



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2016 – 10:32 PM EDT

PDB ID : 5F1C
Title : Crystal structure of an invertebrate P2X receptor from the Gulf Coast tick in the presence of ATP and Zn²⁺ ion at 2.9 Angstroms
Authors : Kasuya, G.; Hattori, M.; Ishitani, R.; Nureki, O.
Deposited on : 2015-11-30
Resolution : 2.90 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0122
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

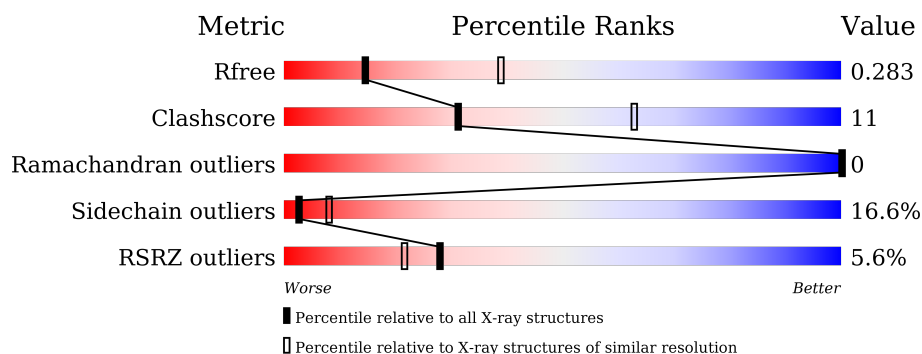
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	358	<div> <div>5%</div> <div> <div></div> <div>66%</div> <div>25%</div> <div>5%</div> <div>.</div> </div> </div>
1	B	358	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>28%</div> <div>5%</div> <div>.</div> </div> </div>
1	C	358	<div> <div>8%</div> <div> <div></div> <div>65%</div> <div>27%</div> <div>.</div> <div>.</div> </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
2	NAG	B	402	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8095 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 Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	0	0
			2569	1646	426	482	15			
1	B	355	Total	C	N	O	S	0	0	0
			2669	1709	442	504	14			
1	C	344	Total	C	N	O	S	0	0	0
			2562	1641	425	482	14			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	GLY	-	expression tag	UNP G3MM57
A	20	SER	-	expression tag	UNP G3MM57
A	21	ARG	-	expression tag	UNP G3MM57
A	22	GLU	-	expression tag	UNP G3MM57
A	23	PHE	-	expression tag	UNP G3MM57
A	171	GLN	ASN	engineered mutation	UNP G3MM57
A	374	LEU	CYS	engineered mutation	UNP G3MM57
B	19	GLY	-	expression tag	UNP G3MM57
B	20	SER	-	expression tag	UNP G3MM57
B	21	ARG	-	expression tag	UNP G3MM57
B	22	GLU	-	expression tag	UNP G3MM57
B	23	PHE	-	expression tag	UNP G3MM57
B	171	GLN	ASN	engineered mutation	UNP G3MM57
B	374	LEU	CYS	engineered mutation	UNP G3MM57
C	19	GLY	-	expression tag	UNP G3MM57
C	20	SER	-	expression tag	UNP G3MM57
C	21	ARG	-	expression tag	UNP G3MM57
C	22	GLU	-	expression tag	UNP G3MM57
C	23	PHE	-	expression tag	UNP G3MM57
C	171	GLN	ASN	engineered mutation	UNP G3MM57
C	374	LEU	CYS	engineered mutation	UNP G3MM57

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).

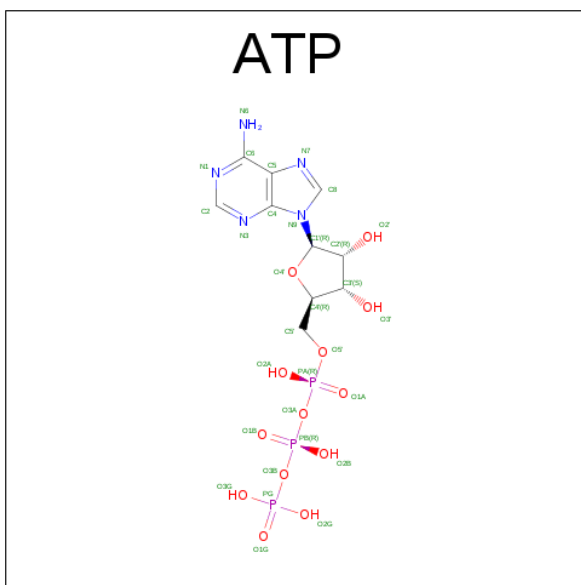


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total	Zn	0	0
			4	4		
3	A	6	Total	Zn	0	0
			6	6		
3	C	3	Total	Zn	0	0
			3	3		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	B	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	C	1	Total 31	C 10	N 5	O 13	P 3	0	0

