	393	ARG	NE-CZ-NH2	-14.85	112.88	120.30
1	A	112	ARG	NE-CZ-NH1	14.71	127.65	120.30
1	A	382	ARG	NE-CZ-NH2	-14.04	113.28	120.30
1	A	393	ARG	NE-CZ-NH1	12.35	126.48	120.30
1	A	284	ARG	CD-NE-CZ	10.98	138.98	123.60
1	A	112	ARG	CD-NE-CZ	10.89	138.84	123.60
1	A	117	ARG	NE-CZ-NH2	-10.34	115.13	120.30
1	A	446	ARG	CD-NE-CZ	10.27	137.98	123.60
1	A	381	ARG	NE-CZ-NH2	-10.10	115.25	120.30
1	A	440	ARG	NE-CZ-NH1	-9.43	115.58	120.30
1	A	382	ARG	NH1-CZ-NH2	8.43	128.67	119.40
1	A	514	ARG	CD-NE-CZ	8.27	135.18	123.60
1	A	320	TYR	CB-CG-CD2	-8.01	116.20	121.00
1	A	194	ARG	CD-NE-CZ	7.92	134.68	123.60
1	A	171	ARG	NE-CZ-NH2	-7.63	116.49	120.30
1	A	450	TYR	CB-CG-CD2	7.41	125.45	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	171	ARG	NE-CZ-NH1	-7.40	116.60	120.30
1	A	215	TYR	CB-CG-CD2	-7.17	116.70	121.00
1	A	320	TYR	CB-CG-CD1	7.14	125.28	121.00
1	A	450	TYR	CB-CG-CD1	-7.09	116.75	121.00
1	A	312	ASP	CB-CG-OD1	7.07	124.66	118.30
1	A	410	TYR	CB-CG-CD2	6.94	125.16	121.00
1	A	171	ARG	NH1-CZ-NH2	6.82	126.91	119.40
1	A	251	ASP	CB-CG-OD1	6.74	124.37	118.30
1	A	284	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	A	462	ARG	NE-CZ-NH1	-6.66	116.97	120.30
1	A	101	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	A	411	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	A	410	TYR	CB-CG-CD1	-6.45	117.13	121.00
1	A	41	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	A	292	ALA	CB-CA-C	-6.33	100.60	110.10
1	A	118	LEU	CB-CG-CD2	-6.31	100.27	111.00
1	A	349	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	A	322	GLN	N-CA-CB	6.28	121.90	110.60
1	A	425	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	43	CYS	CB-CA-C	-6.12	98.16	110.40
1	A	446	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	A	215	TYR	CB-CG-CD1	5.94	124.56	121.00
1	A	419	ALA	CB-CA-C	5.89	118.93	110.10
1	A	329	ARG	CD-NE-CZ	5.88	131.83	123.60
1	A	49	THR	CA-CB-CG2	-5.83	104.23	112.40
1	A	251	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	A	503	ARG	CD-NE-CZ	5.80	131.72	123.60
1	A	250	GLU	OE1-CD-OE2	-5.70	116.47	123.30
1	A	153	GLN	CB-CG-CD	5.64	126.26	111.60
1	A	159	ARG	CA-CB-CG	5.57	125.66	113.40
1	A	411	ASP	CB-CG-OD1	5.44	123.19	118.30
1	A	488	GLN	OE1-CD-NE2	5.42	134.37	121.90
1	A	323	GLU	OE1-CD-OE2	-5.39	116.84	123.30
1	A	334	ALA	N-CA-CB	5.38	117.64	110.10
