



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:30 PM GMT

PDB ID : 3ZKD
Title : CRYSTAL STRUCTURE OF THE ATPASE REGION OF Mycobacterium tuberculosis GyrB WITH AMPPNP
Authors : Agrawal, A.; Roue, M.; Spitzfaden, C.; Petrella, S.; Aubry, A.; Volker, C.; Mossakowska, D.; Hann, M.; Bax, B.; Mayer, C.
Deposited on : 2013-01-22
Resolution : 2.95 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

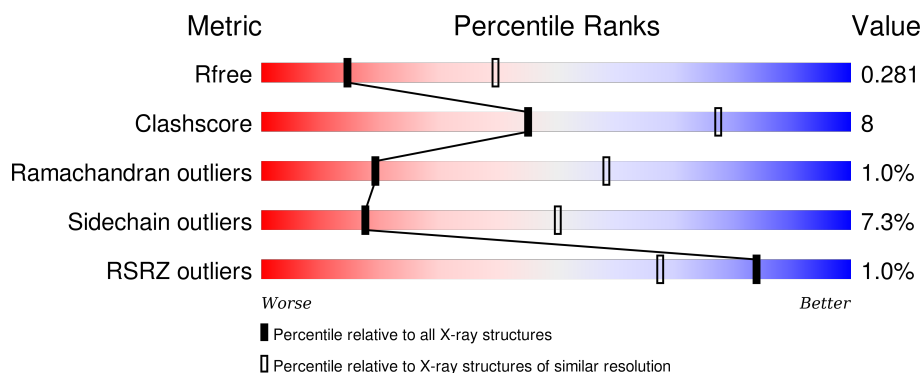
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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 $\leq 5\%$. 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	432	<div> <div> <div></div> <div>65%</div> <div>21%</div> <div>•</div> <div>13%</div> </div> </div>
1	B	432	<div> <div> <div></div> <div>66%</div> <div>20%</div> <div>•</div> <div>13%</div> </div> </div>
1	C	432	<div> <div> <div></div> <div>69%</div> <div>20%</div> <div>•</div> <div>10%</div> </div> </div>
1	D	432	<div> <div> <div></div> <div>69%</div> <div>17%</div> <div>•</div> <div>12%</div> </div> </div>
1	E	432	<div> <div> <div></div> <div>72%</div> <div>16%</div> <div></div> <div>12%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	432	<div><div></div><div>63%22%13%</div><div></div></div>
1	G	432	<div>%<div><div></div><div>68%18%13%</div><div></div></div></div>
1	H	432	<div>%<div><div></div><div>68%19%13%</div><div></div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23192 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 DNA GYRASE SUBUNIT B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			2855	1789	503	557	6			
1	B	375	Total	C	N	O	S	0	0	0
			2843	1783	498	556	6			
1	C	390	Total	C	N	O	S	0	0	0
			2927	1835	519	567	6			
1	D	379	Total	C	N	O	S	0	0	0
			2817	1766	489	556	6			
1	E	382	Total	C	N	O	S	0	0	0
			2878	1803	506	563	6			
1	F	376	Total	C	N	O	S	0	0	0
			2821	1768	497	550	6			
1	G	378	Total	C	N	O	S	0	0	0
			2845	1786	497	556	6			
1	H	378	Total	C	N	O	S	0	0	0
			2835	1776	494	559	6			

There are 40 discrepancies between the modelled and reference sequences:

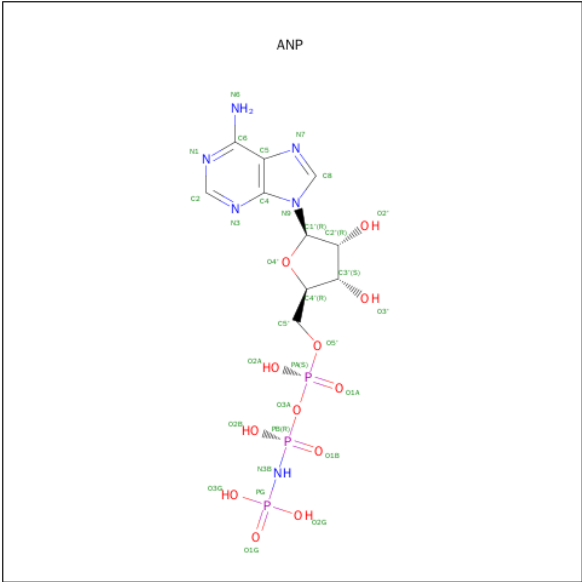
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	EXPRESSION TAG	UNP I6WX66
A	-3	PRO	-	EXPRESSION TAG	UNP I6WX66
A	-2	LEU	-	EXPRESSION TAG	UNP I6WX66
A	-1	GLY	-	EXPRESSION TAG	UNP I6WX66
A	0	SER	-	EXPRESSION TAG	UNP I6WX66
B	-4	GLY	-	EXPRESSION TAG	UNP I6WX66
B	-3	PRO	-	EXPRESSION TAG	UNP I6WX66
B	-2	LEU	-	EXPRESSION TAG	UNP I6WX66
B	-1	GLY	-	EXPRESSION TAG	UNP I6WX66
B	0	SER	-	EXPRESSION TAG	UNP I6WX66
C	-4	GLY	-	EXPRESSION TAG	UNP I6WX66
C	-3	PRO	-	EXPRESSION TAG	UNP I6WX66
C	-2	LEU	-	EXPRESSION TAG	UNP I6WX66

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	EXPRESSION TAG	UNP I6WX66
C	0	SER	-	EXPRESSION TAG	UNP I6WX66
D	-4	GLY	-	EXPRESSION TAG	UNP I6WX66
D	-3	PRO	-	EXPRESSION TAG	UNP I6WX66
D	-2	LEU	-	EXPRESSION TAG	UNP I6WX66
D	-1	GLY	-	EXPRESSION TAG	UNP I6WX66
D	0	SER	-	EXPRESSION TAG	UNP I6WX66
E	-4	GLY	-	EXPRESSION TAG	UNP I6WX66
E	-3	PRO	-	EXPRESSION TAG	UNP I6WX66
E	-2	LEU	-	EXPRESSION TAG	UNP I6WX66
E	-1	GLY	-	EXPRESSION TAG	UNP I6WX66
E	0	SER	-	EXPRESSION TAG	UNP I6WX66
F	-4	GLY	-	EXPRESSION TAG	UNP I6WX66
F	-3	PRO	-	EXPRESSION TAG	UNP I6WX66
F	-2	LEU	-	EXPRESSION TAG	UNP I6WX66
F	-1	GLY	-	EXPRESSION TAG	UNP I6WX66
F	0	SER	-	EXPRESSION TAG	UNP I6WX66
G	-4	GLY	-	EXPRESSION TAG	UNP I6WX66
G	-3	PRO	-	EXPRESSION TAG	UNP I6WX66
G	-2	LEU	-	EXPRESSION TAG	UNP I6WX66
G	-1	GLY	-	EXPRESSION TAG	UNP I6WX66
G	0	SER	-	EXPRESSION TAG	UNP I6WX66
H	-4	GLY	-	EXPRESSION TAG	UNP I6WX66
H	-3	PRO	-	EXPRESSION TAG	UNP I6WX66
H	-2	LEU	-	EXPRESSION TAG	UNP I6WX66
H	-1	GLY	-	EXPRESSION TAG	UNP I6WX66
H	0	SER	-	EXPRESSION TAG	UNP I6WX66

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	G	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	H	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		

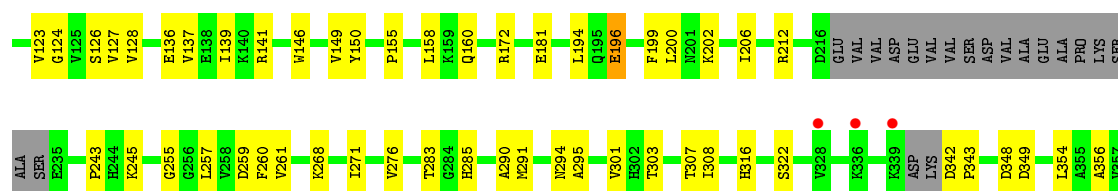
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Mg 1	0	0
3	C	1	Total 1	Mg 1	0	0
3	A	1	Total 1	Mg 1	0	0
3	F	1	Total 1	Mg 1	0	0

- Molecule 4 is water.