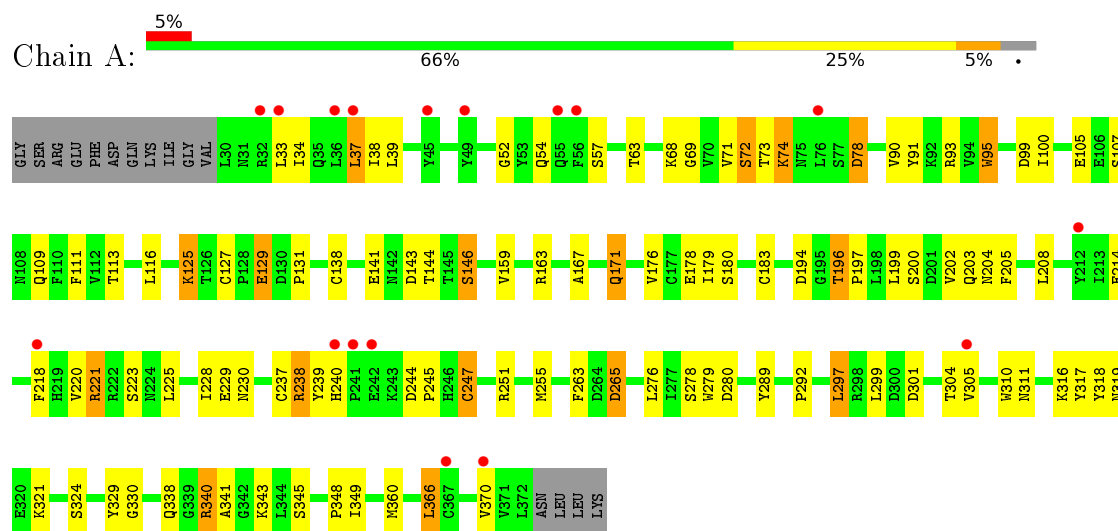
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	38	Total O 38 38	0	0
5	B	50	Total O 50 50	0	0
5	C	31	Total O 31 31	0	0

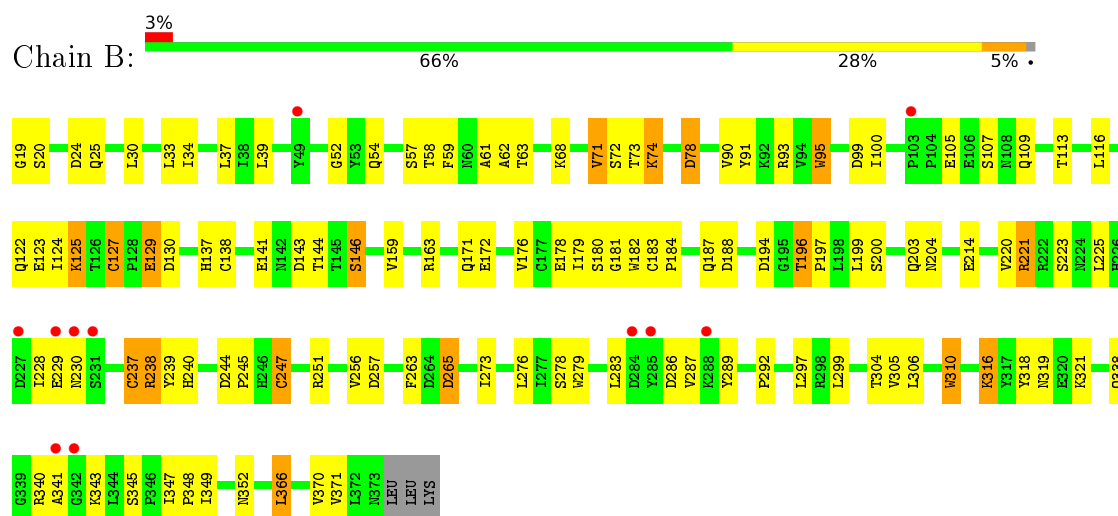
3 Residue-property plots [i](#)

