Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:01 AM GMT

PDB ID	:	2FB3
Title	:	Structure of MoaA in complex with 5'-GTP
Authors	:	Haenzelmann, P.; Schindelin, H.
Deposited on	:	2005-12-08
Resolution	:	2.35 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 ⓘ symbol.

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

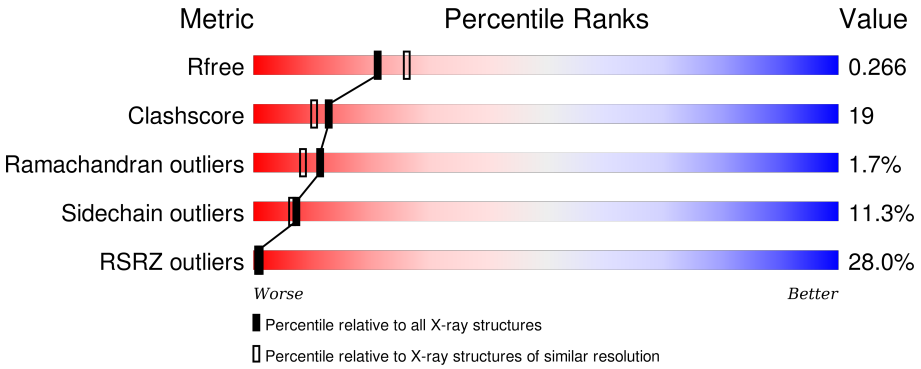
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.35 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	1406 (2.36-2.32)
Clashscore	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)
RSRZ outliers	91569	1412 (2.36-2.32)

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	340	17% 66% 24% 6%
1	B	340	36% 55% 33% 7%

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	SO4	A	403	-	-	-	X
3	MET	B	501	-	-	-	X

2 Entry composition

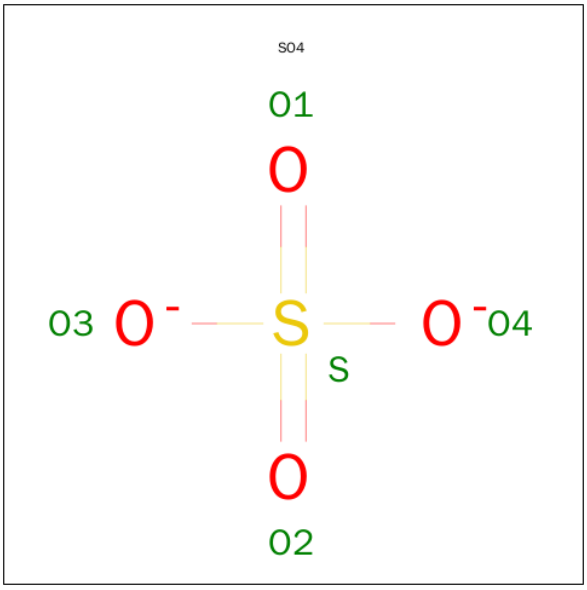
There are 8 unique types of molecules in this entry. The entry contains 5518 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Molybdenum cofactor biosynthesis protein A.

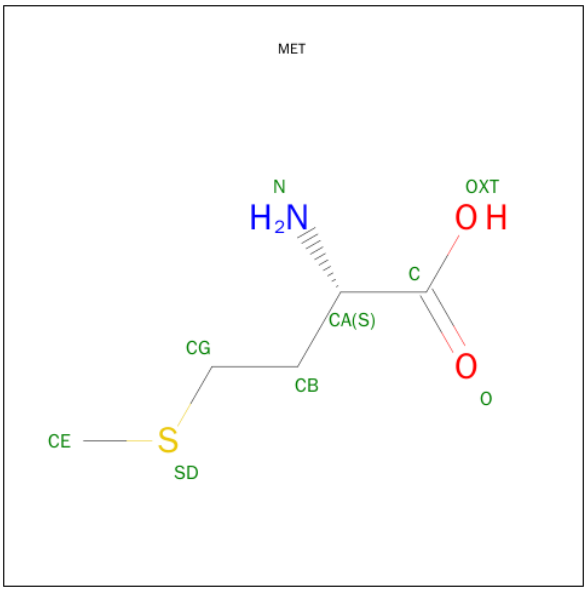
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2641	1673	455	500	13			
1	B	326	Total	C	N	O	S	0	0	0
			2632	1668	454	497	13			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



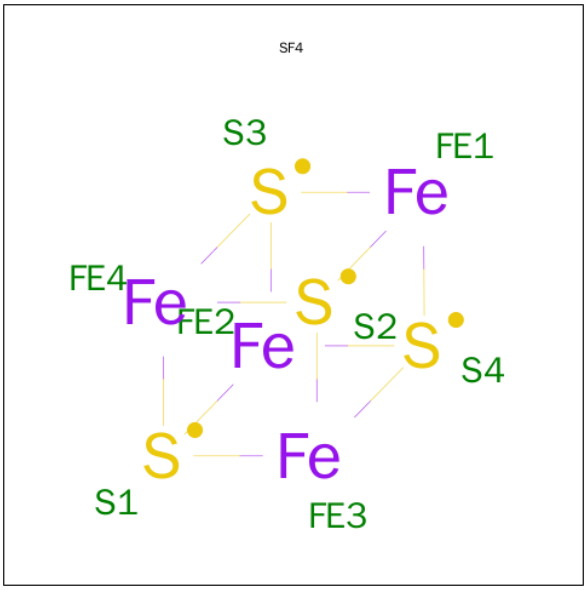
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			9	5	1	2	1		
3	B	1	Total	C	N	O	S	0	0
			9	5	1	2	1		

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	A	1	Total	Fe	S	0	0
			8	4	4		