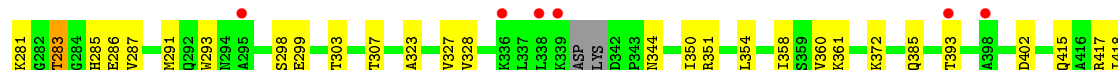
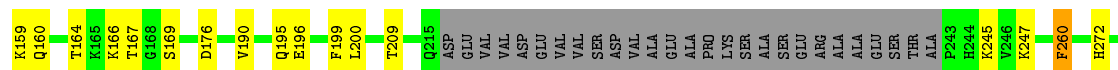
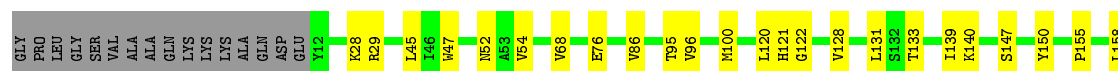
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total 20	O 20	0	0
4	B	11	Total 11	O 11	0	0
4	C	20	Total 20	O 20	0	0
4	D	8	Total 8	O 8	0	0
4	E	15	Total 15	O 15	0	0
4	F	12	Total 12	O 12	0	0
4	G	22	Total 22	O 22	0	0
4	H	7	Total 7	O 7	0	0



- Molecule 1: DNA GYRASE SUBUNIT B



• Molecule 1: DNA GYRASE SUBUNIT B



- Molecule 1: DNA GYRASE SUBUNIT B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.95Å 97.85Å 138.07Å 108.21° 105.18° 91.04°	Depositor
Resolution (Å)	24.81 – 2.95 24.82 – 2.95	Depositor EDS
% Data completeness (in resolution range)	84.6 (24.81-2.95) 75.8 (24.82-2.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.94Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.182 , 0.257 0.196 , 0.281	Depositor DCC
R_{free} test set	2459 reflections (4.20%)	DCC
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.705	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 30.6	EDS
Estimated twinning fraction	0.168 for h,-k,-h-l 0.015 for -h,k,-k-l 0.009 for -h,-k,h+k+l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 61071 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23192	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: MG, ANP

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	0.44	0/2907	0.69	0/3940
1	B	0.44	0/2896	0.67	0/3928
1	C	0.46	0/2981	0.71	0/4044
1	D	0.43	0/2869	0.68	0/3901
1	E	0.44	0/2932	0.69	0/3979
1	F	0.45	0/2873	0.70	0/3900
1	G	0.45	0/2898	0.70	0/3932
1	H	0.44	0/2886	0.68	0/3919
All	All	0.44	0/23242	0.69	0/31543

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	2
1	C	0	1
1	H	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	342	ASP	Mainchain,Peptide
1	C	342	ASP	Mainchain

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Mol	Chain	Res	Type	Group
1	H	342	ASP	Mainchain

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	2855	0	2774	51	0
1	B	2843	0	2764	57	0
1	C	2927	0	2837	46	0
1	D	2817	0	2690	42	0
1	E	2878	0	2780	37	0
1	F	2821	0	2726	54	0
1	G	2845	0	2756	44	0
1	H	2835	0	2723	43	0
2	A	31	0	13	3	0
2	B	31	0	13	1	0
2	C	31	0	13	1	0
2	D	31	0	13	1	0
2	E	31	0	13	2	0
2	F	31	0	13	1	0
2	G	31	0	13	2	0
2	H	31	0	13	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	20	0	0	0	0
4	B	11	0	0	0	0
4	C	20	0	0	0	0
4	D	8	0	0	0	0
4	E	15	0	0	0	0
4	F	12	0	0	0	0
4	G	22	0	0	0	0
4	H	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	23192	0	22154	351	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 8.

