



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:05 am GMT

PDB ID : 3VGA  
Title : Crystal structure of human adenosine A2A receptor with an allosteric inverse-agonist antibody at 3.1 Å resolution  
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Deposited on : 2011-08-04  
Resolution : 3.10 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

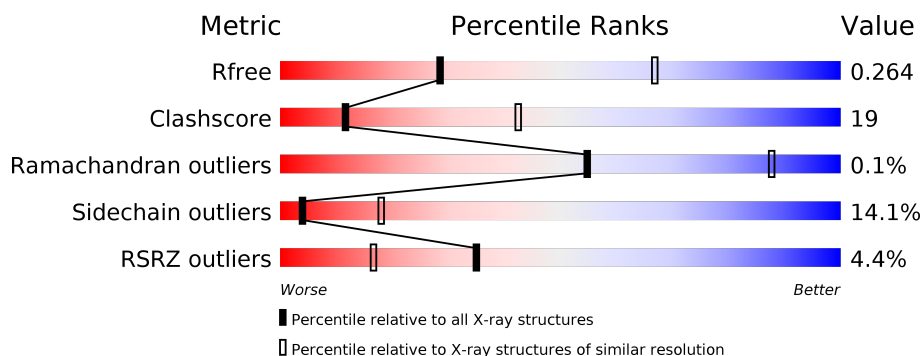
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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  $\geq 3$ , 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	326	<div> <div>10%</div> <div>53%</div> <div>34%</div> <div>9%</div> </div>
2	B	214	<div> <div>60%</div> <div>35%</div> <div>5%</div> </div>
3	C	226	<div> <div>57%</div> <div>34%</div> <div>7%</div> </div>

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	ZMA	A	401	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5635 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 Adenosine receptor A2a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2295	1517	378	380	20			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	154	GLN	ASN	ENGINEERED MUTATION	UNP P29274
A	317	HIS	-	EXPRESSION TAG	UNP P29274
A	318	HIS	-	EXPRESSION TAG	UNP P29274
A	319	HIS	-	EXPRESSION TAG	UNP P29274
A	320	HIS	-	EXPRESSION TAG	UNP P29274
A	321	HIS	-	EXPRESSION TAG	UNP P29274
A	322	HIS	-	EXPRESSION TAG	UNP P29274
A	323	HIS	-	EXPRESSION TAG	UNP P29274
A	324	HIS	-	EXPRESSION TAG	UNP P29274
A	325	HIS	-	EXPRESSION TAG	UNP P29274
A	326	HIS	-	EXPRESSION TAG	UNP P29274

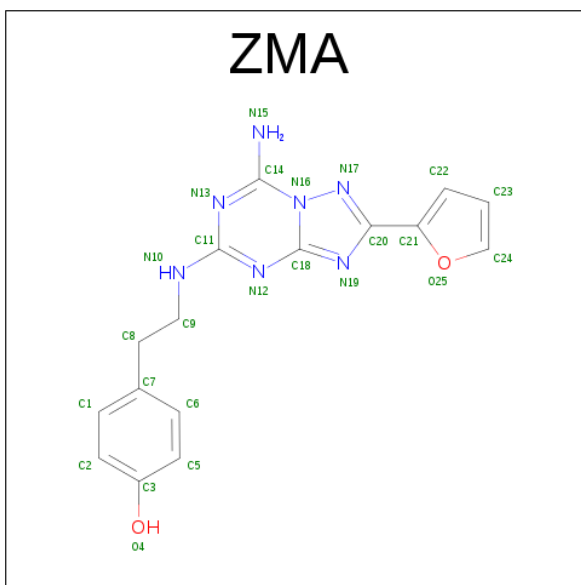
- Molecule 2 is a protein called antibody fab fragment light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1635	1025	274	330	6			

- Molecule 3 is a protein called antibody fab fragment heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	220	Total	C	N	O	S	0	0	0
			1666	1051	274	336	5			