1	A	514	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	484	GLN	O-C-N	5.30	131.18	122.70
1	A	255	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	35	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	A	159	ARG	NE-CZ-NH1	-5.13	117.74	120.30
1	A	410	TYR	N-CA-CB	5.09	119.75	110.60
1	A	246	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	268	ALA	CB-CA-C	-5.08	102.48	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	344	ASP	CB-CG-OD1	5.07	122.87	118.30
1	A	493	GLN	CB-CG-CD	5.07	124.79	111.60
1	A	344	ASP	N-CA-CB	5.02	119.64	110.60
1	A	235	ARG	NE-CZ-NH2	5.02	122.81	120.30

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	THR	Mainchain
1	A	164	ALA	Mainchain
1	A	167	GLN	Mainchain
1	A	219	GLU	Mainchain
1	A	221	PHE	Mainchain
1	A	280	GLU	Mainchain
1	A	289	ILE	Mainchain
1	A	304	ASN	Mainchain
1	A	367	LYS	Mainchain
1	A	387	ASN	Mainchain
1	A	39	SER	Mainchain
1	A	397	CYS	Mainchain
1	A	429	ARG	Mainchain
1	A	449	ASP	Mainchain
1	A	460	MET	Mainchain
1	A	475	GLN	Mainchain
1	A	492	LEU	Mainchain

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	4037	0	4033	170	0
2	A	1	0	0	0	0
3	A	2	0	0	0	0
4	A	31	0	11	5	0
5	A	43	0	0	3	0
All	All	4114	0	4044	174	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (174) 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)
4:A:527:AGS:S1G	4:A:527:AGS:PG	1.49	1.47
1:A:169:ARG:HD3	1:A:197:GLY:HA3	1.52	0.90
1:A:96:ASN:ND2	1:A:98:THR:HG22	1.87	0.90
1:A:366:HIS:HD2	1:A:490:SER:OG	1.55	0.88
1:A:514:ARG:HG3	1:A:516:VAL:HG22	1.58	0.86
1:A:228:MET:O	1:A:232:GLN:HG2	1.78	0.84
1:A:14:LYS:HE3	1:A:31:GLU:OE2	1.78	0.83
1:A:434:TYR:OH	1:A:452:HIS:HD2	1.61	0.82
1:A:112:ARG:HA	1:A:138:TRP:CD1	2.15	0.81
1:A:349:ARG:NH1	1:A:369:ASN:OD1	2.13	0.81
1:A:387:ASN:OD1	1:A:392:GLY:HA2	1.81	0.80
1:A:310:HIS:HE1	1:A:323:GLU:OE1	1.65	0.80
1:A:76:SER:O	1:A:77:LEU:HB2	1.80	0.80
4:A:527:AGS:O3G	4:A:527:AGS:S1G	2.42	0.77
4:A:527:AGS:S1G	4:A:527:AGS:O2G	2.40	0.77
1:A:118:LEU:HD21	1:A:120:TYR:CE1	2.19	0.76
1:A:434:TYR:OH	1:A:452:HIS:CD2	2.37	0.76
1:A:183:THR:HG22	1:A:183:THR:O	1.87	0.74
1:A:382:ARG:O	1:A:386:LEU:HD22	1.86	0.74
4:A:527:AGS:O3B	4:A:527:AGS:S1G	2.47	0.73
1:A:83:ASP:OD2	5:A:547:HOH:O	2.08	0.72
1:A:73:PRO:HD2	1:A:74:LEU:HD22	1.71	0.72
1:A:160:PRO:HG2	1:A:161:GLU:OE1	1.90	0.71