All (351) 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:93:ILE:HG13	1:B:94:PRO:HD2	1.53	0.90
1:C:308:ILE:HD13	1:C:372:LYS:HD3	1.61	0.82
1:D:312:GLU:CG	1:D:373:THR:HB	2.13	0.78
1:D:312:GLU:HG3	1:D:373:THR:HB	1.67	0.76
2:A:601:ANP:H8	2:A:601:ANP:H5'2	1.68	0.75
1:F:61:TYR:CG	1:F:82:ARG:HD2	2.24	0.72
1:G:287:VAL:HG23	1:G:360:VAL:HG12	1.74	0.70
1:G:365:PRO:HA	1:G:377:ASN:HD21	1.55	0.70
1:F:34:ILE:HG13	1:F:44:HIS:HB3	1.72	0.70
1:F:135:LEU:HD12	1:F:173:PHE:HB3	1.74	0.69
1:E:303:THR:HG22	1:E:358:ILE:HB	1.74	0.68
1:B:131:LEU:HG	1:B:179:VAL:HG11	1.74	0.68
1:D:190:VAL:HG12	1:D:194:LEU:HD11	1.76	0.68
1:H:140:LYS:O	1:H:167:THR:HA	1.93	0.67
1:F:34:ILE:HD12	1:F:44:HIS:HD2	1.60	0.67
1:G:303:THR:HB	1:G:316:HIS:CE1	2.29	0.67
1:E:272:HIS:HE1	1:E:293:TRP:H	1.44	0.66
1:F:276:VAL:O	1:F:290:ALA:HA	1.95	0.66
1:B:276:VAL:HB	1:B:291:MET:HG2	1.77	0.65
1:D:131:LEU:HG	1:D:179:VAL:HG11	1.79	0.65
1:C:36:SER:O	1:C:41:GLY:HA3	1.97	0.64
1:F:287:VAL:HG23	1:F:360:VAL:HG12	1.78	0.64
1:C:291:MET:HB2	1:C:354:LEU:HD11	1.79	0.64
1:G:29:ARG:HH21	1:H:109:PHE:HA	1.60	0.64
1:F:187:PHE:CD1	1:F:210:ASP:HB2	2.33	0.63
1:E:140:LYS:O	1:E:167:THR:HA	1.99	0.63
1:E:86:VAL:HG22	1:E:158:LEU:HD21	1.81	0.62
1:B:136:GLU:HB2	1:B:172:ARG:HB2	1.82	0.62
1:D:312:GLU:HG2	1:D:373:THR:HB	1.81	0.62
1:B:308:ILE:HD13	1:B:372:LYS:HD3	1.80	0.62
1:F:291:MET:HB2	1:F:354:LEU:HD11	1.82	0.61
1:F:67:VAL:HB	1:F:77:VAL:HG22	1.80	0.61
1:B:329:ASN:HD21	1:B:345:LEU:H	1.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:GLU:HG2	1:A:149:VAL:HG22	1.81	0.61
1:E:272:HIS:CE1	1:E:293:TRP:H	2.18	0.61
1:G:98:VAL:HG13	1:H:19:ILE:HD11	1.82	0.61
2:A:601:ANP:C8	2:A:601:ANP:H5'2	2.31	0.60
1:A:272:HIS:CE1	1:A:293:TRP:H	2.18	0.60
1:H:303:THR:HB	1:H:316:HIS:CE1	2.36	0.60
1:C:103:LEU:HD22	1:C:123:VAL:HG13	1.83	0.60
1:A:272:HIS:HE1	1:A:293:TRP:H	1.50	0.60
1:D:327:VAL:HG11	1:D:392:LEU:HB3	1.83	0.60
1:E:147:SER:HB3	1:E:159:LYS:HB2	1.83	0.60
1:C:109:PHE:HA	1:D:29:ARG:HH21	1.66	0.60
2:A:601:ANP:H5'1	2:A:601:ANP:PB	2.42	0.60
1:E:164:THR:OG1	1:E:166:LYS:HB2	2.01	0.59
1:A:281:LYS:HG2	1:A:286:GLU:HG3	1.84	0.59
1:E:29:ARG:HH21	1:F:109:PHE:HA	1.68	0.59
1:G:100:MET:HG2	1:G:150:TYR:CE2	2.38	0.59
1:C:76:GLU:HG3	1:C:172:ARG:HH11	1.68	0.59
1:B:316:HIS:H	1:B:316:HIS:CD2	2.21	0.59
1:B:139:ILE:HA	1:B:169:SER:HA	1.85	0.58
1:A:17:ILE:HG13	1:B:95:THR:HG21	1.85	0.58
1:A:321:ARG:HG2	1:A:351:ARG:HD3	1.86	0.58
1:G:37:THR:HG23	1:H:366:GLN:HE22	1.69	0.57
1:F:276:VAL:HG22	1:F:395:TRP:CE2	2.39	0.57
1:A:65:VAL:HG23	1:A:204:LEU:HD11	1.87	0.57
1:H:323:ALA:HB1	1:H:388:CYS:HB3	1.85	0.57
1:A:45:LEU:HD22	1:A:128:VAL:HA	1.87	0.57
1:F:303:THR:HB	1:F:316:HIS:CE1	2.40	0.57
1:B:86:VAL:HG11	1:B:146:TRP:CD2	2.40	0.57
1:E:86:VAL:HA	1:E:96:VAL:HG23	1.87	0.57
1:B:34:ILE:HD13	1:B:44:HIS:HD2	1.69	0.56
1:D:86:VAL:HG11	1:D:146:TRP:CD2	2.40	0.56
1:C:308:ILE:CD1	1:C:372:LYS:HD3	2.33	0.56
1:H:276:VAL:O	1:H:290:ALA:HA	2.05	0.56
1:E:287:VAL:HG23	1:E:360:VAL:HG12	1.87	0.56
1:D:54:VAL:HG21	1:D:197:MET:HE2	1.87	0.56
1:G:35:GLY:HA2	1:H:368:GLU:HG3	1.87	0.56
1:A:95:THR:CG2	1:B:17:ILE:HG13	2.36	0.56
1:F:276:VAL:HB	1:F:291:MET:HG2	1.88	0.56
1:B:196:GLU:HA	1:B:199:PHE:HD2	1.71	0.56
1:H:148:GLN:HB2	1:H:158:LEU:HD12	1.88	0.56
1:D:315:THR:HB	1:D:381:LYS:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:ILE:HD12	1:D:295:ALA:HA	1.88	0.55
1:F:299:GLU:HG3	1:F:351:ARG:HB3	1.88	0.55
1:A:47:TRP:HH2	1:A:190:VAL:HA	1.71	0.55
1:G:291:MET:HB2	1:G:354:LEU:HD11	1.88	0.55
1:A:245:LYS:HA	1:E:160:GLN:HB3	1.88	0.55
1:C:245:LYS:HA	1:G:160:GLN:HB3	1.88	0.55
1:G:196:GLU:HA	1:G:199:PHE:HD2	1.72	0.55
1:B:45:LEU:HD22	1:B:128:VAL:HA	1.88	0.55
1:D:388:CYS:O	1:D:392:LEU:HB2	2.05	0.55
1:H:187:PHE:CD2	1:H:210:ASP:HB2	2.40	0.55
1:E:293:TRP:CD1	1:E:354:LEU:HB2	2.42	0.54
1:F:308:ILE:HD13	1:F:372:LYS:HD2	1.89	0.54
1:G:282:GLY:HA3	1:G:285:HIS:CE1	2.42	0.54
1:F:271:ILE:HD12	1:F:293:TRP:HB3	1.88	0.54
1:A:131:LEU:HG	1:A:179:VAL:HG11	1.90	0.54
1:E:45:LEU:HD22	1:E:128:VAL:HA	1.90	0.54
1:G:131:LEU:HG	1:G:179:VAL:HG11	1.90	0.54
1:D:371:THR:HG22	1:D:373:THR:HG23	1.89	0.53
1:G:210:ASP:HB3	1:G:247:LYS:HB3	1.89	0.53
1:A:137:VAL:HG12	1:A:171:VAL:HG22	1.91	0.53
1:C:86:VAL:HG11	1:C:146:TRP:CD2	2.43	0.53
1:A:287:VAL:HG23	1:A:360:VAL:HG12	1.90	0.52
1:H:291:MET:HB2	1:H:354:LEU:HD11	1.90	0.52
1:F:301:VAL:HG22	1:F:356:ALA:HB3	1.91	0.52
1:A:43:HIS:CE1	1:A:186:ASP:H	2.27	0.52
1:E:95:THR:CG2	1:F:17:ILE:HG13	2.40	0.52
1:D:144:TYR:HA	1:D:163:PRO:HA	1.91	0.52
1:G:65:VAL:HG23	1:G:204:LEU:HD11	1.91	0.52
1:C:303:THR:HG22	1:C:358:ILE:HB	1.91	0.52
1:E:54:VAL:HG11	1:E:307:THR:HG21	1.91	0.52
1:H:303:THR:HB	1:H:316:HIS:HE1	1.75	0.51
1:A:17:ILE:HG13	1:B:95:THR:CG2	2.40	0.51
1:F:86:VAL:HG13	1:F:158:LEU:HD21	1.91	0.51
1:E:100:MET:HG2	1:E:150:TYR:CE2	2.46	0.51
1:E:291:MET:HB2	1:E:354:LEU:HD11	1.93	0.51
1:A:196:GLU:HA	1:A:199:PHE:HD2	1.75	0.51
1:A:44:HIS:HA	1:A:47:TRP:CD1	2.45	0.51
1:D:34:ILE:HG22	1:D:36:SER:O	2.10	0.51
1:C:93:ILE:HD13	1:C:94:PRO:HD2	1.91	0.51
1:H:83:GLY:HA2	1:H:169:SER:OG	2.10	0.51
1:C:34:ILE:HD12	1:C:36:SER:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:THR:HG23	1:D:176:ASP:HA	1.93	0.51
1:B:324:LEU:HG	1:B:350:ILE:HD13	1.93	0.51
1:A:196:GLU:O	1:A:200:LEU:HG	2.11	0.50
1:A:68:VAL:HB	1:A:76:GLU:HB3	1.93	0.50