- Molecule 4 is 4-{2-[(7-AMINO-2-FURAN-2-YL[1,2,4]TRIAZOLO[1,5-A][1,3,5]TRIAZIN-5-YL)AMINO]ETHYL}PHENOL (three-letter code: ZMA) (formula: C<sub>16</sub>H<sub>15</sub>N<sub>7</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			25	16	7	2		

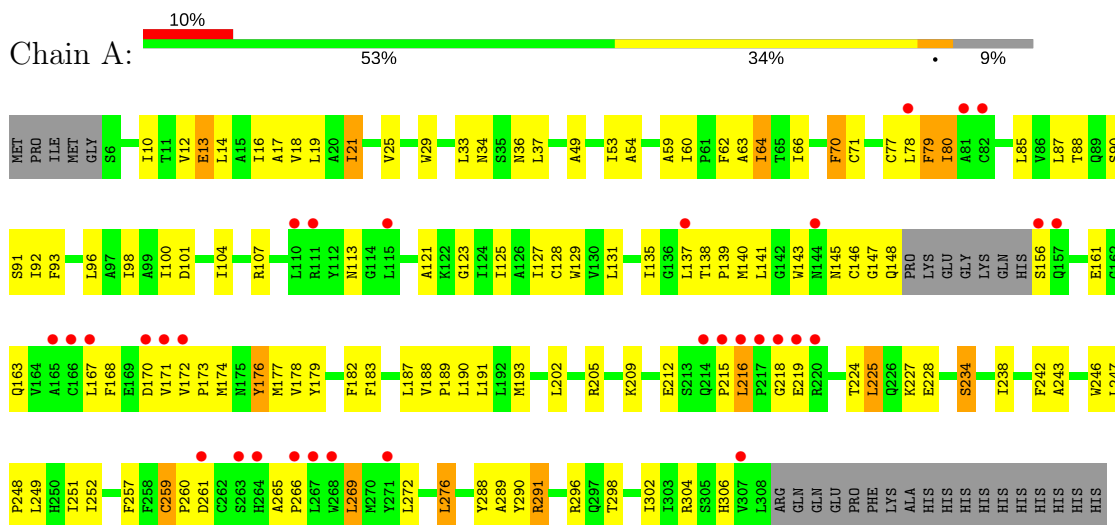
- Molecule 5 is water.

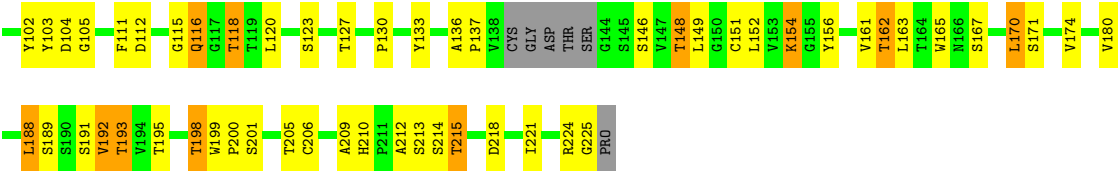
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	O	0	0
			2	2		
5	B	5	Total	O	0	0
			5	5		
5	C	7	Total	O	0	0
			7	7		

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

- Molecule 1: Adenosine receptor A2a





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.31Å 89.77Å 110.68Å 90.00° 96.14° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 71.80 – 2.62	Depositor EDS
% Data completeness (in resolution range)	88.4 (20.00-3.10) 74.4 (71.80-2.62)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.196 , 0.263 0.200 , 0.264	Depositor DCC
$R_{free}$ test set	971 reflections (5.13%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.6	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 56.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	5635	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZMA

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	0.36	0/2351	0.56	0/3208
2	B	0.48	0/1674	0.64	0/2275
3	C	0.48	0/1707	0.65	0/2328
All	All	0.44	0/5732	0.61	0/7811