1:A:366:HIS:CD2	1:A:490:SER:OG	2.45	0.68
1:A:267:HIS:HD2	1:A:269:GLY:H	1.43	0.67
1:A:209:ASP:OD1	1:A:382:ARG:HD3	1.94	0.66
1:A:124:GLU:N	1:A:124:GLU:OE1	2.17	0.66
1:A:220:LYS:O	1:A:221:PHE:HB2	1.94	0.66
1:A:94:CYS:HA	1:A:120:TYR:O	1.96	0.65
1:A:499:ARG:HB3	1:A:500:PRO:HD3	1.78	0.65
1:A:5:GLU:HG3	1:A:62:LEU:O	1.96	0.65
1:A:118:LEU:O	1:A:118:LEU:HD23	1.97	0.65
1:A:1:MET:HA	1:A:114:GLY:O	1.98	0.64
1:A:464:LYS:HD3	1:A:468:HIS:CE1	2.33	0.64
1:A:46:VAL:HG21	1:A:189:ARG:HD2	1.78	0.64
1:A:75:ILE:H	1:A:75:ILE:HD12	1.62	0.64
1:A:2:ALA:O	1:A:65:ASN:HA	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LEU:HD23	1:A:121:ILE:HD12	1.78	0.63
1:A:310:HIS:HD2	5:A:540:HOH:O	1.80	0.63
1:A:30:GLN:O	1:A:34:ILE:HG13	1.98	0.63
1:A:341:ASP:OD1	1:A:343:ALA:N	2.31	0.63
1:A:267:HIS:CD2	1:A:269:GLY:H	2.17	0.62
1:A:160:PRO:CD	1:A:161:GLU:OE1	2.47	0.62
1:A:202:LEU:HD21	1:A:204:GLN:HB2	1.80	0.62
1:A:109:THR:OG1	1:A:112:ARG:NH2	2.33	0.62
1:A:75:ILE:O	1:A:76:SER:CB	2.48	0.62
1:A:169:ARG:CD	1:A:197:GLY:HA3	2.27	0.61
1:A:101:ARG:O	1:A:105:LEU:HG	2.01	0.60
1:A:33:ILE:HD12	1:A:45:VAL:HG22	1.83	0.60
1:A:160:PRO:CG	1:A:161:GLU:OE1	2.51	0.59
1:A:345:MET:O	1:A:349:ARG:HG3	2.03	0.58
1:A:214:ARG:HB2	1:A:399:ASN:OD1	2.03	0.58
1:A:1:MET:O	1:A:2:ALA:HB3	2.01	0.58
1:A:199:ASN:O	1:A:200:ASP:C	2.38	0.58
1:A:160:PRO:HD2	1:A:161:GLU:OE1	2.04	0.58
1:A:193:VAL:HG22	1:A:198:LEU:HD12	1.86	0.57
1:A:109:THR:HG22	1:A:109:THR:O	2.02	0.57
1:A:303:PRO:HA	1:A:329:ARG:HB2	1.87	0.57
1:A:174:THR:O	1:A:176:PRO:HD3	2.05	0.56
1:A:127:MET:CE	1:A:165:LEU:HD23	2.36	0.56
1:A:53:LYS:NZ	1:A:182:ALA:HB2	2.20	0.56
1:A:96:ASN:HD21	1:A:99:GLN:HG3	1.71	0.56
1:A:109:THR:CG2	1:A:109:THR:O	2.53	0.56
1:A:161:GLU:OE1	1:A:161:GLU:N	2.32	0.56
1:A:118:LEU:C	1:A:118:LEU:HD23	2.25	0.55
1:A:220:LYS:HG2	1:A:223:PRO:HB3	1.87	0.55
1:A:1:MET:CA	1:A:114:GLY:O	2.55	0.55
1:A:33:ILE:O	1:A:37:VAL:HG23	2.07	0.55
1:A:47:MET:HB2	1:A:53:LYS:HG3	1.89	0.54
1:A:127:MET:HE2	1:A:165:LEU:HD23	1.89	0.54
1:A:352:LEU:O	1:A:352:LEU:HD12	2.06	0.54
1:A:75:ILE:O	1:A:76:SER:HB2	2.07	0.54
1:A:413:SER:O	1:A:417:GLN:HG3	2.08	0.54
1:A:32:GLU:O	1:A:36:THR:OG1	2.16	0.54
1:A:53:LYS:HB2	4:A:527:AGS:O2B	2.07	0.54
1:A:308:VAL:HG23	1:A:327:ALA:HB2	1.90	0.54
1:A:20:THR:HG21	1:A:62:LEU:HD11	1.90	0.53