1:F:140:LYS:O	1:F:167:THR:HA	2.12	0.50
1:G:75:VAL:O	1:G:172:ARG:HA	2.11	0.50
1:F:315:THR:HB	1:F:381:LYS:HB2	1.93	0.50
1:A:271:ILE:HD12	1:A:293:TRP:HB3	1.93	0.50
1:C:136:GLU:HG2	1:C:149:VAL:HG22	1.93	0.50
1:C:276:VAL:O	1:C:290:ALA:HA	2.11	0.50
1:A:293:TRP:CD1	1:A:354:LEU:HB2	2.46	0.50
1:C:86:VAL:HG11	1:C:146:TRP:CE2	2.46	0.50
1:H:276:VAL:HB	1:H:291:MET:HG2	1.94	0.50
1:C:86:VAL:HG13	1:C:158:LEU:HD21	1.94	0.50
1:B:34:ILE:CD1	1:B:44:HIS:HD2	2.24	0.49
1:E:68:VAL:HG13	1:E:209:THR:HG23	1.93	0.49
1:B:388:CYS:HB3	1:B:392:LEU:HD12	1.94	0.49
1:C:106:GLY:HA2	2:C:601:ANP:H4'	1.94	0.49
1:F:135:LEU:HB3	1:F:150:TYR:HB2	1.93	0.49
1:A:26:VAL:HG11	1:A:127:VAL:HG22	1.93	0.49
1:F:10:ASP:HB3	1:F:12:TYR:HB3	1.93	0.49
1:C:54:VAL:O	1:C:58:MET:HG3	2.11	0.49
1:F:34:ILE:CD1	1:F:44:HIS:HD2	2.24	0.49
1:B:291:MET:HB2	1:B:354:LEU:HD11	1.95	0.49
1:B:324:LEU:HG	1:B:350:ILE:CD1	2.42	0.49
1:D:75:VAL:O	1:D:172:ARG:HA	2.13	0.49
1:G:86:VAL:HG12	1:G:158:LEU:HD21	1.95	0.49
1:B:52:ASN:OD1	2:B:601:ANP:O2B	2.31	0.49
1:G:285:HIS:HA	1:G:361:LYS:O	2.13	0.49
1:A:75:VAL:O	1:A:172:ARG:HA	2.13	0.49
1:F:54:VAL:HG21	1:F:197:MET:HG2	1.94	0.49
1:G:47:TRP:HH2	1:G:190:VAL:HA	1.77	0.49
1:C:301:VAL:HG22	1:C:356:ALA:HB3	1.95	0.49
1:H:52:ASN:HB3	2:H:601:ANP:N7	2.28	0.49
1:B:316:HIS:CD2	1:B:316:HIS:N	2.80	0.48
1:B:289:ILE:HG12	1:B:358:ILE:HG13	1.95	0.48
1:D:286:GLU:HB3	1:D:361:LYS:HB2	1.94	0.48
1:F:61:TYR:CD2	1:F:82:ARG:HD2	2.48	0.48
1:C:54:VAL:HG11	1:C:307:THR:HG21	1.95	0.48
1:E:68:VAL:HB	1:E:76:GLU:HB3	1.94	0.48
1:A:140:LYS:HG2	1:A:145:GLU:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:141:ARG:HA	1:G:167:THR:HG22	1.95	0.48
1:D:44:HIS:HA	1:D:47:TRP:CD1	2.48	0.48
1:C:415:GLN:HA	1:C:418:ILE:HG13	1.94	0.48
1:H:47:TRP:HH2	1:H:190:VAL:HA	1.78	0.48
1:H:75:VAL:O	1:H:172:ARG:HA	2.13	0.48
1:B:276:VAL:HG22	1:B:395:TRP:CE2	2.48	0.48
1:C:123:VAL:HG12	1:C:127:VAL:HG23	1.95	0.48
1:B:272:HIS:HE1	1:B:293:TRP:H	1.62	0.48
1:A:384:VAL:O	1:A:388:CYS:HB2	2.14	0.48
1:H:54:VAL:HG11	1:H:307:THR:HG21	1.95	0.48
1:B:137:VAL:HG13	1:B:171:VAL:HG22	1.94	0.48
1:B:299:GLU:HG3	1:B:351:ARG:HB3	1.95	0.47
1:F:195:GLN:HG2	1:F:199:PHE:CE2	2.49	0.47
1:H:45:LEU:HD22	1:H:128:VAL:HA	1.96	0.47
1:E:47:TRP:HH2	1:E:190:VAL:HA	1.78	0.47
1:F:135:LEU:HA	1:F:172:ARG:O	2.14	0.47
1:E:196:GLU:HA	1:E:199:PHE:HD2	1.79	0.47
1:B:321:ARG:HG2	1:B:351:ARG:HD3	1.95	0.47
1:E:195:GLN:HG2	1:E:199:PHE:CE2	2.50	0.47
1:A:194:LEU:HD22	1:A:206:ILE:HG21	1.97	0.47
1:G:53:ALA:HB1	1:G:79:ASP:HB3	1.96	0.47
1:D:303:THR:HG22	1:D:358:ILE:HB	1.97	0.47
1:C:29:ARG:HD2	1:D:120:LEU:HG	1.97	0.47
1:D:308:ILE:HD13	1:D:372:LYS:HD2	1.97	0.47
1:F:86:VAL:HG11	1:F:146:TRP:CD2	2.49	0.47
1:B:272:HIS:CE1	1:B:293:TRP:H	2.33	0.47
1:D:85:PRO:O	1:D:95:THR:HB	2.14	0.46
1:H:286:GLU:HB3	1:H:361:LYS:HB2	1.97	0.46
1:H:67:VAL:HA	1:H:76:GLU:O	2.15	0.46
1:E:415:GLN:HA	1:E:418:ILE:HD12	1.97	0.46
1:H:133:THR:HG23	1:H:176:ASP:HA	1.96	0.46
1:B:316:HIS:H	1:B:316:HIS:HD2	1.62	0.46
1:B:136:GLU:HG2	1:B:149:VAL:HG22	1.97	0.46
1:H:187:PHE:HD2	1:H:210:ASP:HB2	1.81	0.46
1:H:329:ASN:HD21	1:H:345:LEU:H	1.62	0.46
1:B:263:HIS:O	1:B:266:ARG:HG2	2.16	0.46
1:A:195:GLN:HG2	1:A:199:PHE:CE2	2.50	0.46
1:C:45:LEU:HD22	1:C:128:VAL:HA	1.98	0.46
1:H:276:VAL:HG22	1:H:395:TRP:CE2	2.50	0.46
1:G:276:VAL:O	1:G:290:ALA:HA	2.15	0.46
1:A:303:THR:HG22	1:A:358:ILE:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:45:LEU:HD22	1:F:128:VAL:HA	1.98	0.46
1:B:270:ALA:HA	1:B:294:ASN:HA	1.97	0.46
1:E:299:GLU:HG3	1:E:351:ARG:HB3	1.98	0.46
1:D:276:VAL:O	1:D:290:ALA:HA	2.15	0.46
1:B:139:ILE:HG23	1:B:169:SER:HB3	1.98	0.46
1:C:45:LEU:O	1:C:49:VAL:HG23	2.16	0.46
1:C:93:ILE:HG22	1:C:98:VAL:HG23	1.98	0.46
1:D:190:VAL:HG12	1:D:194:LEU:CD1	2.44	0.45
1:G:116:ILE:HG21	1:G:361:LYS:HG2	1.98	0.45
1:E:200:LEU:HD13	1:E:307:THR:HA	1.97	0.45
1:D:68:VAL:HB	1:D:76:GLU:HB3	1.98	0.45
1:G:145:GLU:HG3	1:G:162:ALA:O	2.16	0.45
1:C:367:PHE:HB3	1:C:372:LYS:HA	1.99	0.45
1:B:365:PRO:HA	1:B:377:ASN:HD21	1.81	0.45
1:C:243:PRO:HB3	1:G:158:LEU:HD23	1.97	0.45
1:D:328:VAL:HG13	1:D:407:VAL:HG22	1.99	0.45
1:B:34:ILE:HD13	1:B:44:HIS:CD2	2.50	0.45
1:B:377:ASN:HB2	1:B:380:VAL:HG23	1.99	0.45
1:C:160:GLN:HB3	1:G:245:LYS:HA	1.97	0.45
1:A:86:VAL:HG11	1:A:146:TRP:CE2	2.52	0.45
1:F:287:VAL:HG23	1:F:360:VAL:CG1	2.46	0.45
1:B:271:ILE:HD12	1:B:405:VAL:HG12	1.98	0.45
1:E:122:GLY:HA2	2:E:601:ANP:O3A	2.17	0.45
1:B:301:VAL:HG22	1:B:356:ALA:HB3	1.98	0.45
1:H:346:THR:HG22	1:H:348:ASP:H	1.82	0.44
1:A:82:ARG:HD2	1:B:12:TYR:CD2	2.53	0.44
1:D:138:GLU:HB2	1:D:170:THR:HB	1.99	0.44
1:C:57:ALA:HA	1:C:62:ALA:O	2.18	0.44
1:E:286:GLU:HB3	1:E:361:LYS:HB2	1.99	0.44
1:D:76:GLU:HA	1:D:172:ARG:HG2	1.99	0.44
1:F:388:CYS:O	1:F:392:LEU:HB2	2.17	0.44
1:B:93:ILE:CG1	1:B:94:PRO:HD2	2.35	0.44
1:G:46:ILE:HD11	1:G:185:TYR:CD1	2.52	0.44
1:A:335:ARG:HH12	1:A:400:PRO:HB3	1.83	0.44
1:C:200:LEU:HD13	1:C:307:THR:HA	1.99	0.44
1:C:85:PRO:HB2	1:C:95:THR:HG21	2.00	0.44
1:A:85:PRO:HB2	1:A:95:THR:HG21	1.99	0.44
1:E:120:LEU:HD21	1:E:121:HIS:CE1	2.52	0.44
1:C:194:LEU:HB3	1:C:206:ILE:HG21	2.00	0.44
1:F:44:HIS:HA	1:F:47:TRP:CD1	2.53	0.43
1:F:316:HIS:CD2	1:F:316:HIS:H	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:ILE:HG22	1:B:36:SER:O	2.18	0.43
1:F:23:LEU:HD22	1:F:130:ALA:HB2	1.99	0.43
1:F:93:ILE:HG22	1:F:97:ASP:HB2	2.00	0.43