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2295	0	2356	99	0
2	B	1635	0	1558	59	0
3	C	1666	0	1609	69	0
4	A	25	0	15	2	0
5	A	2	0	0	1	0
5	B	5	0	0	0	0
5	C	7	0	0	0	0
All	All	5635	0	5538	217	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 (217) 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)
3:C:6:GLN:HE21	3:C:115:GLY:HA3	1.32	0.94
2:B:77:ARG:CZ	2:B:77:ARG:HB3	2.02	0.90
1:A:243:ALA:O	1:A:247:LEU:HB2	1.72	0.89
2:B:8:PRO:O	2:B:102:THR:HB	1.77	0.84
1:A:143:TRP:CD1	1:A:173:PRO:HG3	2.13	0.84
2:B:31:SER:O	2:B:32:SER:HB2	1.78	0.83
3:C:148:THR:HG22	3:C:193:THR:HB	1.60	0.82
1:A:259:CYS:C	1:A:261:ASP:H	1.83	0.81
3:C:174:VAL:HG22	3:C:192:VAL:HG13	1.62	0.80
2:B:133:VAL:HG22	2:B:178:THR:HB	1.64	0.80
1:A:248:PRO:HG2	1:A:276:LEU:HD21	1.63	0.79
1:A:167:LEU:O	1:A:171:VAL:HG22	1.84	0.77
3:C:162:THR:HG23	3:C:209:ALA:HB3	1.69	0.73
1:A:238:ILE:HD11	1:A:288:TYR:CE1	2.26	0.70
3:C:170:LEU:HD13	3:C:192:VAL:HG11	1.74	0.69
1:A:218:GLY:HA2	1:A:219:GLU:C	2.13	0.69
3:C:103:TYR:CZ	3:C:105:GLY:HA2	2.28	0.68
2:B:48:VAL:HG22	2:B:54:LEU:HD23	1.75	0.68
2:B:31:SER:O	2:B:32:SER:CB	2.42	0.67
1:A:298:THR:O	1:A:302:ILE:HG13	1.95	0.67
2:B:193:THR:HG23	2:B:208:SER:HB2	1.78	0.66
2:B:77:ARG:NH1	2:B:77:ARG:HB3	2.11	0.65
1:A:257:PHE:O	1:A:260:PRO:HD3	1.97	0.65
2:B:135:PHE:CE2	3:C:191:SER:HB3	2.31	0.65
1:A:18:VAL:HA	1:A:21:ILE:HD12	1.78	0.65
1:A:238:ILE:HD11	1:A:288:TYR:HE1	1.61	0.65
3:C:148:THR:HA	3:C:193:THR:HA	1.79	0.64
3:C:6:GLN:OE1	3:C:118:THR:HG22	1.98	0.63
2:B:160:LEU:HD13	3:C:180:VAL:HG11	1.79	0.63
2:B:45:GLN:OE1	2:B:45:GLN:HA	1.99	0.63
2:B:29:ILE:O	2:B:31:SER:O	2.16	0.62
2:B:33:LEU:HD21	2:B:88:CYS:HB2	1.80	0.62
1:A:173:PRO:HG2	1:A:176:TYR:HB3	1.81	0.62
2:B:150:ILE:HD11	2:B:179:LEU:HD21	1.81	0.62
3:C:156:TYR:CE2	3:C:161:VAL:HG13	2.35	0.61
1:A:188:VAL:HB	1:A:189:PRO:HD3	1.82	0.61
1:A:143:TRP:HD1	1:A:143:TRP:O	1.85	0.60
1:A:234:SER:OG	1:A:291:ARG:HB3	2.02	0.60
3:C:67:LYS:HE2	3:C:84(A):ASN:O	2.00	0.60