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: Putative uncharacterized protein

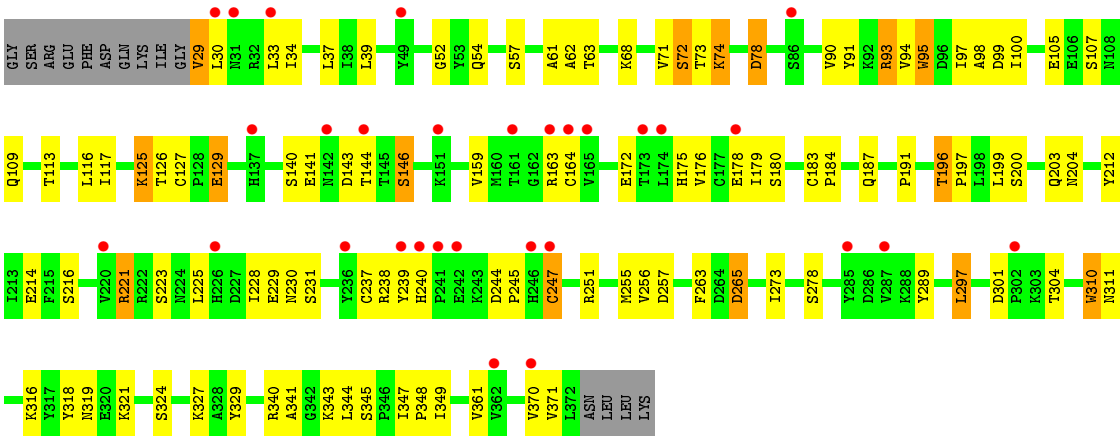


• Molecule 1: Putative uncharacterized protein



• Molecule 1: Putative uncharacterized protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.46Å 139.90Å 202.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.07 – 2.90 43.07 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.07-2.90) 99.1 (43.07-2.89)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.90Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.255 , 0.289 0.249 , 0.283	Depositor DCC
R_{free} test set	1994 reflections (3.81%)	DCC
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 33.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 52452 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8095	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NAG, ATP

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	0.68	3/2628 (0.1%)	0.77	0/3592
1	B	0.68	3/2729 (0.1%)	0.77	0/3729
1	C	0.65	0/2620	0.80	2/3586 (0.1%)
All	All	0.67	6/7977 (0.1%)	0.78	2/10907 (0.0%)

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	1
1	B	0	2
1	C	0	2
All	All	0	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	CYS	CB-SG	-8.18	1.68	1.82
1	B	138	CYS	CB-SG	-7.04	1.70	1.82
1	A	141	GLU	CG-CD	5.87	1.60	1.51
1	B	141	GLU	CG-CD	5.78	1.60	1.51
1	B	127	CYS	CB-SG	-5.69	1.72	1.81
1	A	138	CYS	CB-SG	-5.17	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	344	LEU	CA-CB-CG	5.09	127.01	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	29	VAL	C-N-CA	5.04	134.31	121.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	289	TYR	Peptide
1	B	289	TYR	Peptide
1	B	371	VAL	Peptide
1	C	289	TYR	Peptide
1	C	371	VAL	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	2569	0	2416	60	0
1	B	2669	0	2524	64	0
1	C	2562	0	2399	55	0
2	A	28	0	26	0	0
2	B	28	0	26	0	0
2	C	14	0	13	0	0
3	A	6	0	0	0	0
3	B	4	0	0	0	0
3	C	3	0	0	0	0
4	A	31	0	12	2	0
4	B	31	0	12	2	0
4	C	31	0	12	3	0
5	A	38	0	0	2	0
5	B	50	0	0	6	0
5	C	31	0	0	5	0
All	All	8095	0	7440	167	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 11.