1:F:365:PRO:HA	1:F:377:ASN:HD21	1.83	0.43
1:C:276:VAL:HB	1:C:291:MET:HG2	1.99	0.43
1:A:68:VAL:HG22	1:A:209:THR:HG22	1.99	0.43
1:E:196:GLU:HB2	1:E:260:PHE:CZ	2.52	0.43
1:A:400:PRO:HA	1:A:403:ALA:HB3	2.01	0.43
1:A:96:VAL:O	1:A:100:MET:HB2	2.18	0.43
1:C:271:ILE:HD11	1:C:295:ALA:HB2	2.00	0.43
1:G:118:GLY:HA3	1:G:308:ILE:HD13	2.01	0.43
1:F:138:GLU:HB2	1:F:170:THR:HB	1.98	0.43
1:B:44:HIS:CE1	1:B:371:THR:HA	2.53	0.43
1:G:86:VAL:HG11	1:G:146:TRP:CD2	2.54	0.43
1:G:52:ASN:HB3	2:G:601:ANP:N7	2.33	0.43
1:E:96:VAL:HG21	1:E:139:ILE:HD13	2.00	0.43
1:A:23:LEU:HA	1:A:26:VAL:HG23	2.00	0.43
1:G:86:VAL:HA	1:G:96:VAL:HG22	2.01	0.43
1:C:139:ILE:HG22	1:C:141:ARG:HG2	2.00	0.43
1:A:160:GLN:HB3	1:E:245:LYS:HA	2.00	0.43
1:F:131:LEU:HG	1:F:179:VAL:HG11	1.99	0.43
1:G:276:VAL:HG22	1:G:395:TRP:CE2	2.54	0.43
1:F:194:LEU:HB3	1:F:206:ILE:HG21	2.01	0.43
1:H:311:HIS:NE2	1:H:373:THR:HG22	2.33	0.43
1:F:120:LEU:HD13	1:F:365:PRO:HG2	2.00	0.43
1:G:109:PHE:HB3	1:H:28:LYS:HE3	2.01	0.43
1:D:365:PRO:HA	1:D:377:ASN:HD21	1.83	0.43
1:G:196:GLU:O	1:G:200:LEU:HG	2.18	0.43
1:F:190:VAL:O	1:F:194:LEU:HG	2.17	0.43
1:G:301:VAL:HG22	1:G:356:ALA:HB3	2.00	0.43
1:F:187:PHE:CE1	1:F:210:ASP:HB2	2.54	0.43
1:H:323:ALA:CB	1:H:388:CYS:HB3	2.46	0.43
1:H:312:GLU:HB2	1:H:373:THR:HB	2.01	0.43
1:E:281:LYS:HB3	1:E:286:GLU:HG3	2.00	0.42
1:A:58:MET:HE2	1:A:116:ILE:HG22	2.01	0.42
1:D:45:LEU:HD11	1:D:180:PHE:CZ	2.54	0.42
1:H:145:GLU:HG2	1:H:162:ALA:H	1.83	0.42
1:H:136:GLU:HB2	1:H:172:ARG:HB2	2.01	0.42
1:B:186:ASP:HB3	1:B:189:THR:HB	2.01	0.42
1:A:53:ALA:O	1:A:56:GLU:HB2	2.19	0.42
1:G:282:GLY:HA3	1:G:285:HIS:ND1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:HIS:HA	1:B:14:ALA:HB1	2.01	0.42
1:C:377:ASN:O	1:C:380:VAL:HB	2.19	0.42
1:B:193:ARG:O	1:B:197:MET:HG3	2.19	0.42
1:B:367:PHE:CD1	1:B:372:LYS:HB3	2.54	0.42
1:B:272:HIS:CD2	1:B:274:SER:O	2.72	0.42
1:H:89:HIS:HB2	1:H:95:THR:OG1	2.19	0.42
1:H:129:ASN:HA	1:H:135:LEU:HD13	2.00	0.42
1:D:65:VAL:O	1:D:206:ILE:HA	2.19	0.42
1:H:306:ASN:OD1	1:H:361:LYS:HA	2.19	0.42
1:B:88:THR:HA	1:B:94:PRO:HA	2.01	0.42
1:B:23:LEU:HD22	1:B:130:ALA:HB2	2.01	0.42
1:D:415:GLN:HA	1:D:418:ILE:HD12	2.02	0.42
1:C:12:TYR:CD2	1:D:82:ARG:HD2	2.54	0.42
1:G:100:MET:O	1:G:126:SER:HA	2.20	0.42
1:A:137:VAL:HG23	1:A:148:GLN:HB3	2.01	0.42
1:B:346:THR:O	1:B:350:ILE:HG22	2.19	0.42
1:F:312:GLU:HG3	1:F:373:THR:HB	2.01	0.42
1:H:64:THR:HG23	1:H:205:THR:HB	2.01	0.42
1:C:255:GLY:HA3	1:C:259:ASP:HB2	2.01	0.42
1:F:46:ILE:HD11	1:F:75:VAL:HG21	2.01	0.42
1:D:34:ILE:HD12	1:D:44:HIS:HB3	2.01	0.42
1:D:393:THR:O	1:D:397:GLU:HG2	2.20	0.42
1:B:367:PHE:HB3	1:B:372:LYS:HA	2.02	0.42
1:H:67:VAL:HG22	1:H:77:VAL:HG22	2.02	0.42
1:F:129:ASN:OD1	1:F:153:SER:HA	2.20	0.42
1:E:323:ALA:HB2	1:E:385:GLN:HG3	2.02	0.42
1:A:164:THR:HG23	1:A:166:LYS:H	1.84	0.42
1:A:210:ASP:HB3	1:A:247:LYS:HB3	2.02	0.42
1:G:377:ASN:HB2	1:G:380:VAL:HG23	2.01	0.41
1:G:86:VAL:HG13	1:G:158:LEU:HD11	2.03	0.41
1:C:71:GLU:HA	1:C:212:ARG:HG2	2.01	0.41
1:F:34:ILE:HD13	1:F:127:VAL:HG11	2.02	0.41
1:D:116:ILE:HD13	1:D:361:LYS:HB3	2.03	0.41
1:D:99:VAL:HG13	2:D:601:ANP:H5'1	2.02	0.41
1:A:369:GLY:HA2	1:B:32:MET:HA	2.01	0.41
1:E:327:VAL:HG22	1:E:393:THR:HG23	2.02	0.41
1:A:176:ASP:O	1:A:180:PHE:HD2	2.03	0.41
1:G:276:VAL:HB	1:G:291:MET:HG2	2.00	0.41
1:F:196:GLU:HA	1:F:199:PHE:HD2	1.86	0.41
1:G:303:THR:HG22	1:G:358:ILE:HB	2.02	0.41
1:H:194:LEU:HB3	1:H:206:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:LYS:HB3	1:C:294:ASN:HB2	2.03	0.41
1:B:200:LEU:HD13	1:B:307:THR:HA	2.01	0.41
1:G:54:VAL:HG22	1:G:204:LEU:HD21	2.03	0.41
1:A:200:LEU:HB2	1:A:307:THR:HG23	2.02	0.41
1:E:52:ASN:HB3	2:E:601:ANP:N7	2.35	0.41
1:G:106:GLY:HA2	2:G:601:ANP:H4'	2.02	0.41
1:G:34:ILE:HD12	1:G:44:HIS:HB3	2.03	0.41
1:A:104:HIS:HB3	1:B:20:LEU:HB2	2.03	0.41
1:H:123:VAL:HG13	1:H:127:VAL:HG23	2.03	0.41
1:C:196:GLU:HA	1:C:199:PHE:HD2	1.85	0.41
1:D:33:TYR:HB3	1:D:127:VAL:HG21	2.02	0.41
1:H:23:LEU:HD11	1:H:101:THR:HA	2.03	0.41
1:F:122:GLY:HA2	2:F:601:ANP:O3A	2.20	0.41
1:C:87:ALA:HB3	1:D:14:ALA:HB2	2.02	0.41
1:H:323:ALA:HB2	1:H:385:GLN:HA	2.02	0.41
1:A:95:THR:HG21	1:B:17:ILE:HG13	2.02	0.41
1:F:47:TRP:CE3	1:F:193:ARG:HG2	2.56	0.40
1:F:148:GLN:HG3	1:F:150:TYR:CE1	2.55	0.40
1:B:196:GLU:HA	1:B:199:PHE:CD2	2.52	0.40
1:E:150:TYR:CE1	1:E:155:PRO:HB3	2.56	0.40
1:A:139:ILE:O	1:A:146:TRP:HD1	2.02	0.40
1:C:276:VAL:HG22	1:C:395:TRP:CE2	2.56	0.40
1:F:318:GLU:HB3	1:F:381:LYS:HE2	2.04	0.40
1:H:190:VAL:O	1:H:194:LEU:HG	2.21	0.40
1:F:281:LYS:HG3	1:F:286:GLU:HG2	2.03	0.40
1:C:369:GLY:HA2	1:D:32:MET:HA	2.03	0.40
1:D:186:ASP:O	1:D:190:VAL:HG23	2.21	0.40
1:A:86:VAL:O	1:A:87:ALA:CB	2.69	0.40
1:C:150:TYR:CE1	1:C:155:PRO:HB3	2.57	0.40
1:E:95:THR:HG21	1:F:17:ILE:HG13	2.03	0.40
1:H:43:HIS:CE1	1:H:186:ASP:H	2.39	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	371/432 (86%)	342 (92%)	22 (6%)	7 (2%)	10	40
1	B	369/432 (85%)	346 (94%)	22 (6%)	1 (0%)	46	81
1	C	384/432 (89%)	359 (94%)	21 (6%)	4 (1%)	19	58
1	D	373/432 (86%)	351 (94%)	15 (4%)	7 (2%)	10	40
1	E	376/432 (87%)	355 (94%)	20 (5%)	1 (0%)	46	81
1	F	370/432 (86%)	349 (94%)	19 (5%)	2 (0%)	34	74
1	G	372/432 (86%)	349 (94%)	18 (5%)	5 (1%)	15	51
1	H	372/432 (86%)	349 (94%)	19 (5%)	4 (1%)	17	56
All	All	2987/3456 (86%)	2800 (94%)	156 (5%)	31 (1%)	19	58