1:A:208:PHE:N	1:A:391:GLU:OE1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:PRO:HB2	1:A:311:PHE:CZ	2.44	0.53
1:A:130:ASN:O	1:A:134:HIS:HD2	1.92	0.53
1:A:234:GLN:HG3	1:A:307:PHE:CD1	2.44	0.53
1:A:169:ARG:HD3	1:A:197:GLY:CA	2.34	0.52
1:A:202:LEU:HD23	1:A:202:LEU:C	2.30	0.52
1:A:352:LEU:HD11	1:A:361:GLN:HG3	1.91	0.52
1:A:175:LEU:HD12	1:A:176:PRO:HD2	1.92	0.52
1:A:12:GLY:O	1:A:16:VAL:HG23	2.11	0.51
1:A:2:ALA:HB1	1:A:66:GLY:H	1.76	0.51
1:A:183:THR:HG21	1:A:318:GLU:HB3	1.93	0.50
1:A:17:LEU:HD13	1:A:26:PHE:CE1	2.46	0.50
1:A:96:ASN:C	1:A:96:ASN:HD22	2.15	0.50
1:A:96:ASN:HD21	1:A:98:THR:HG22	1.74	0.50
1:A:1:MET:SD	1:A:115:GLN:OE1	2.70	0.50
1:A:229:ARG:HG2	1:A:229:ARG:O	2.12	0.50
1:A:246:ARG:NH1	1:A:269:GLY:HA3	2.26	0.49
1:A:266:TYR:HD2	1:A:278:VAL:HG11	1.76	0.49
1:A:110:GLY:HA3	1:A:116:ILE:HD12	1.95	0.49
1:A:47:MET:O	1:A:182:ALA:HA	2.13	0.49
1:A:378:GLN:HE22	1:A:513:PRO:HA	1.76	0.49
1:A:313:ILE:HG13	1:A:338:LEU:HD11	1.95	0.49
1:A:310:HIS:CE1	1:A:323:GLU:OE1	2.55	0.48
1:A:435:VAL:HG21	1:A:492:LEU:HD12	1.95	0.48
1:A:222:LYS:N	1:A:223:PRO:CD	2.76	0.48
1:A:59:ILE:N	1:A:60:PRO:HD2	2.28	0.48
1:A:127:MET:HE3	1:A:165:LEU:HA	1.96	0.48
1:A:468:HIS:O	1:A:472:VAL:HG23	2.14	0.48
1:A:302:LYS:HE2	1:A:304:ASN:OD1	2.13	0.47
1:A:4:ALA:N	1:A:65:ASN:OD1	2.32	0.47
1:A:156:HIS:HD1	1:A:156:HIS:H	1.62	0.47
1:A:14:LYS:HG2	1:A:26:PHE:CE2	2.49	0.47
1:A:275:ARG:O	1:A:278:VAL:HB	2.14	0.47
1:A:153:GLN:HG3	1:A:359:GLN:HE22	1.79	0.47
1:A:3:GLN:HA	1:A:65:ASN:OD1	2.14	0.47
1:A:332:LEU:HB3	1:A:333:PRO:CD	2.45	0.47
1:A:234:GLN:HG3	1:A:307:PHE:CE1	2.50	0.46
1:A:27:ARG:O	1:A:28:PRO:C	2.53	0.46
1:A:415:ASP:OD2	1:A:468:HIS:HE1	1.98	0.46
1:A:117:ARG:HH11	1:A:117:ARG:HG3	1.81	0.46
1:A:78:MET:O	1:A:82:VAL:HG23	2.16	0.46
1:A:143:LEU:HD13	1:A:168:LEU:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LYS:HZ1	1:A:182:ALA:HB2	1.82	0.45
1:A:434:TYR:CZ	1:A:452:HIS:HD2	2.34	0.45
1:A:20:THR:HG21	1:A:62:LEU:CD1	2.47	0.45
1:A:279:GLN:HG3	1:A:300:ILE:HB	1.98	0.45
1:A:467:GLU:OE2	1:A:515:ILE:HA	2.17	0.44
1:A:496:GLU:OE1	1:A:499:ARG:NH1	2.35	0.44
1:A:251:ASP:O	1:A:255:ARG:HG3	2.17	0.44
1:A:263:ALA:HA	1:A:289:ILE:O	2.18	0.44
1:A:184:ALA:HB1	1:A:188:THR:CG2	2.47	0.44
1:A:156:HIS:NE2	1:A:322:GLN:NE2	2.65	0.44
1:A:46:VAL:HB	1:A:205:ILE:HA	2.00	0.43
1:A:76:SER:O	1:A:77:LEU:CB	2.58	0.43