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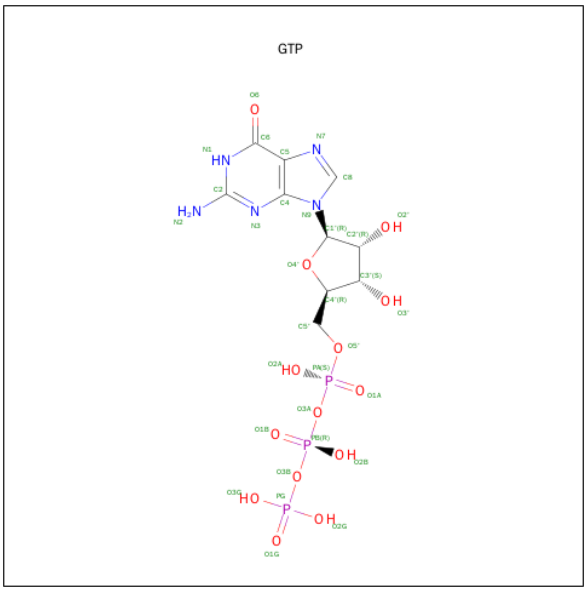
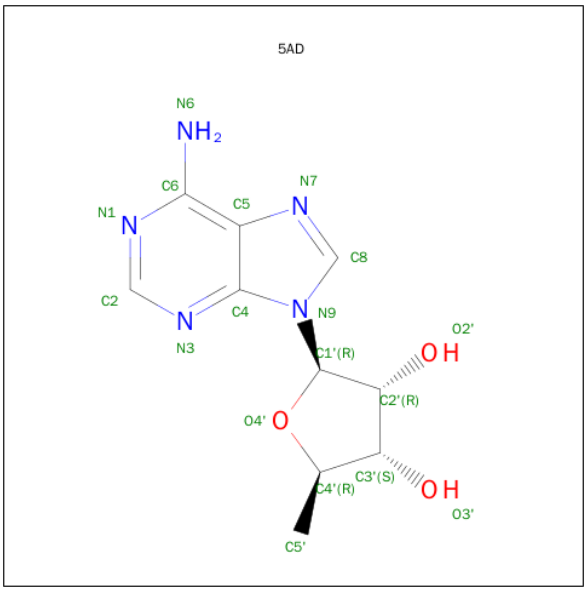
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Fe S 8 4 4	0	0
4	B	1	Total Fe S 8 4 4	0	0

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



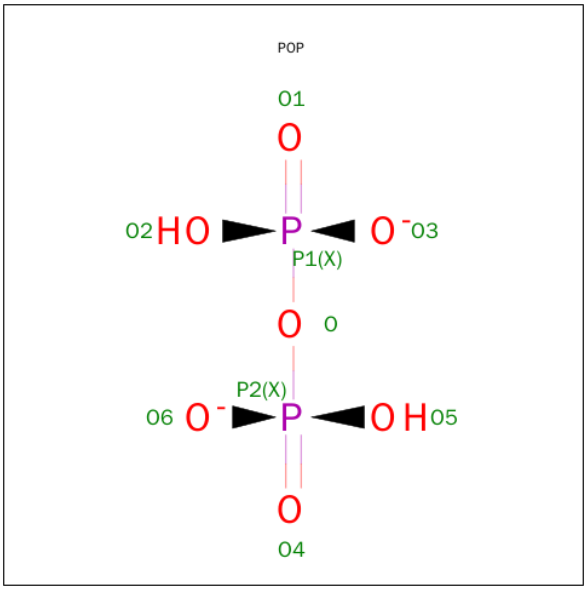
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 32 10 5 14 3	0	0

- Molecule 6 is 5'-DEOXYADENOSINE (three-letter code: 5AD) (formula: $C_{10}H_{13}N_5O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 17 9 5 3	0	0

- Molecule 7 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total O P 9 7 2	0	0

- Molecule 8 is water.

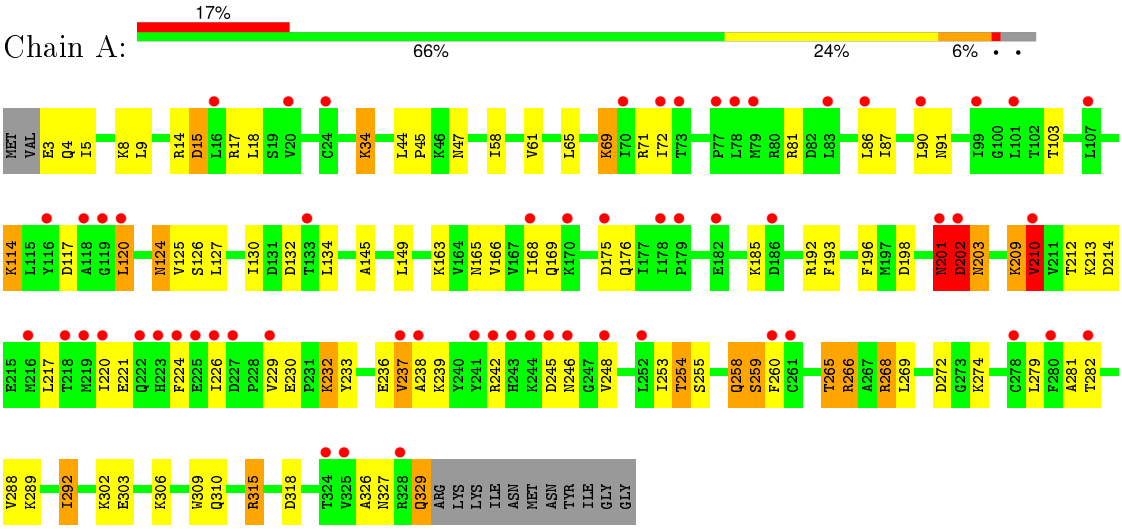
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	94	Total O 94 94	0	0
8	B	33	Total O 33 33	0	0

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.