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	343	PRO
1	C	343	PRO
1	H	343	PRO
1	A	87	ALA
1	A	124	GLY
1	C	124	GLY
1	D	377	ASN
1	H	124	GLY
1	H	336	LYS
1	A	283	THR
1	C	414	ALA
1	D	120	LEU
1	D	283	THR
1	D	316	HIS
1	D	341	LYS
1	F	21	GLU
1	A	377	ASN
1	C	283	THR
1	G	87	ALA
1	G	124	GLY
1	G	141	ARG
1	B	124	GLY
1	D	22	GLY
1	E	283	THR

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Mol	Chain	Res	Type
1	G	120	LEU
1	A	22	GLY
1	A	247	LYS
1	D	124	GLY
1	F	120	LEU
1	G	11	GLU
1	H	81	GLY

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	297/350 (85%)	280 (94%)	17 (6%)	25	62
1	B	298/350 (85%)	273 (92%)	25 (8%)	14	42
1	C	301/350 (86%)	280 (93%)	21 (7%)	19	53
1	D	289/350 (83%)	270 (93%)	19 (7%)	21	55
1	E	299/350 (85%)	283 (95%)	16 (5%)	27	64
1	F	292/350 (83%)	261 (89%)	31 (11%)	8	29
1	G	296/350 (85%)	272 (92%)	24 (8%)	15	44
1	H	293/350 (84%)	273 (93%)	20 (7%)	20	54
All	All	2365/2800 (84%)	2192 (93%)	173 (7%)	17	50

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	THR
1	A	72	ASP
1	A	110	ASP
1	A	126	SER
1	A	164	THR
1	A	181	GLU
1	A	257	LEU
1	A	260	PHE

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Mol	Chain	Res	Type
1	A	275	ILE
1	A	285	HIS
1	A	307	THR
1	A	316	HIS
1	A	346	THR
1	A	361	LYS
1	A	363	SER
1	A	388	CYS
1	A	421	ARG
1	B	63	THR
1	B	67	VAL
1	B	93	ILE
1	B	97	ASP
1	B	110	ASP
1	B	131	LEU
1	B	135	LEU
1	B	141	ARG
1	B	188	GLU
1	B	209	THR
1	B	247	LYS
1	B	248	SER
1	B	260	PHE
1	B	279	SER
1	B	285	HIS
1	B	300	SER
1	B	316	HIS
1	B	318	GLU
1	B	350	ILE
1	B	362	VAL
1	B	364	GLU
1	B	377	ASN
1	B	389	ASN
1	B	402	ASP
1	B	404	LYS
1	C	16	SER
1	C	36	SER
1	C	67	VAL
1	C	93	ILE
1	C	126	SER
1	C	137	VAL
1	C	181	GLU
1	C	196	GLU

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Mol	Chain	Res	Type
1	C	202	LYS
1	C	257	LEU
1	C	260	PHE
1	C	261	VAL
1	C	285	HIS
1	C	316	HIS
1	C	322	SER
1	C	348	ASP
1	C	349	ASP
1	C	386	LYS
1	C	389	ASN
1	C	394	HIS
1	C	404	LYS
1	D	34	ILE
1	D	71	GLU
1	D	72	ASP
1	D	95	THR
1	D	110	ASP
1	D	126	SER
1	D	131	LEU
1	D	137	VAL
1	D	156	LEU
1	D	164	THR
1	D	182	THR
1	D	209	THR
1	D	260	PHE
1	D	271	ILE
1	D	274	SER
1	D	335	ARG
1	D	348	ASP
1	D	388	CYS
1	D	392	LEU
1	E	28	LYS
1	E	131	LEU
1	E	133	THR
1	E	169	SER
1	E	176	ASP
1	E	247	LYS
1	E	260	PHE
1	E	283	THR
1	E	285	HIS
1	E	298	SER

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Mol	Chain	Res	Type
1	E	328	VAL
1	E	344	ASN
1	E	350	ILE
1	E	372	LYS
1	E	402	ASP
1	E	417	ARG
1	F	10	ASP
1	F	12	TYR
1	F	16	SER
1	F	37	THR
1	F	39	GLU
1	F	40	ARG
1	F	64	THR
1	F	67	VAL
1	F	72	ASP
1	F	108	LYS
1	F	134	ARG
1	F	135	LEU
1	F	164	THR
1	F	181	GLU
1	F	197	MET
1	F	209	THR
1	F	247	LYS
1	F	260	PHE
1	F	268	LYS
1	F	299	GLU
1	F	300	SER
1	F	308	ILE
1	F	322	SER
1	F	334	ASP
1	F	348	ASP
1	F	378	THR
1	F	379	GLU
1	F	382	SER
1	F	389	ASN
1	F	391	GLN
1	F	401	THR
1	G	34	ILE
1	G	88	THR
1	G	96	VAL
1	G	110	ASP
1	G	131	LEU