1:A:10:ILE:HA	1:A:64:ILE:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:136:ALA:O	3:C:224:ARG:NH1	2.35	0.59
3:C:6:GLN:HE21	3:C:115:GLY:CA	2.11	0.59
3:C:60:TYR:HE1	3:C:70:LEU:HG	1.68	0.58
1:A:29:TRP:HZ2	1:A:306:HIS:CD2	2.21	0.58
2:B:183:LYS:O	2:B:187:GLU:HG3	2.04	0.58
2:B:163:TRP:CD1	2:B:163:TRP:N	2.70	0.58
2:B:79:GLN:HB3	2:B:80:PRO:HD2	1.86	0.58
1:A:246:TRP:HZ3	1:A:249:LEU:HD13	1.69	0.57
1:A:10:ILE:HG23	1:A:64:ILE:CD1	2.34	0.57
2:B:79:GLN:HE21	2:B:80:PRO:HD2	1.69	0.57
1:A:10:ILE:HG23	1:A:64:ILE:HD11	1.86	0.57
2:B:33:LEU:C	2:B:33:LEU:HD13	2.25	0.57
1:A:96:LEU:CD1	1:A:193:MET:HG3	2.35	0.56
3:C:210:HIS:CE1	3:C:212:ALA:HB3	2.40	0.56
1:A:93:PHE:HB3	1:A:128:CYS:SG	2.45	0.56
1:A:190:LEU:HD23	1:A:193:MET:HE3	1.86	0.56
1:A:13:GLU:CG	1:A:60:ILE:HG23	2.36	0.56
1:A:147:GLY:O	1:A:148:GLN:HG3	2.05	0.56
2:B:124:GLN:O	2:B:127:SER:HB3	2.05	0.56
1:A:171:VAL:HG23	1:A:172:VAL:HG23	1.88	0.56
1:A:259:CYS:C	1:A:261:ASP:N	2.54	0.55
2:B:8:PRO:HG3	2:B:11:LEU:HD23	1.88	0.55
1:A:143:TRP:CD1	1:A:143:TRP:O	2.60	0.55
1:A:29:TRP:CZ2	1:A:306:HIS:CD2	2.95	0.55
1:A:137:LEU:HB3	1:A:140:MET:HE2	1.88	0.54
1:A:249:LEU:O	1:A:249:LEU:HD23	2.08	0.54
3:C:163:LEU:C	3:C:163:LEU:HD23	2.28	0.54
1:A:174:MET:CE	1:A:257:PHE:HB2	2.38	0.54
3:C:210:HIS:HD2	3:C:213:SER:OG	1.91	0.53
2:B:48:VAL:CG2	2:B:54:LEU:HD23	2.38	0.53
3:C:18:VAL:O	3:C:82:GLN:HA	2.09	0.53
1:A:178:VAL:HG21	1:A:257:PHE:CB	2.38	0.53
2:B:149:LYS:HB2	2:B:193:THR:HB	1.89	0.53
1:A:49:ALA:O	1:A:53:ILE:HG13	2.08	0.53
1:A:289:ALA:O	1:A:296:ARG:HD3	2.08	0.53
3:C:72:VAL:CG1	3:C:73:ASP:N	2.72	0.52
2:B:117:ILE:HG22	2:B:207:LYS:HB3	1.91	0.52
2:B:181:LEU:N	2:B:181:LEU:HD12	2.25	0.52
2:B:167:ASP:O	2:B:171:SER:HA	2.10	0.52
3:C:37:VAL:HG13	3:C:46:GLU:O	2.09	0.52
1:A:54:ALA:HB3	1:A:87:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:GLY:O	1:A:127:ILE:HG13	2.10	0.52
3:C:148:THR:CG2	3:C:193:THR:HB	2.34	0.51
2:B:160:LEU:HD13	3:C:180:VAL:CG1	2.40	0.51