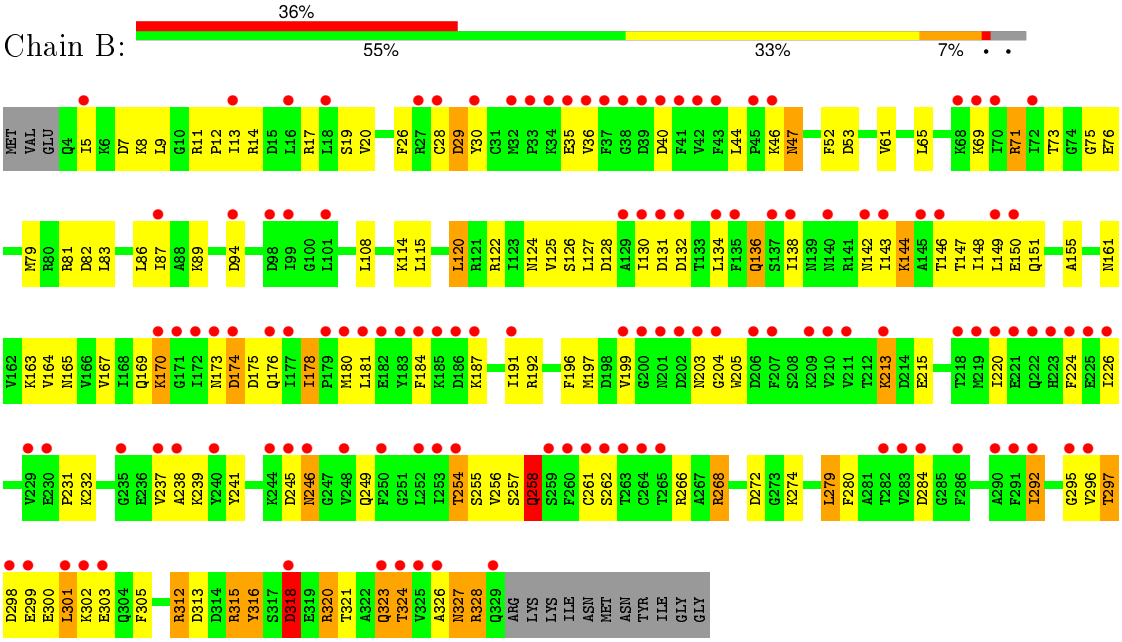
- Molecule 1: Molybdenum cofactor biosynthesis protein A

Chain A:



- Molecule 1: Molybdenum cofactor biosynthesis protein A

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	48.02Å 103.45Å 191.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35 43.39 – 2.35	Depositor EDS
% Data completeness (in resolution range)	91.1 (20.00-2.35) 90.9 (43.39-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.220 , 0.271 0.215 , 0.266	Depositor DCC
R_{free} test set	1859 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	56.5	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 73.6	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 37061 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5518	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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: GTP, SF4, SO4, POP, 5AD

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	1.10	4/2684 (0.1%)	0.95	8/3613 (0.2%)
1	B	0.98	16/2675 (0.6%)	0.82	7/3601 (0.2%)
All	All	1.04	20/5359 (0.4%)	0.89	15/7214 (0.2%)

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	1	0
1	B	0	1
All	All	1	1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	329	GLN	C-O	25.59	1.72	1.23
1	A	329	GLN	CD-NE2	17.63	1.76	1.32
1	B	318	ASP	CG-OD2	15.85	1.61	1.25
1	A	329	GLN	CD-OE1	11.90	1.50	1.24
1	B	215	GLU	CD-OE2	11.49	1.38	1.25
1	B	327	ASN	CG-ND2	10.87	1.60	1.32
1	B	323	GLN	CG-CD	10.19	1.74	1.51
1	B	11	ARG	CZ-NH1	9.96	1.46	1.33
1	B	318	ASP	CB-CG	8.70	1.70	1.51
1	B	215	GLU	CD-OE1	7.55	1.33	1.25
1	B	312	ARG	CZ-NH1	7.25	1.42	1.33
1	B	323	GLN	C-N	7.00	1.50	1.34
1	B	262	SER	CB-OG	6.59	1.50	1.42
1	B	328	ARG	CZ-NH1	6.34	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	323	GLN	CD-NE2	6.32	1.48	1.32
1	A	114	LYS	CD-CE	6.13	1.66	1.51
1	B	323	GLN	CD-OE1	5.81	1.36	1.24
1	B	316	TYR	C-O	5.51	1.33	1.23
1	B	327	ASN	CG-OD1	5.15	1.35	1.24
1	B	323	GLN	C-O	5.08	1.32	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	11	ARG	NE-CZ-NH2	-10.36	115.12	120.30
1	B	312	ARG	NE-CZ-NH2	-8.37	116.11	120.30
1	A	117	ASP	CB-CG-OD2	7.15	124.74	118.30
1	A	15	ASP	CB-CA-C	-6.59	97.22	110.40
1	B	318	ASP	CB-CG-OD2	-6.54	112.42	118.30
1	B	318	ASP	OD1-CG-OD2	-6.29	111.36	123.30
1	A	120	LEU	CB-CG-CD2	6.21	121.55	111.00
1	A	117	ASP	CB-CG-OD1	-6.04	112.87	118.30
1	A	329	GLN	CA-C-O	-5.67	108.19	120.10
1	A	210	VAL	N-CA-C	5.49	125.83	111.00
1	B	315	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	A	209	LYS	C-N-CA	5.32	134.99	121.70
1	B	328	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	201	ASN	C-N-CA	5.03	134.28	121.70
1	B	11	ARG	NE-CZ-NH1	5.02	122.81	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	210	VAL	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	318	ASP	Sidechain

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	2641	0	2637	106	0
1	B	2632	0	2631	102	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
3	A	9	0	8	2	0
3	B	9	0	8	2	0
4	A	16	0	0	0	0
4	B	16	0	0	0	0
5	A	32	0	11	3	0
6	A	17	0	9	1	0
7	B	9	0	0	0	0
8	A	94	0	0	13	0
8	B	33	0	0	7	0
All	All	5518	0	5304	205	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 19.