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Mol	Chain	Res	Type
1	G	147	SER
1	G	153	SER
1	G	156	LEU
1	G	209	THR
1	G	260	PHE
1	G	271	ILE
1	G	277	ASP
1	G	289	ILE
1	G	308	ILE
1	G	316	HIS
1	G	330	LYS
1	G	333	LYS
1	G	334	ASP
1	G	344	ASN
1	G	364	GLU
1	G	378	THR
1	G	381	LYS
1	G	382	SER
1	G	415	GLN
1	H	64	THR
1	H	111	SER
1	H	112	ASP
1	H	126	SER
1	H	135	LEU
1	H	160	GLN
1	H	165	LYS
1	H	169	SER
1	H	181	GLU
1	H	247	LYS
1	H	260	PHE
1	H	277	ASP
1	H	285	HIS
1	H	298	SER
1	H	300	SER
1	H	334	ASP
1	H	386	LYS
1	H	388	CYS
1	H	389	ASN
1	H	391	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	265	ASN
1	A	272	HIS
1	A	292	GLN
1	A	316	HIS
1	B	44	HIS
1	B	272	HIS
1	B	316	HIS
1	B	329	ASN
1	C	89	HIS
1	C	302	HIS
1	C	309	ASN
1	D	102	GLN
1	E	89	HIS
1	E	272	HIS
1	F	44	HIS
1	F	316	HIS
1	H	102	GLN
1	H	195	GLN
1	H	316	HIS
1	H	329	ASN
1	H	366	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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
2	ANP	A	601	3	27,33,33	4.13	12 (44%)	30,52,52	2.46	9 (30%)
2	ANP	B	601	3	27,33,33	3.99	12 (44%)	30,52,52	2.32	8 (26%)
2	ANP	C	601	3	27,33,33	4.19	10 (37%)	30,52,52	2.48	6 (20%)
2	ANP	D	601	3	27,33,33	4.14	11 (40%)	30,52,52	2.38	6 (20%)
2	ANP	E	601	3	27,33,33	4.09	10 (37%)	30,52,52	2.49	5 (16%)
2	ANP	F	601	3	27,33,33	4.13	10 (37%)	30,52,52	2.70	7 (23%)
2	ANP	G	601	3	27,33,33	4.11	11 (40%)	30,52,52	2.36	7 (23%)
2	ANP	H	601	3	27,33,33	4.03	11 (40%)	30,52,52	2.54	5 (16%)

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
2	ANP	A	601	3	-	0/12/38/38	0/3/3/3
2	ANP	B	601	3	-	0/12/38/38	0/3/3/3
2	ANP	C	601	3	-	0/12/38/38	0/3/3/3
2	ANP	D	601	3	-	0/12/38/38	0/3/3/3
2	ANP	E	601	3	-	0/12/38/38	0/3/3/3
2	ANP	F	601	3	-	1/12/38/38	0/3/3/3
2	ANP	G	601	3	-	0/12/38/38	0/3/3/3
2	ANP	H	601	3	-	0/12/38/38	0/3/3/3

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	601	ANP	PG-N3B	-4.74	1.50	1.63
2	B	601	ANP	PG-N3B	-4.38	1.51	1.63
2	C	601	ANP	PG-N3B	-4.31	1.51	1.63
2	G	601	ANP	PG-N3B	-4.28	1.52	1.63
2	H	601	ANP	PG-N3B	-4.19	1.52	1.63
2	D	601	ANP	PG-N3B	-4.12	1.52	1.63
2	E	601	ANP	PG-N3B	-3.86	1.53	1.63
2	A	601	ANP	PG-N3B	-3.66	1.53	1.63
2	B	601	ANP	C3'-C4'	-3.65	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	ANP	C3'-C4'	-3.53	1.43	1.53
2	F	601	ANP	C3'-C4'	-3.47	1.43	1.53
2	A	601	ANP	C3'-C4'	-3.43	1.43	1.53
2	H	601	ANP	C3'-C4'	-3.34	1.44	1.53
2	E	601	ANP	C3'-C4'	-3.25	1.44	1.53
2	G	601	ANP	C2'-C3'	-3.21	1.44	1.53
2	C	601	ANP	C3'-C4'	-3.19	1.44	1.53
2	G	601	ANP	C3'-C4'	-3.17	1.44	1.53
2	F	601	ANP	PB-N3B	-2.90	1.55	1.63
2	E	601	ANP	C2'-C3'	-2.86	1.45	1.53
2	H	601	ANP	C2'-C3'	-2.76	1.45	1.53
2	B	601	ANP	C2'-C3'	-2.75	1.45	1.53
2	C	601	ANP	C2'-C3'	-2.75	1.45	1.53
2	D	601	ANP	C2'-C3'	-2.68	1.46	1.53
2	A	601	ANP	C2'-C3'	-2.64	1.46	1.53
2	G	601	ANP	PB-N3B	-2.62	1.56	1.63
2	C	601	ANP	PB-N3B	-2.56	1.56	1.63
2	F	601	ANP	C2'-C3'	-2.52	1.46	1.53
2	H	601	ANP	PB-N3B	-2.49	1.56	1.63
2	D	601	ANP	PB-N3B	-2.39	1.57	1.63
2	G	601	ANP	C2-N3	-2.36	1.28	1.32
2	B	601	ANP	PB-N3B	-2.28	1.57	1.63
2	A	601	ANP	C5'-C4'	-2.22	1.44	1.51
2	B	601	ANP	C2-N3	-2.18	1.28	1.32
2	B	601	ANP	O4'-C4'	-2.12	1.40	1.45
2	H	601	ANP	C2-N3	-2.12	1.28	1.32
2	E	601	ANP	C2-N3	-2.08	1.28	1.32
2	A	601	ANP	C2-N3	-2.07	1.28	1.32
2	A	601	ANP	PB-N3B	-2.07	1.57	1.63
2	D	601	ANP	C2-N3	-2.04	1.28	1.32
2	G	601	ANP	C2-N1	3.45	1.40	1.33
2	A	601	ANP	C2-N1	3.76	1.41	1.33
2	C	601	ANP	C2-N1	3.80	1.41	1.33
2	D	601	ANP	C2-N1	3.82	1.41	1.33
2	B	601	ANP	C2-N1	4.04	1.41	1.33
2	H	601	ANP	C8-N7	4.06	1.42	1.34
2	D	601	ANP	C8-N7	4.11	1.42	1.34
2	E	601	ANP	C2-N1	4.13	1.41	1.33
2	F	601	ANP	C2-N1	4.15	1.41	1.33
2	B	601	ANP	C8-N7	4.17	1.42	1.34
2	F	601	ANP	C8-N7	4.21	1.42	1.34
2	A	601	ANP	C8-N7	4.22	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	ANP	C8-N7	4.28	1.42	1.34
2	H	601	ANP	C2-N1	4.31	1.42	1.33
2	C	601	ANP	C8-N7	4.36	1.43	1.34
2	G	601	ANP	C8-N7	4.59	1.43	1.34
2	A	601	ANP	C6-N6	5.11	1.50	1.34
2	H	601	ANP	C6-N6	5.31	1.51	1.34
2	C	601	ANP	C6-N6	5.32	1.51	1.34
2	E	601	ANP	C6-N6	5.35	1.51	1.34
2	D	601	ANP	C6-N6	5.38	1.51	1.34
2	G	601	ANP	C4-N3	5.39	1.43	1.35
2	G	601	ANP	C6-N6	5.39	1.51	1.34
2	F	601	ANP	C6-N6	5.42	1.51	1.34
2	B	601	ANP	C6-N6	5.60	1.52	1.34
2	B	601	ANP	C4-N3	5.80	1.44	1.35
2	E	601	ANP	C4-N3	5.94	1.44	1.35
2	D	601	ANP	C4-N3	6.26	1.44	1.35
2	H	601	ANP	C4-N3	6.28	1.44	1.35
2	C	601	ANP	C4-N3	6.44	1.45	1.35
2	A	601	ANP	C4-N3	6.47	1.45	1.35
2	F	601	ANP	C4-N3	6.65	1.45	1.35
2	B	601	ANP	PG-O1G	8.82	1.56	1.46
2	C	601	ANP	PG-O1G	9.59	1.57	1.46
2	H	601	ANP	PG-O1G	9.76	1.57	1.46
2	A	601	ANP	PG-O1G	9.76	1.57	1.46
2	F	601	ANP	PG-O1G	9.83	1.57	1.46
2	G	601	ANP	PG-O1G	9.94	1.57	1.46
2	D	601	ANP	PG-O1G	10.09	1.57	1.46
2	E	601	ANP	PG-O1G	10.17	1.57	1.46
2	H	601	ANP	PB-O1B	13.44	1.61	1.46
2	B	601	ANP	PB-O1B	13.84	1.62	1.46
2	F	601	ANP	PB-O1B	13.87	1.62	1.46
2	E	601	ANP	PB-O1B	14.01	1.62	1.46
2	D	601	ANP	PB-O1B	14.30	1.62	1.46
2	G	601	ANP	PB-O1B	14.31	1.62	1.46
2	A	601	ANP	PB-O1B	14.62	1.63	1.46
2	C	601	ANP	PB-O1B	14.81	1.63	1.46