2:B:17:ASP:O	2:B:78:LEU:HB2	2.09	0.51
2:B:61:ARG:NH2	2:B:82:ASP:OD1	2.34	0.51
3:C:188:LEU:HG	3:C:189:SER:N	2.25	0.51
3:C:137:PRO:O	3:C:224:ARG:HD2	2.11	0.51
3:C:161:VAL:HG12	3:C:210:HIS:HB2	1.92	0.51
3:C:12:VAL:HG13	3:C:16:SER:OG	2.09	0.51
2:B:106:ILE:HD12	2:B:166:GLN:OE1	2.10	0.51
2:B:120:PRO:HD3	2:B:132:VAL:HG22	1.92	0.51
3:C:130:PRO:HB3	3:C:156:TYR:HB3	1.93	0.50
1:A:246:TRP:CZ3	1:A:249:LEU:HD13	2.46	0.50
2:B:76:ASN:O	2:B:77:ARG:C	2.50	0.50
3:C:224:ARG:O	3:C:225:GLY:C	2.49	0.50
1:A:143:TRP:HD1	1:A:173:PRO:HG3	1.74	0.50
1:A:13:GLU:HG3	1:A:60:ILE:HG23	1.93	0.50
3:C:17:SER:HA	3:C:83:LEU:O	2.12	0.49
3:C:35:ASN:HD21	3:C:99:GLU:HB2	1.78	0.49
3:C:51:ILE:HD13	3:C:72:VAL:HG23	1.93	0.49
3:C:213:SER:OG	3:C:215:THR:HG23	2.13	0.49
2:B:110:ASP:OD2	2:B:199:LYS:HD2	2.13	0.49
1:A:54:ALA:HB3	1:A:87:LEU:CD1	2.42	0.49
1:A:98:ILE:O	1:A:101:ASP:HB3	2.13	0.49
1:A:143:TRP:CE2	1:A:176:TYR:HB2	2.48	0.49
1:A:131:LEU:O	1:A:135:ILE:HB	2.13	0.49
1:A:63:ALA:O	1:A:66:ILE:HG22	2.13	0.49
1:A:77:CYS:HA	1:A:80:ILE:HD12	1.94	0.48
3:C:40:SER:O	3:C:41:HIS:CD2	2.66	0.48
1:A:54:ALA:CB	1:A:87:LEU:HD11	2.43	0.48
1:A:177:MET:HE1	4:A:401:ZMA:C21	2.44	0.48
3:C:149:LEU:HD22	3:C:221:ILE:HG21	1.95	0.48
1:A:85:LEU:CD2	4:A:401:ZMA:H23	2.44	0.48
3:C:72:VAL:HG12	3:C:73:ASP:N	2.29	0.48
3:C:206:CYS:O	3:C:218:ASP:HA	2.14	0.48
1:A:145:ASN:HB3	1:A:170:ASP:O	2.14	0.47
1:A:179:TYR:O	1:A:183:PHE:HB2	2.13	0.47
3:C:195:THR:OG1	3:C:198:THR:CG2	2.62	0.47
1:A:174:MET:HE2	1:A:257:PHE:HB2	1.96	0.47
2:B:124:GLN:HG3	3:C:133:TYR:CZ	2.49	0.47
3:C:60:TYR:CE1	3:C:70:LEU:HG	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:LEU:HD13	1:A:193:MET:HG3	1.96	0.47
2:B:159:VAL:O	2:B:160:LEU:HD23	2.15	0.47
1:A:13:GLU:HG2	1:A:60:ILE:HG23	1.96	0.47
3:C:35:ASN:ND2	3:C:99:GLU:HB2	2.30	0.47
1:A:113:ASN:HB2	5:A:328:HOH:O	2.14	0.47
2:B:91:PHE:HE1	3:C:111:PHE:CE1	2.33	0.47
1:A:71:CYS:HB3	1:A:163:GLN:HB3	1.97	0.46
1:A:139:PRO:HA	1:A:143:TRP:HB3	1.97	0.46