All (205) 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:323:GLN:CG	1:B:323:GLN:CD	1.74	1.53
1:A:329:GLN:CD	1:A:329:GLN:NE2	1.76	1.36
1:A:329:GLN:O	1:A:329:GLN:C	1.72	1.28
1:A:266:ARG:HD2	5:A:404:GTP:O6	1.38	1.21
1:A:245:ASP:HB2	1:A:246:ASN:HB3	1.28	1.12
1:A:245:ASP:CB	1:A:246:ASN:HB3	1.78	1.12
1:A:201:ASN:HB3	1:A:202:ASP:HB3	1.15	1.10
1:A:246:ASN:HD21	1:A:248:VAL:HG23	1.28	0.96
1:B:292:ILE:HD11	1:B:301:LEU:HD21	1.50	0.94
1:A:201:ASN:CB	1:A:202:ASP:HB3	1.98	0.94
1:A:201:ASN:HB3	1:A:202:ASP:CB	1.98	0.94
1:A:34:LYS:HD2	8:A:584:HOH:O	1.70	0.90
1:A:237:VAL:HG23	1:A:238:ALA:H	1.37	0.90
1:B:30:TYR:CD1	1:B:196:PHE:HE1	1.91	0.88
1:B:178:ILE:HD12	1:B:178:ILE:H	1.41	0.85
3:A:500:MET:SD	6:A:501:5AD:C4'	2.67	0.83
1:B:124:ASN:HB3	1:B:165:ASN:ND2	1.95	0.81
1:A:245:ASP:CB	1:A:246:ASN:CB	2.58	0.80
1:B:261:CYS:HB2	1:B:318:ASP:OD2	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ARG:HD3	8:A:525:HOH:O	1.84	0.76
1:A:315:ARG:NH2	1:B:9:LEU:O	2.19	0.76
1:A:329:GLN:HA	1:B:14:ARG:NH2	2.02	0.75
1:A:9:LEU:O	1:B:315:ARG:NH2	2.20	0.74
1:B:268:ARG:HD2	1:B:279:LEU:HD23	1.70	0.74
1:B:301:LEU:HD22	1:B:305:PHE:CE1	2.22	0.74
1:A:303:GLU:HG2	8:A:552:HOH:O	1.86	0.73
1:A:58:ILE:HD13	1:A:269:LEU:HD11	1.71	0.72
1:B:266:ARG:HD3	8:B:510:HOH:O	1.88	0.72
1:A:266:ARG:CD	5:A:404:GTP:O6	2.30	0.71
1:A:245:ASP:HB3	1:A:246:ASN:CB	2.20	0.71
1:A:245:ASP:HB3	1:A:246:ASN:HB3	1.71	0.71
1:A:237:VAL:HG23	1:A:238:ALA:N	2.06	0.70
1:A:81:ARG:CD	8:A:525:HOH:O	2.37	0.69
1:B:128:ASP:O	1:B:173:ASN:ND2	2.25	0.69
1:A:69:LYS:HD3	8:A:539:HOH:O	1.93	0.69
1:A:224:PHE:HB2	1:A:226:ILE:HD11	1.75	0.68
1:B:30:TYR:CD1	1:B:196:PHE:CE1	2.78	0.68
1:B:87:ILE:CD1	1:B:115:LEU:HD22	2.23	0.68
1:B:199:VAL:HG13	1:B:204:GLY:O	1.94	0.68
1:B:324:THR:O	1:B:328:ARG:HG2	1.95	0.66
1:B:292:ILE:HD11	1:B:301:LEU:CD2	2.26	0.66
1:B:87:ILE:HD12	1:B:115:LEU:CD2	2.25	0.66
1:A:213:LYS:NZ	1:A:239:LYS:HG3	2.10	0.66
1:A:202:ASP:CG	1:A:203:ASN:HA	2.17	0.65
1:A:14:ARG:NE	8:A:579:HOH:O	2.30	0.64
1:B:124:ASN:HB3	1:B:165:ASN:HD21	1.62	0.64
1:A:126:SER:HB3	2:A:403:SO4:O1	1.96	0.64
1:B:87:ILE:HD12	1:B:115:LEU:HD22	1.78	0.64
1:B:124:ASN:HD21	1:B:192:ARG:NH2	1.97	0.64
1:A:17:ARG:HD3	1:A:71:ARG:HB3	1.80	0.63
1:A:229:VAL:HG12	1:A:230:GLU:O	1.99	0.63
1:B:146:THR:HG22	1:B:150:GLU:OE2	1.98	0.63
1:A:8:LYS:HE2	1:A:310:GLN:O	1.99	0.63
1:A:47:ASN:H	1:A:47:ASN:ND2	1.95	0.63
1:A:202:ASP:OD1	1:A:203:ASN:HA	1.99	0.62
1:A:163:LYS:NZ	5:A:404:GTP:O3G	2.33	0.62
1:B:71:ARG:NH2	1:B:124:ASN:OD1	2.33	0.61
1:B:161:ASN:HD21	1:B:163:LYS:HE2	1.67	0.60
1:A:14:ARG:HB2	1:A:265:THR:HG23	1.83	0.60
1:B:71:ARG:HD3	8:B:531:HOH:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ARG:HB2	1:A:265:THR:CG2	2.32	0.59
1:A:169:GLN:HE21	1:A:209:LYS:NZ	2.00	0.59
1:B:323:GLN:CB	1:B:323:GLN:CD	2.69	0.58
1:B:132:ASP:OD2	1:B:144:LYS:HB3	2.04	0.58
1:B:124:ASN:HD21	1:B:192:ARG:HH22	1.50	0.58
1:A:237:VAL:CG2	1:A:238:ALA:H	2.12	0.58
1:B:30:TYR:HD1	1:B:196:PHE:HE1	1.47	0.58
1:A:329:GLN:CG	1:A:329:GLN:NE2	2.66	0.57