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	601	ANP	N3-C2-N1	-11.98	119.72	128.89
2	E	601	ANP	N3-C2-N1	-11.61	120.00	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	ANP	N3-C2-N1	-11.41	120.16	128.89
2	H	601	ANP	N3-C2-N1	-11.19	120.32	128.89
2	D	601	ANP	N3-C2-N1	-10.97	120.49	128.89
2	G	601	ANP	N3-C2-N1	-10.60	120.78	128.89
2	A	601	ANP	N3-C2-N1	-10.46	120.89	128.89
2	B	601	ANP	N3-C2-N1	-10.08	121.17	128.89
2	F	601	ANP	O1B-PB-N3B	-4.18	105.49	111.90
2	H	601	ANP	C2'-C1'-N9	-3.87	108.38	114.29
2	H	601	ANP	O1G-PG-N3B	-3.64	106.32	111.90
2	E	601	ANP	C2'-C1'-N9	-3.59	108.80	114.29
2	F	601	ANP	O3G-PG-O1G	-3.44	104.34	113.49
2	C	601	ANP	O1B-PB-N3B	-3.30	106.83	111.90
2	A	601	ANP	C2'-C1'-N9	-3.13	109.52	114.29
2	F	601	ANP	C2'-C1'-N9	-3.05	109.63	114.29
2	G	601	ANP	C2'-C1'-N9	-2.92	109.83	114.29
2	H	601	ANP	O1B-PB-N3B	-2.91	107.43	111.90
2	B	601	ANP	O1B-PB-N3B	-2.90	107.45	111.90
2	C	601	ANP	C2'-C1'-N9	-2.82	109.98	114.29
2	D	601	ANP	PA-O3A-PB	-2.78	123.36	132.67
2	B	601	ANP	O2G-PG-O1G	-2.67	106.39	113.49
2	E	601	ANP	PA-O3A-PB	-2.64	123.83	132.67
2	B	601	ANP	PA-O3A-PB	-2.56	124.09	132.67
2	C	601	ANP	PA-O3A-PB	-2.53	124.17	132.67
2	A	601	ANP	C5'-C4'-C3'	-2.50	105.29	115.21
2	G	601	ANP	PA-O3A-PB	-2.50	124.30	132.67
2	F	601	ANP	PA-O3A-PB	-2.43	124.52	132.67
2	B	601	ANP	O1G-PG-N3B	-2.34	108.31	111.90
2	A	601	ANP	O2G-PG-O1G	-2.23	107.57	113.49
2	G	601	ANP	C4-C5-N7	-2.22	107.44	109.48
2	A	601	ANP	PA-O3A-PB	-2.21	125.27	132.67
2	D	601	ANP	O3G-PG-O1G	-2.19	107.66	113.49
2	G	601	ANP	O3G-PG-O1G	-2.15	107.78	113.49
2	A	601	ANP	C1'-N9-C4	-2.14	123.70	126.94
2	D	601	ANP	O1G-PG-N3B	-2.12	108.64	111.90
2	G	601	ANP	O1B-PB-N3B	-2.11	108.66	111.90
2	B	601	ANP	C1'-N9-C4	-2.09	123.78	126.94
2	A	601	ANP	C4-C5-N7	-2.05	107.59	109.48
2	E	601	ANP	C1'-N9-C4	-2.01	123.91	126.94
2	H	601	ANP	O5'-C5'-C4'	2.13	116.95	109.12
2	C	601	ANP	O5'-C5'-C4'	2.13	116.98	109.12
2	B	601	ANP	O3A-PA-O5'	2.15	108.65	102.94
2	E	601	ANP	O3A-PA-O5'	2.27	108.97	102.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	601	ANP	O5'-C5'-C4'	2.28	117.53	109.12
2	F	601	ANP	O3A-PA-O5'	2.33	109.11	102.94
2	A	601	ANP	C2'-C3'-C4'	2.33	107.41	102.61
2	G	601	ANP	O3A-PA-O5'	2.43	109.39	102.94
2	D	601	ANP	O5'-C5'-C4'	2.67	118.97	109.12
2	C	601	ANP	O3A-PA-O5'	2.73	110.17	102.94
2	A	601	ANP	O5'-C5'-C4'	2.80	119.45	109.12
2	D	601	ANP	O3A-PA-O5'	2.96	110.80	102.94
2	B	601	ANP	O5'-C5'-C4'	3.12	120.61	109.12

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	601	ANP	O1G-PG-N3B-PB

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	ANP	3	0
2	B	601	ANP	1	0
2	C	601	ANP	1	0
2	D	601	ANP	1	0
2	E	601	ANP	2	0
2	F	601	ANP	1	0
2	G	601	ANP	2	0
2	H	601	ANP	1	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	377/432 (87%)	-0.20	4 (1%)	82 65	47, 74, 130, 156	0
1	B	375/432 (86%)	-0.27	1 (0%)	94 87	46, 75, 110, 129	0
1	C	390/432 (90%)	-0.30	4 (1%)	84 67	39, 71, 129, 179	0
1	D	379/432 (87%)	-0.28	3 (0%)	87 73	51, 83, 124, 160	0
1	E	382/432 (88%)	-0.23	6 (1%)	74 55	41, 70, 135, 171	0
1	F	376/432 (87%)	-0.30	2 (0%)	91 81	44, 72, 123, 160	0
1	G	378/432 (87%)	-0.30	4 (1%)	82 65	41, 70, 132, 155	0
1	H	378/432 (87%)	-0.21	6 (1%)	74 55	49, 82, 130, 149	0
All	All	3035/3456 (87%)	-0.26	30 (0%)	84 67	39, 75, 128, 179	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	340	ASP	5.4
1	E	339	LYS	5.1
1	E	338	LEU	4.8
1	C	339	LYS	4.5
1	H	338	LEU	3.9
1	G	402	ASP	3.4
1	B	21	GLU	3.3
1	G	338	LEU	3.1
1	G	337	LEU	3.1
1	E	295	ALA	3.0
1	C	328	VAL	3.0
1	C	336	LYS	3.0
1	F	333	LYS	2.9
1	E	336	LYS	2.9
1	A	331	TYR	2.9
1	H	333	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	419	ALA	2.6
1	G	406	VAL	2.6
1	D	341	LYS	2.6
1	F	421	ARG	2.5
1	A	329	ASN	2.5
1	E	393	THR	2.4
1	H	156	LEU	2.4
1	C	410	ALA	2.3
1	H	414	ALA	2.2
1	A	396	PHE	2.2
1	D	87	ALA	2.2
1	A	395	TRP	2.2
1	H	84	ILE	2.1
1	E	398	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	MG	D	602	1/1	0.97	0.20	1.91	60,60,60,60	0
3	MG	A	602	1/1	0.99	0.19	1.67	38,38,38,38	0
3	MG	E	602	1/1	0.98	0.17	1.07	51,51,51,51	0
3	MG	H	602	1/1	0.99	0.17	0.80	37,37,37,37	0
2	ANP	E	601	31/31	0.98	0.16	0.20	42,51,57,58	0
2	ANP	D	601	31/31	0.98	0.17	0.12	49,76,86,87	0
2	ANP	G	601	31/31	0.99	0.16	0.12	44,49,55,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ANP	C	601	31/31	0.99	0.16	0.09	48,59,66,69	0
3	MG	G	602	1/1	0.98	0.16	-0.10	35,35,35,35	0
2	ANP	H	601	31/31	0.98	0.17	-0.11	51,80,88,92	0
2	ANP	F	601	31/31	0.98	0.15	-0.25	38,54,60,61	0
3	MG	C	602	1/1	0.98	0.15	-0.29	35,35,35,35	0
2	ANP	B	601	31/31	0.98	0.15	-0.33	52,64,69,71	0
2	ANP	A	601	31/31	0.98	0.15	-0.33	49,58,62,63	0
3	MG	B	602	1/1	0.98	0.13	-0.80	37,37,37,37	0
3	MG	F	602	1/1	0.96	0.20	-	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.