1:A:46:VAL:HG21	1:A:189:ARG:CD	2.47	0.43
1:A:78:MET:SD	1:A:94:CYS:HB2	2.58	0.43
1:A:1:MET:HB3	1:A:3:GLN:HE21	1.84	0.43
1:A:84:GLN:O	1:A:87:ALA:HB3	2.19	0.43
1:A:307:PHE:CD2	1:A:309:VAL:HG23	2.54	0.43
1:A:254:ALA:O	1:A:257:GLN:HB2	2.18	0.43
1:A:25:GLN:HG2	1:A:26:PHE:N	2.34	0.43
1:A:492:LEU:O	1:A:493:GLN:HG2	2.19	0.43
1:A:353:GLU:OE1	1:A:365:ARG:NE	2.47	0.43
1:A:313:ILE:HA	1:A:314:PRO:HD3	1.75	0.43
1:A:350:ARG:O	1:A:351:CYS:C	2.56	0.43
1:A:223:PRO:HB2	1:A:311:PHE:HZ	1.84	0.42
1:A:441:GLY:HA2	1:A:458:TYR:CE1	2.54	0.42
1:A:332:LEU:HB3	1:A:333:PRO:HD2	2.00	0.42
1:A:379:THR:HG22	1:A:380:CYS:N	2.33	0.42
1:A:104:GLN:O	1:A:108:MET:HG2	2.19	0.42
1:A:354:GLU:HG3	1:A:354:GLU:O	2.19	0.42
1:A:29:GLY:CA	1:A:204:GLN:OE1	2.68	0.42
1:A:5:GLU:OE2	1:A:117:ARG:NH2	2.53	0.42
1:A:503:ARG:HB3	1:A:505:GLU:HG3	2.01	0.42
1:A:426:VAL:O	1:A:427:ASN:HB2	2.20	0.42
1:A:43:CYS:O	1:A:178:MET:HA	2.19	0.42
1:A:478:HIS:HD2	5:A:533:HOH:O	2.01	0.42
1:A:73:PRO:CD	1:A:74:LEU:HD22	2.46	0.41
1:A:477:ILE:HA	1:A:482:VAL:O	2.20	0.41
1:A:355:LYS:HB3	1:A:356:PRO:HD2	2.02	0.41
1:A:49:THR:HG23	1:A:321:TYR:CE2	2.55	0.41
1:A:415:ASP:OD2	1:A:468:HIS:CE1	2.74	0.41
1:A:146:ASP:O	1:A:147:GLU:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:PRO:HG3	1:A:162:TYR:CE2	2.55	0.41
1:A:489:HIS:O	1:A:490:SER:HB2	2.20	0.41
1:A:352:LEU:O	1:A:361:GLN:NE2	2.54	0.41
1:A:305:VAL:HB	1:A:327:ALA:HA	2.03	0.41
1:A:109:THR:HA	1:A:112:ARG:NH2	2.36	0.40
1:A:92:ALA:HA	1:A:118:LEU:O	2.21	0.40
1:A:18:GLN:HA	1:A:23:TYR:O	2.21	0.40
1:A:202:LEU:CD2	1:A:204:GLN:HB2	2.50	0.40
1:A:184:ALA:O	1:A:189:ARG:NH1	2.51	0.40
1:A:162:TYR:O	1:A:165:LEU:HB2	2.21	0.40
1:A:59:ILE:N	1:A:60:PRO:CD	2.84	0.40
1:A:70:VAL:O	1:A:120:TYR:HA	2.21	0.40
1:A:162:TYR:O	1:A:163:ALA:C	2.59	0.40
1:A:61:ALA:HB2	1:A:68:THR:HG21	2.04	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	508/523 (97%)	476 (94%)	28 (6%)	4 (1%)	24 41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	SER
1	A	221	PHE
1	A	77	LEU
1	A	28	PRO

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	432/439 (98%)	403 (93%)	29 (7%)	20 37

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	28	PRO
1	A	43	CYS
1	A	49	THR
1	A	54	SER
1	A	72	SER
1	A	74	LEU
1	A	76	SER
1	A	78	MET
1	A	96	ASN
1	A	97	SER
1	A	98	THR
1	A	128	LEU
1	A	153	GLN