1:B:46:LYS:HG2	8:B:529:HOH:O	2.03	0.57
1:B:205:TRP:CZ2	1:B:320:ARG:HB2	2.39	0.57
1:B:237:VAL:HG23	1:B:238:ALA:H	1.69	0.57
1:A:237:VAL:HG12	8:A:594:HOH:O	2.04	0.56
1:B:130:ILE:HG22	1:B:176:GLN:OE1	2.06	0.56
1:A:246:ASN:ND2	1:A:248:VAL:HG23	2.10	0.56
1:A:259:SER:HB2	1:A:318:ASP:OD1	2.06	0.55
1:B:205:TRP:CD2	1:B:256:VAL:HG13	2.42	0.55
1:A:71:ARG:NH1	1:A:124:ASN:ND2	2.56	0.54
1:A:268:ARG:HH11	1:A:268:ARG:CG	2.20	0.54
1:B:184:PHE:CD1	1:B:191:ILE:HD12	2.43	0.54
1:B:170:LYS:O	1:B:174:ASP:HB2	2.07	0.54
1:B:181:LEU:HD11	1:B:220:ILE:HG12	1.90	0.54
1:A:3:GLU:O	1:A:3:GLU:OE2	2.26	0.54
1:A:5:ILE:HD13	1:A:65:LEU:HD22	1.90	0.53
1:B:197:MET:CE	1:B:280:PHE:CZ	2.92	0.53
1:A:169:GLN:HA	1:A:209:LYS:O	2.08	0.53
1:A:47:ASN:H	1:A:47:ASN:HD22	1.57	0.53
1:B:205:TRP:CE2	1:B:320:ARG:HB2	2.43	0.53
1:A:14:ARG:CD	8:A:579:HOH:O	2.56	0.52
1:A:4:GLN:HG3	1:A:14:ARG:NH2	2.23	0.52
1:B:266:ARG:NH2	8:B:524:HOH:O	2.42	0.52
1:A:72:ILE:CD1	1:A:87:ILE:CD1	2.88	0.52
1:A:185:LYS:NZ	1:A:245:ASP:OD2	2.37	0.52
1:A:202:ASP:N	1:A:203:ASN:HB3	2.25	0.51
1:B:127:LEU:HD13	1:B:148:ILE:CG2	2.40	0.51
1:B:184:PHE:HD1	1:B:191:ILE:HD12	1.74	0.51
1:B:53:ASP:HA	1:B:89:LYS:HE2	1.91	0.51
1:B:169:GLN:H	1:B:173:ASN:HB3	1.74	0.51
1:B:280:PHE:CD2	1:B:316:TYR:CE2	2.99	0.51
1:B:30:TYR:CE1	1:B:196:PHE:CE1	2.98	0.51
1:B:318:ASP:O	1:B:321:THR:HB	2.11	0.50
1:A:202:ASP:OD2	1:A:327:ASN:ND2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:LYS:HD2	8:B:533:HOH:O	2.11	0.50
1:B:7:ASP:HB2	1:B:312:ARG:O	2.11	0.50
1:A:165:ASN:HD21	1:A:192:ARG:HH11	1.60	0.50
1:B:29:ASP:N	1:B:29:ASP:OD1	2.44	0.50
1:B:197:MET:CE	1:B:280:PHE:HZ	2.24	0.50
1:A:268:ARG:NH1	1:A:268:ARG:CG	2.75	0.49
1:A:5:ILE:HG22	1:A:309:TRP:HD1	1.77	0.49
1:B:75:GLY:O	3:B:501:MET:HG3	2.13	0.49
1:A:254:THR:OG1	1:A:258:GLN:HB3	2.11	0.49
1:B:316:TYR:O	1:B:320:ARG:HG2	2.12	0.49
1:A:288:VAL:O	1:A:292:ILE:HG12	2.12	0.49
1:B:300:GLU:O	1:B:303:GLU:HG2	2.13	0.49
1:A:201:ASN:CA	1:A:202:ASP:HB3	2.43	0.49
1:B:5:ILE:HD12	1:B:5:ILE:H	1.77	0.49
1:A:4:GLN:HG3	1:A:14:ARG:HH21	1.78	0.48
1:A:71:ARG:HH12	1:A:124:ASN:ND2	2.10	0.48
1:B:203:ASN:O	1:B:320:ARG:HD3	2.13	0.48
1:B:323:GLN:O	1:B:326:ALA:HB3	2.13	0.48
1:A:268:ARG:HE	1:A:279:LEU:HD23	1.77	0.48
1:B:5:ILE:HG12	1:B:65:LEU:HD22	1.95	0.48
1:A:233:TYR:O	1:A:236:GLU:HB2	2.14	0.48
1:B:241:TYR:O	1:B:249:GLN:HG2	2.13	0.48
1:A:242:ARG:HD2	8:A:567:HOH:O	2.13	0.47
1:B:254:THR:HB	1:B:258:GLN:HB3	1.96	0.47
1:A:268:ARG:HH11	1:A:268:ARG:HG3	1.78	0.47
1:A:169:GLN:HE21	1:A:209:LYS:HZ2	1.61	0.47
1:A:196:PHE:CE2	1:A:198:ASP:HB2	2.49	0.47
1:A:220:ILE:HG22	1:A:226:ILE:CD1	2.45	0.47
1:A:268:ARG:NH2	1:A:279:LEU:HG	2.29	0.47
1:A:315:ARG:HD2	8:A:588:HOH:O	2.15	0.47
1:B:231:PRO:O	1:B:232:LYS:C	2.53	0.47
1:B:127:LEU:HD13	1:B:148:ILE:HG21	1.96	0.47
1:B:224:PHE:HB2	1:B:226:ILE:HD13	1.96	0.47
1:B:274:LYS:NZ	1:B:284:ASP:HB3	2.30	0.46
1:B:131:ASP:HB2	1:B:176:GLN:HE22	1.80	0.46
1:B:61:VAL:CG1	1:B:302:LYS:HA	2.45	0.46
1:A:14:ARG:HD2	8:A:579:HOH:O	2.16	0.46
1:B:132:ASP:O	1:B:136:GLN:HB2	2.15	0.46