1:A:125:ILE:O	1:A:129:TRP:HD1	1.99	0.46
1:A:259:CYS:O	1:A:261:ASP:N	2.48	0.46
1:A:269:LEU:O	1:A:272:LEU:HB3	2.15	0.46
2:B:79:GLN:NE2	2:B:80:PRO:HD2	2.30	0.46
1:A:96:LEU:HD12	1:A:193:MET:HG3	1.98	0.46
3:C:188:LEU:HG	3:C:189:SER:H	1.81	0.46
2:B:12:SER:HA	2:B:105:GLU:O	2.15	0.46
3:C:12:VAL:CG1	3:C:16:SER:OG	2.64	0.46
1:A:92:ILE:HD11	1:A:242:PHE:CZ	2.51	0.46
3:C:195:THR:O	3:C:198:THR:HG23	2.16	0.45
1:A:121:ALA:O	1:A:125:ILE:HG13	2.16	0.45
3:C:221:ILE:N	3:C:221:ILE:HD12	2.31	0.45
3:C:195:THR:OG1	3:C:198:THR:HG23	2.16	0.45
3:C:210:HIS:CD2	3:C:213:SER:OG	2.70	0.45
1:A:79:PHE:HD2	1:A:79:PHE:O	2.00	0.45
3:C:165:TRP:CE2	3:C:192:VAL:HG22	2.52	0.45
3:C:20:ILE:HB	3:C:81:ILE:CG2	2.47	0.45
2:B:121:SER:OG	3:C:133:TYR:HB3	2.17	0.44
1:A:21:ILE:HG23	1:A:53:ILE:HG23	1.98	0.44
1:A:227:LYS:HD3	1:A:227:LYS:HA	1.82	0.44
1:A:248:PRO:CG	1:A:276:LEU:HD21	2.43	0.44
2:B:199:LYS:HB2	2:B:199:LYS:HE2	1.78	0.44
1:A:79:PHE:O	1:A:79:PHE:CD2	2.70	0.44
2:B:86:TYR:O	2:B:101:GLY:HA2	2.17	0.44
1:A:79:PHE:C	1:A:79:PHE:CD2	2.91	0.44
3:C:137:PRO:HD2	3:C:199:TRP:CH2	2.52	0.44
1:A:187:LEU:HD13	1:A:191:LEU:HD13	2.00	0.44
1:A:269:LEU:HD13	1:A:269:LEU:HA	1.83	0.44
3:C:81:ILE:O	3:C:81:ILE:HG23	2.17	0.44
1:A:304:ARG:HG3	1:A:304:ARG:O	2.17	0.44
1:A:209:LYS:HD3	1:A:209:LYS:O	2.18	0.44
1:A:34:ASN:HB3	1:A:37:LEU:HD12	1.98	0.44
2:B:43:SER:HB3	3:C:95:TYR:HE1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:VAL:HG23	1:A:53:ILE:HD13	2.00	0.43
2:B:115:VAL:HG12	2:B:207:LYS:HG3	2.00	0.43
2:B:135:PHE:CE2	3:C:191:SER:CB	3.01	0.43
2:B:47:LEU:HD11	2:B:62:PHE:CE1	2.53	0.43
2:B:113:PRO:HG3	2:B:144:ILE:HD11	2.00	0.43
1:A:247:LEU:HD12	1:A:247:LEU:HA	1.80	0.43
3:C:76:SER:OG	3:C:78:THR:HG23	2.19	0.43
2:B:6:GLN:NE2	2:B:102:THR:HG23	2.33	0.43
2:B:11:LEU:HB3	2:B:104:LEU:HD12	2.00	0.43
2:B:4:MET:HE2	2:B:33:LEU:HD23	1.99	0.43
1:A:12:VAL:O	1:A:16:ILE:HD13	2.19	0.43
1:A:70:PHE:C	1:A:70:PHE:CD1	2.92	0.43
3:C:20:ILE:HG21	3:C:118:THR:HG21	2.00	0.43