1	A	161	GLU
1	A	169	ARG
1	A	171	ARG
1	A	258	SER
1	A	273	ASN
1	A	357	GLN
1	A	364	GLU
1	A	386	LEU
1	A	395	GLU
1	A	417	GLN
1	A	448	ARG
1	A	474	ARG
1	A	506	SER
1	A	507	SER
1	A	516	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	15	GLN
1	A	96	ASN
1	A	134	HIS
1	A	267	HIS
1	A	310	HIS
1	A	322	GLN
1	A	357	GLN
1	A	359	GLN
1	A	366	HIS
1	A	378	GLN
1	A	427	ASN
1	A	452	HIS
1	A	468	HIS
1	A	478	HIS
1	A	488	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 3 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	AGS	A	527	3	24,33,33	4.55	5 (20%)	28,52,52	2.09	7 (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
4	AGS	A	527	3	1/1/7/7	0/15/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	527	AGS	PG-S1G	-21.21	1.49	1.90
4	A	527	AGS	C8-N7	-3.98	1.27	1.34
4	A	527	AGS	C5-N7	-2.29	1.31	1.39
4	A	527	AGS	PG-O2G	-2.02	1.48	1.55
4	A	527	AGS	C2-N1	2.30	1.38	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	527	AGS	O3'-C3'-C4'	-2.56	103.37	111.05
4	A	527	AGS	C4-C5-N7	2.34	111.64	109.48
4	A	527	AGS	O2G-PG-O3B	2.92	118.36	105.09
4	A	527	AGS	O4'-C1'-N9	3.45	115.32	108.10
4	A	527	AGS	O2B-PB-O3B	3.56	121.24	105.09
4	A	527	AGS	PB-O3B-PG	4.16	146.61	132.67
4	A	527	AGS	O2'-C2'-C3'	5.86	130.90	111.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	527	AGS	C2'

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	527	AGS	5	0

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	512/523 (97%)	0.27	27 (5%) 30 34	27, 50, 95, 128	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	PRO	4.7
1	A	1	MET	4.5
1	A	76	SER	4.5
1	A	84	GLN	4.1
1	A	515	ILE	3.8
1	A	83	ASP	3.7
1	A	77	LEU	3.5
1	A	301	ASN	3.2
1	A	271	GLU	3.2
1	A	300	ILE	3.0
1	A	87	ALA	3.0
1	A	129	ASP	3.0
1	A	82	VAL	2.7
1	A	75	ILE	2.7
1	A	443	ASN	2.6
1	A	80	ASP	2.5
1	A	2	ALA	2.4
1	A	22	GLY	2.4
1	A	25	GLN	2.4
1	A	95	LEU	2.3
1	A	516	VAL	2.3
1	A	49	THR	2.2
1	A	221	PHE	2.2
1	A	23	TYR	2.1
1	A	81	GLN	2.1
1	A	126	LEU	2.1
1	A	346	ALA	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, 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
4	AGS	A	527	31/31	0.89	0.23	0.10	51,66,94,98	0
2	ZN	A	524	1/1	0.99	0.09	-1.53	32,32,32,32	0
3	MN	A	525	1/1	0.96	0.07	-	83,83,83,83	0
3	MN	A	526	1/1	0.91	0.07	-	69,69,69,69	0

6.5 Other polymers (i)

There are no such residues in this entry.