1:B:122:ARG:HD2	8:B:515:HOH:O	2.14	0.46
1:A:5:ILE:HG22	1:A:309:TRP:CD1	2.51	0.45
1:A:272:ASP:OD2	1:A:274:LYS:CE	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:PHE:HA	1:B:187:LYS:HB2	1.98	0.45
1:A:127:LEU:O	1:A:166:VAL:HG22	2.16	0.45
1:A:169:GLN:NE2	1:A:209:LYS:NZ	2.65	0.45
1:A:132:ASP:OD1	1:A:145:ALA:N	2.50	0.45
1:B:125:VAL:O	1:B:164:VAL:HA	2.16	0.45
1:B:197:MET:HE1	1:B:280:PHE:CZ	2.51	0.45
1:A:114:LYS:HE3	8:A:510:HOH:O	2.17	0.45
1:A:329:GLN:HA	1:B:14:ARG:CZ	2.47	0.44
1:B:254:THR:HG22	1:B:257:SER:OG	2.16	0.44
1:B:26:PHE:HZ	1:B:148:ILE:HD11	1.80	0.44
1:A:245:ASP:HB3	1:A:246:ASN:HB2	1.95	0.44
1:A:72:ILE:CD1	1:A:87:ILE:HD11	2.47	0.44
1:A:326:ALA:HB2	1:B:12:PRO:HD3	1.99	0.44
1:B:237:VAL:HG23	1:B:238:ALA:N	2.33	0.44
1:A:213:LYS:HZ3	1:A:239:LYS:HG3	1.80	0.44
1:A:217:LEU:O	1:A:221:GLU:HG2	2.18	0.44
1:B:115:LEU:O	1:B:120:LEU:HB2	2.18	0.44
1:B:44:LEU:HD11	1:B:272:ASP:HB3	1.99	0.44
1:A:232:LYS:HB3	1:A:233:TYR:HD2	1.83	0.43
1:B:213:LYS:HB3	1:B:254:THR:HG23	2.01	0.43
1:A:5:ILE:HG12	1:A:306:LYS:HG3	2.00	0.43
1:B:130:ILE:HB	1:B:180:MET:HG2	2.00	0.43
1:B:130:ILE:HD11	1:B:149:LEU:HD21	1.99	0.43
1:B:323:GLN:O	1:B:327:ASN:N	2.49	0.43
1:A:265:THR:O	1:A:265:THR:HG23	2.18	0.43
1:A:130:ILE:HG22	1:A:176:GLN:OE1	2.19	0.43
1:B:178:ILE:CD1	1:B:178:ILE:H	2.13	0.43
3:A:500:MET:SD	3:A:500:MET:C	2.97	0.42
1:A:221:GLU:OE2	1:A:226:ILE:HB	2.19	0.42
1:A:268:ARG:NE	1:A:279:LEU:HD23	2.34	0.42
1:B:167:VAL:HG11	8:B:522:HOH:O	2.17	0.42
1:B:47:ASN:HD22	1:B:47:ASN:C	2.21	0.42
1:A:272:ASP:OD2	1:A:274:LYS:HE3	2.20	0.42
1:B:246:ASN:HD22	1:B:246:ASN:H	1.68	0.42
1:A:114:LYS:HB3	1:A:114:LYS:HE2	1.81	0.42
1:B:76:GLU:HB3	1:B:79:MET:CG	2.49	0.42
1:A:81:ARG:HD2	8:A:525:HOH:O	2.14	0.42
1:A:289:LYS:HE2	1:A:289:LYS:HB3	1.60	0.42
1:B:297:THR:OG1	1:B:300:GLU:HB2	2.20	0.42
1:B:108:LEU:HD13	1:B:155:ALA:HB2	2.02	0.41
1:A:202:ASP:H	1:A:203:ASN:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:THR:O	1:A:125:VAL:HA	2.20	0.41
1:A:238:ALA:HB2	1:A:253:ILE:HG12	2.02	0.41
1:B:126:SER:HB2	3:B:501:MET:O	2.21	0.41
1:B:8:LYS:HB2	1:B:313:ASP:HB3	2.01	0.41
1:A:86:LEU:O	1:A:90:LEU:HG	2.20	0.41
1:A:168:ILE:HD11	1:A:193:PHE:CD2	2.56	0.41
1:A:61:VAL:HG13	1:A:302:LYS:HG3	2.02	0.41
1:B:124:ASN:HB3	1:B:165:ASN:HD22	1.79	0.41
1:A:145:ALA:O	1:A:149:LEU:HG	2.21	0.41
1:B:124:ASN:HA	1:B:163:LYS:O	2.20	0.41
1:B:81:ARG:O	1:B:82:ASP:HB2	2.20	0.41
1:B:147:THR:O	1:B:151:GLN:HG2	2.21	0.41
1:B:28:CYS:HA	1:B:138:ILE:O	2.20	0.41
1:B:279:LEU:H	1:B:279:LEU:HG	1.77	0.41
1:B:301:LEU:CD2	1:B:305:PHE:CE1	2.99	0.40
1:A:237:VAL:CG2	1:A:238:ALA:N	2.75	0.40
1:A:213:LYS:HZ1	1:A:239:LYS:HG3	1.86	0.40
1:A:71:ARG:HH12	1:A:124:ASN:HD22	1.70	0.40
1:B:52:PHE:CD2	1:B:86:LEU:HB2	2.56	0.40
1:B:254:THR:HB	1:B:258:GLN:CB	2.51	0.40
1:A:44:LEU:HA	1:A:45:PRO:HD3	1.99	0.40
1:B:205:TRP:CE3	1:B:256:VAL:HG13	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	325/340 (96%)	296 (91%)	22 (7%)	7 (2%)	8 5
1	B	324/340 (95%)	297 (92%)	23 (7%)	4 (1%)	16 14
All	All	649/680 (95%)	593 (91%)	45 (7%)	11 (2%)	11 8