2:B:124:GLN:HG3	3:C:133:TYR:CE1	2.54	0.43
3:C:116:GLN:H	3:C:116:GLN:HG3	1.36	0.43
1:A:215:PRO:O	1:A:216:LEU:HB3	2.19	0.43
2:B:30:TYR:HE2	2:B:92:TYR:CE1	2.37	0.43
2:B:47:LEU:HD12	2:B:73:LEU:HD11	2.01	0.42
3:C:151:CYS:HB2	3:C:165:TRP:CH2	2.54	0.42
1:A:100:ILE:O	1:A:104:ILE:HG13	2.19	0.42
3:C:149:LEU:N	3:C:192:VAL:O	2.50	0.42
3:C:199:TRP:CG	3:C:200:PRO:HA	2.54	0.42
1:A:59:ALA:HA	1:A:62:PHE:HB2	2.01	0.42
2:B:34:THR:O	2:B:88:CYS:HA	2.18	0.42
3:C:20:ILE:CG2	3:C:118:THR:HG21	2.49	0.42
3:C:23:LYS:HG3	3:C:78:THR:HG22	2.01	0.42
1:A:156:SER:O	1:A:156:SER:OG	2.35	0.42
1:A:88:THR:O	1:A:91:SER:HB2	2.20	0.42
1:A:138:THR:O	1:A:141:LEU:N	2.52	0.41
1:A:265:ALA:HA	1:A:266:PRO:HD3	1.67	0.41
1:A:272:LEU:O	1:A:272:LEU:HD23	2.20	0.41
2:B:47:LEU:HD11	2:B:62:PHE:CD1	2.55	0.41
1:A:202:LEU:HD22	1:A:205:ARG:NH2	2.35	0.41
1:A:34:ASN:OD1	1:A:36:ASN:N	2.49	0.41
1:A:17:ALA:O	1:A:21:ILE:HG13	2.20	0.41
1:A:228:GLU:CG	3:C:102:TYR:HB2	2.51	0.41
2:B:50:ALA:O	2:B:51:ALA:HB3	2.20	0.41
1:A:178:VAL:HG21	1:A:257:PHE:HB3	2.02	0.41
1:A:190:LEU:HD23	1:A:193:MET:CE	2.50	0.41
2:B:32:SER:O	2:B:90:HIS:HA	2.21	0.41
3:C:37:VAL:HG12	3:C:38:LYS:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:VAL:HG21	1:A:257:PHE:CG	2.56	0.41
2:B:6:GLN:HE21	2:B:102:THR:CG2	2.33	0.41
1:A:96:LEU:O	1:A:100:ILE:HD12	2.20	0.41
1:A:225:LEU:O	1:A:228:GLU:N	2.53	0.41
1:A:290:TYR:CD1	1:A:291:ARG:HG2	2.55	0.41
1:A:29:TRP:HZ2	1:A:306:HIS:HD2	1.67	0.41
3:C:137:PRO:HD3	3:C:149:LEU:HD23	2.02	0.41
3:C:154:LYS:HB2	3:C:154:LYS:HE2	1.78	0.41
3:C:6:GLN:NE2	3:C:96:CYS:H	2.18	0.41
2:B:61:ARG:HH21	2:B:82:ASP:CG	2.20	0.41
1:A:187:LEU:O	1:A:191:LEU:HD13	2.21	0.40
2:B:182:THR:O	2:B:183:LYS:C	2.57	0.40
1:A:178:VAL:O	1:A:182:PHE:HB3	2.21	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	292/326 (90%)	266 (91%)	26 (9%)	0	100	100
2	B	210/214 (98%)	201 (96%)	8 (4%)	1 (0%)	32	71
3	C	216/226 (96%)	209 (97%)	7 (3%)	0	100	100
All	All	718/766 (94%)	676 (94%)	41 (6%)	1 (0%)	55	88