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	201	ASN
1	A	202	ASP
1	A	237	VAL
1	B	36	VAL
1	B	170	LYS
1	B	258	GLN
1	A	281	ALA
1	A	212	THR
1	A	258	GLN
1	B	295	GLY
1	A	210	VAL

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	291/302 (96%)	267 (92%)	24 (8%)	14 14
1	B	290/302 (96%)	250 (86%)	40 (14%)	4 4
All	All	581/604 (96%)	517 (89%)	64 (11%)	7 7

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	18	LEU
1	A	34	LYS
1	A	69	LYS
1	A	91	ASN
1	A	120	LEU
1	A	124	ASN
1	A	134	LEU
1	A	175	ASP
1	A	202	ASP
1	A	203	ASN
1	A	210	VAL

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Mol	Chain	Res	Type
1	A	214	ASP
1	A	232	LYS
1	A	254	THR
1	A	255	SER
1	A	259	SER
1	A	260	PHE
1	A	265	THR
1	A	266	ARG
1	A	268	ARG
1	A	282	THR
1	A	292	ILE
1	A	315	ARG
1	B	13	ILE
1	B	17	ARG
1	B	19	SER
1	B	20	VAL
1	B	29	ASP
1	B	35	GLU
1	B	40	ASP
1	B	47	ASN
1	B	69	LYS
1	B	71	ARG
1	B	73	THR
1	B	83	LEU
1	B	94	ASP
1	B	114	LYS
1	B	120	LEU
1	B	134	LEU
1	B	136	GLN
1	B	142	ASN
1	B	143	ILE
1	B	144	LYS
1	B	174	ASP
1	B	175	ASP
1	B	178	ILE
1	B	213	LYS
1	B	239	LYS
1	B	245	ASP
1	B	246	ASN
1	B	254	THR
1	B	255	SER
1	B	258	GLN

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Mol	Chain	Res	Type
1	B	268	ARG
1	B	279	LEU
1	B	292	ILE
1	B	296	VAL
1	B	297	THR
1	B	298	ASP
1	B	299	GLU
1	B	301	LEU
1	B	320	ARG
1	B	324	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	47	ASN
1	A	91	ASN
1	A	92	GLN
1	A	124	ASN
1	A	136	GLN
1	A	165	ASN
1	A	169	GLN
1	A	203	ASN
1	A	246	ASN
1	A	249	GLN
1	A	258	GLN
1	B	47	ASN
1	B	136	GLN
1	B	161	ASN
1	B	169	GLN
1	B	243	HIS
1	B	246	ASN
1	B	258	GLN

5.3.3 RNA

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)

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SF4	A	401	1,3	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	A	402	1,5	0,12,12	0.00	-	0,24,24	0.00	-
2	SO4	A	403	-	4,4,4	0.49	0	6,6,6	0.93	0
5	GTP	A	404	4	25,34,34	1.07	1 (4%)	34,54,54	2.24	8 (23%)
3	MET	A	500	4	5,8,8	0.39	0	3,9,9	1.05	0
6	5AD	A	501	-	14,19,20	0.93	1 (7%)	13,28,30	3.27	5 (38%)
4	SF4	B	401	1,3	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	B	402	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SO4	B	403	-	4,4,4	0.17	0	6,6,6	0.29	0
7	POP	B	404	-	8,8,8	0.81	0	13,13,13	0.88	0
3	MET	B	501	4	5,8,8	0.53	0	3,9,9	0.71	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
4	SF4	A	401	1,3	-	0/0/48/48	0/6/5/5
4	SF4	A	402	1,5	-	0/0/48/48	0/6/5/5
2	SO4	A	403	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	A	404	4	-	0/18/38/38	0/3/3/3
3	MET	A	500	4	-	0/4/8/8	0/0/0/0
6	5AD	A	501	-	-	0/0/17/20	0/3/3/3
4	SF4	B	401	1,3	-	0/0/48/48	0/6/5/5
4	SF4	B	402	1	-	0/0/48/48	0/6/5/5
2	SO4	B	403	-	-	0/0/0/0	0/0/0/0
7	POP	B	404	-	-	0/6/6/6	0/0/0/0
3	MET	B	501	4	-	0/4/8/8	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	501	5AD	C3'-C2'	-2.03	1.50	1.53
5	A	404	GTP	C6-N1	3.23	1.39	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	501	5AD	N3-C2-N1	-9.18	121.87	128.89
5	A	404	GTP	C2'-C1'-N9	-8.31	101.60	114.29
5	A	404	GTP	N3-C2-N1	-5.85	118.54	127.44
6	A	501	5AD	O2'-C2'-C3'	-4.98	99.85	111.68
6	A	501	5AD	C4-C5-N7	-3.33	106.42	109.48
5	A	404	GTP	PA-O3A-PB	-3.33	123.38	132.73
6	A	501	5AD	O3'-C3'-C2'	-2.23	106.96	111.23
5	A	404	GTP	C5-C6-N1	-2.17	120.62	123.59
5	A	404	GTP	O3G-PG-O3B	2.26	115.35	105.09
5	A	404	GTP	O4'-C1'-N9	2.30	112.92	108.10
6	A	501	5AD	C4'-C3'-C2'	2.37	105.46	101.64
5	A	404	GTP	N2-C2-N3	2.90	123.36	117.80
5	A	404	GTP	C6-N1-C2	3.66	121.02	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	403	SO4	1	0
5	A	404	GTP	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	MET	2	0
6	A	501	5AD	1	0
3	B	501	MET	2	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