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	32	SER

### 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	247/276 (90%)	220 (89%)	27 (11%)	7	30
2	B	183/186 (98%)	159 (87%)	24 (13%)	5	20
3	C	189/195 (97%)	153 (81%)	36 (19%)	2	7
All	All	619/657 (94%)	532 (86%)	87 (14%)	4	18

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	14	LEU
1	A	19	LEU
1	A	21	ILE
1	A	33	LEU
1	A	64	ILE
1	A	70	PHE
1	A	78	LEU
1	A	79	PHE
1	A	80	ILE
1	A	90	SER
1	A	107	ARG
1	A	146	CYS
1	A	161	GLU
1	A	168	PHE
1	A	176	TYR
1	A	212	GLU
1	A	216	LEU
1	A	224	THR
1	A	225	LEU
1	A	234	SER
1	A	251	ILE
1	A	252	ILE
1	A	259	CYS
1	A	269	LEU
1	A	276	LEU

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Mol	Chain	Res	Type
1	A	291	ARG
2	B	5	THR
2	B	7	SER
2	B	18	THR
2	B	22	THR
2	B	47	LEU
2	B	65	SER
2	B	73	LEU
2	B	77	ARG
2	B	85	THR
2	B	95	THR
2	B	102	THR
2	B	106	ILE
2	B	116	SER
2	B	145	ASN
2	B	165	ASP
2	B	175	MET
2	B	178	THR
2	B	181	LEU
2	B	184	ASP
2	B	188	ARG
2	B	191	SER
2	B	194	CYS
2	B	199	LYS
2	B	211	ARG
3	C	7	SER
3	C	11	LEU
3	C	17	SER
3	C	19	LYS
3	C	24	THR
3	C	35	ASN
3	C	40	SER
3	C	54	TYR
3	C	57	SER
3	C	69	THR
3	C	71	THR
3	C	78	THR
3	C	89	GLU
3	C	104	ASP
3	C	112	ASP
3	C	116	GLN
3	C	118	THR

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Mol	Chain	Res	Type
3	C	120	LEU
3	C	123	SER
3	C	127	THR
3	C	146	SER
3	C	148	THR
3	C	152	LEU
3	C	154	LYS
3	C	162	THR
3	C	167	SER
3	C	170	LEU
3	C	171	SER
3	C	188	LEU
3	C	192	VAL
3	C	193	THR
3	C	198	THR
3	C	201	SER
3	C	205	THR
3	C	214	SER
3	C	215	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	GLN
2	B	79	GLN
3	C	6	GLN
3	C	41	HIS
3	C	210	HIS

### 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

1 ligand is 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	ZMA	A	401	-	21,28,28	1.86	3 (14%)	22,39,39	2.96	9 (40%)

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	ZMA	A	401	-	-	0/6/10/10	0/3/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	ZMA	C18-N19	3.97	1.41	1.35
4	A	401	ZMA	C14-N15	4.37	1.43	1.34
4	A	401	ZMA	C11-N10	5.59	1.43	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	ZMA	N17-C20-N19	-10.16	107.85	114.58
4	A	401	ZMA	N12-C11-N13	-3.93	120.28	126.23
4	A	401	ZMA	C9-N10-C11	-2.30	119.49	123.68
4	A	401	ZMA	N13-C14-N16	-2.06	119.52	124.22
4	A	401	ZMA	C9-C8-C7	2.08	117.16	112.81
4	A	401	ZMA	N10-C11-N12	2.10	121.02	117.19
4	A	401	ZMA	C21-C20-N19	2.88	127.24	123.64
4	A	401	ZMA	N15-C14-N16	3.83	120.62	117.95
4	A	401	ZMA	C8-C9-N10	4.61	117.98	111.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	401	ZMA	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	296/326 (90%)	0.34	31 (10%) <b>7</b> <b>2</b>	62, 101, 165, 212	0
2	B	212/214 (99%)	-0.34	0 <b>100</b> <b>100</b>	50, 71, 107, 125	0
3	C	220/226 (97%)	-0.34	1 (0%) <b>90</b> <b>80</b>	48, 71, 101, 141	0
All	All	728/766 (95%)	-0.06	32 (4%) <b>35</b> <b>17</b>	48, 79, 142, 212	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	215	PRO	9.3
1	A	216	LEU	8.6
1	A	217	PRO	7.3
1	A	267	LEU	6.0
1	A	271	TYR	5.3
1	A	219	GLU	5.2
1	A	78	LEU	4.9
1	A	82	CYS	4.7
3	C	27	ASP	4.5
1	A	218	GLY	4.4
1	A	307	VAL	3.8
1	A	111	ARG	3.6
1	A	167	LEU	3.5
1	A	264	HIS	3.5
1	A	214	GLN	3.5
1	A	81	ALA	3.4
1	A	220	ARG	3.3
1	A	166	CYS	3.3
1	A	170	ASP	3.2
1	A	266	PRO	3.1
1	A	172	VAL	3.1
1	A	157	GLN	2.9
1	A	137	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	268	TRP	2.7
1	A	115	LEU	2.7
1	A	165	ALA	2.6
1	A	144	ASN	2.5
1	A	261	ASP	2.4
1	A	110	LEU	2.4
1	A	263	SER	2.4
1	A	156	SER	2.0
1	A	171	VAL	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	ZMA	A	401	25/25	0.88	0.68	2.45	123,130,140,143	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.