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	327/340 (96%)	1.19	59 (18%)	2	3	54, 63, 72, 83	0
1	B	326/340 (95%)	1.82	124 (38%)	0	0	54, 63, 71, 75	0
All	All	653/680 (96%)	1.50	183 (28%)	1	1	54, 63, 72, 83	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	41	PHE	9.5
1	B	30	TYR	7.5
1	B	282	THR	7.3
1	B	226	ILE	7.2
1	B	135	PHE	6.4
1	A	244	LYS	6.1
1	B	283	VAL	6.1
1	B	130	ILE	5.9
1	B	36	VAL	5.7
1	B	42	VAL	5.6
1	A	201	ASN	5.6
1	B	222	GLN	5.6
1	B	140	ASN	5.3
1	A	248	VAL	5.2
1	B	37	PHE	5.1
1	B	223	HIS	5.0
1	A	224	PHE	4.8
1	A	222	GLN	4.8
1	A	226	ILE	4.7
1	B	40	ASP	4.6
1	B	171	GLY	4.6
1	B	225	GLU	4.5
1	B	202	ASP	4.3
1	B	146	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	246	ASN	4.2
1	B	179	PRO	4.1
1	B	296	VAL	4.1
1	B	32	MET	4.1
1	B	149	LEU	4.1
1	A	242	ARG	4.0
1	B	132	ASP	4.0
1	B	246	ASN	3.9
1	B	325	VAL	3.9
1	B	33	PRO	3.9
1	B	181	LEU	3.9
1	A	220	ILE	3.8
1	A	227	ASP	3.6
1	B	176	GLN	3.6
1	A	219	MET	3.6
1	A	245	ASP	3.6
1	B	35	GLU	3.6
1	B	183	TYR	3.5
1	A	237	VAL	3.5
1	B	43	PHE	3.5
1	B	261	CYS	3.5
1	B	235	GLY	3.5
1	B	299	GLU	3.5
1	B	284	ASP	3.4
1	B	131	ASP	3.4
1	B	200	GLY	3.4
1	B	70	ILE	3.4
1	B	263	THR	3.3
1	B	206	ASP	3.3
1	B	240	TYR	3.3
1	B	219	MET	3.3
1	B	220	ILE	3.3
1	B	253	ILE	3.3
1	B	129	ALA	3.2
1	A	225	GLU	3.2
1	B	245	ASP	3.2
1	B	254	THR	3.2
1	B	203	ASN	3.2
1	B	177	ILE	3.1
1	B	244	LYS	3.1
1	B	238	ALA	3.1
1	B	224	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	223	HIS	3.1
1	B	38	GLY	3.0
1	A	243	HIS	3.0
1	B	201	ASN	3.0
1	B	174	ASP	3.0
1	A	179	PRO	3.0
1	B	182	GLU	3.0
1	B	99	ILE	2.9
1	B	173	ASN	2.9
1	B	209	LYS	2.9
1	B	172	ILE	2.9
1	A	328	ARG	2.9
1	A	99	ILE	2.9
1	B	13	ILE	2.8
1	B	250	PHE	2.8
1	B	292	ILE	2.8
1	B	39	ASP	2.8
1	B	265	THR	2.8
1	B	185	LYS	2.8
1	B	45	PRO	2.8
1	A	83	LEU	2.7
1	B	230	GLU	2.7
1	B	262	SER	2.7
1	A	78	LEU	2.7
1	B	72	ILE	2.7
1	A	118	ALA	2.7
1	B	290	ALA	2.7
1	A	252	LEU	2.7
1	B	259	SER	2.7
1	B	143	ILE	2.7
1	B	229	VAL	2.7
1	B	134	LEU	2.6
1	A	218	THR	2.6
1	B	264	CYS	2.6
1	B	137	SER	2.6
1	B	324	THR	2.6
1	B	187	LYS	2.6
1	A	238	ALA	2.6
1	B	180	MET	2.6
1	A	133	THR	2.6
1	A	175	ASP	2.6
1	B	101	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	145	ALA	2.6
1	B	237	VAL	2.6
1	A	72	ILE	2.6
1	B	34	LYS	2.6
1	A	186	ASP	2.5
1	B	138	ILE	2.5
1	B	142	ASN	2.5
1	B	218	THR	2.5
1	A	325	VAL	2.5
1	A	79	MET	2.5
1	A	168	ILE	2.4
1	B	184	PHE	2.4
1	B	207	PHE	2.4
1	B	301	LEU	2.4
1	B	329	GLN	2.4
1	B	46	LYS	2.4
1	A	216	MET	2.4
1	B	221	GLU	2.4
1	A	101	LEU	2.4
1	A	210	VAL	2.4
1	B	303	GLU	2.4
1	A	170	LYS	2.4
1	A	20	VAL	2.3
1	B	98	ASP	2.3
1	B	252	LEU	2.3
1	A	178	ILE	2.3
1	A	182	GLU	2.3
1	B	186	ASP	2.3
1	A	229	VAL	2.3
1	B	323	GLN	2.3
1	A	120	LEU	2.3
1	A	260	PHE	2.3
1	A	73	THR	2.3
1	B	291	PHE	2.3
1	B	295	GLY	2.2
1	A	282	THR	2.2
1	B	191	ILE	2.2
1	B	213	LYS	2.2
1	A	202	ASP	2.2
1	B	260	PHE	2.2
1	A	107	LEU	2.2
1	B	16	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	119	GLY	2.2
1	B	150	GLU	2.2
1	A	116	TYR	2.2
1	A	77	PRO	2.2
1	B	211	VAL	2.2
1	B	248	VAL	2.2
1	B	18	LEU	2.2
1	A	70	ILE	2.2
1	B	298	ASP	2.2
1	A	16	LEU	2.2
1	A	24	CYS	2.2
1	B	28	CYS	2.2
1	B	199	VAL	2.1
1	A	324	THR	2.1
1	B	68	LYS	2.1
1	B	318	ASP	2.1
1	B	87	ILE	2.1
1	B	286	PHE	2.1
1	B	204	GLY	2.1
1	A	90	LEU	2.1
1	B	302	LYS	2.1
1	A	278	CYS	2.1
1	B	27	ARG	2.1
1	A	86	LEU	2.1
1	B	69	LYS	2.1
1	B	326	ALA	2.1
1	B	5	ILE	2.1
1	B	94	ASP	2.1
1	B	210	VAL	2.1
1	A	280	PHE	2.1
1	A	261	CYS	2.0
1	A	241	TYR	2.0
1	B	170	LYS	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 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	SO4	A	403	5/5	0.98	0.26	6.85	65,66,67,72	0
3	MET	B	501	9/9	0.91	0.31	3.95	83,85,85,85	0
2	SO4	B	403	5/5	0.94	0.25	0.16	94,95,96,98	0
6	5AD	A	501	17/18	0.92	0.14	-1.05	77,78,82,82	0
7	POP	B	404	9/9	0.89	0.17	-1.47	114,115,116,117	0
5	GTP	A	404	32/32	0.94	0.14	-1.73	74,78,81,85	0
4	SF4	B	401	8/8	0.98	0.05	-2.42	64,67,68,69	0
3	MET	A	500	9/9	0.98	0.09	-3.69	49,55,60,60	0
4	SF4	A	402	8/8	0.98	0.06	-4.31	52,53,54,61	0
4	SF4	B	402	8/8	0.96	0.05	-5.02	68,70,72,77	0
4	SF4	A	401	8/8	0.99	0.04	-5.48	42,46,48,48	0

6.5 Other polymers (i)

There are no such residues in this entry.