All (167) 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:19:GLY:N	1:B:24:ASP:OD2	2.06	0.87
1:B:34:ILE:HD13	1:B:366:LEU:HD13	1.63	0.80
1:B:214:GLU:OE2	5:B:501:HOH:O	2.02	0.75
1:A:34:ILE:HD13	1:A:366:LEU:HD13	1.68	0.75
1:B:214:GLU:HG3	1:B:221:ARG:HG2	1.69	0.74
1:B:194:ASP:O	5:B:502:HOH:O	2.06	0.74
1:C:214:GLU:HG3	1:C:221:ARG:HG2	1.71	0.72
1:A:125:LYS:HG3	1:A:183:CYS:HB2	1.72	0.72
1:A:71:VAL:HG22	1:A:95:TRP:HB2	1.72	0.71
1:A:214:GLU:HG3	1:A:221:ARG:HG2	1.70	0.71
1:A:73:THR:HG1	1:A:95:TRP:HZ3	1.39	0.70
1:C:318:TYR:O	5:C:501:HOH:O	2.09	0.69
1:C:71:VAL:HG22	1:C:95:TRP:HB2	1.75	0.69
1:B:125:LYS:HG3	1:B:183:CYS:HB2	1.73	0.69
1:B:306:LEU:HD11	1:C:231:SER:HA	1.75	0.68
1:A:69:GLY:N	5:A:501:HOH:O	2.19	0.67
1:C:125:LYS:HG3	1:C:183:CYS:HB2	1.78	0.66
1:B:71:VAL:HG22	1:B:95:TRP:HB2	1.76	0.66
1:B:137:HIS:HE1	5:B:536:HOH:O	1.79	0.65
4:B:407:ATP:C6	1:C:68:LYS:HD3	2.33	0.64
1:C:73:THR:OG1	1:C:95:TRP:HZ3	1.80	0.64
1:C:129:GLU:HG2	1:C:179:ILE:HG12	1.80	0.64
1:A:73:THR:OG1	1:A:95:TRP:HZ3	1.81	0.63
1:A:71:VAL:HG21	1:A:199:LEU:HD22	1.81	0.63
1:B:73:THR:OG1	1:B:95:TRP:HZ3	1.82	0.62
1:A:129:GLU:HG2	1:A:179:ILE:HG12	1.83	0.61
1:B:265:ASP:N	1:B:265:ASP:OD1	2.34	0.59
1:C:73:THR:HG1	1:C:95:TRP:HZ3	1.50	0.59
1:A:299:LEU:HB3	1:B:62:ALA:HB2	1.84	0.58
1:A:95:TRP:HD1	1:A:99:ASP:HB3	1.68	0.58
1:B:129:GLU:HG2	1:B:179:ILE:HG12	1.86	0.57
1:B:163:ARG:HD3	1:B:178:GLU:OE2	2.05	0.57
1:B:52:GLY:O	1:B:348:PRO:HB2	2.05	0.57
1:A:163:ARG:HD3	1:A:178:GLU:OE2	2.04	0.57
1:A:78:ASP:OD1	1:A:78:ASP:N	2.37	0.56
1:C:71:VAL:HG21	1:C:199:LEU:HD22	1.88	0.56
1:A:68:LYS:HD3	4:C:401:ATP:C6	2.40	0.56
1:A:265:ASP:OD1	1:A:265:ASP:N	2.38	0.56
1:C:78:ASP:N	1:C:78:ASP:OD1	2.39	0.55
1:C:265:ASP:OD1	1:C:265:ASP:N	2.38	0.55
4:B:407:ATP:C5	1:C:68:LYS:HD3	2.42	0.55
1:B:73:THR:HG1	1:B:95:TRP:HZ3	1.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ASP:OD1	1:B:78:ASP:N	2.39	0.54
1:C:163:ARG:HD3	1:C:178:GLU:OE2	2.06	0.54
1:C:212:TYR:HE2	5:C:520:HOH:O	1.90	0.54
1:A:34:ILE:HG21	1:A:366:LEU:HD22	1.89	0.54
1:B:220:VAL:HG11	1:B:283:LEU:HD21	1.90	0.54
4:A:409:ATP:C5	1:B:68:LYS:HD3	2.43	0.53
1:B:310:TRP:HH2	1:C:105:GLU:HG3	1.73	0.53
1:C:143:ASP:OD2	1:C:146:SER:OG	2.27	0.53
4:A:409:ATP:C6	1:B:68:LYS:HD3	2.44	0.53
1:A:52:GLY:O	1:A:348:PRO:HB2	2.09	0.53
1:A:100:ILE:CD1	1:A:199:LEU:HD13	2.39	0.53
1:B:143:ASP:OD2	1:B:146:SER:OG	2.27	0.52
1:C:54:GLN:HG2	1:C:343:LYS:C	2.29	0.52
1:A:167:ALA:HB3	1:A:171:GLN:O	2.10	0.52
1:A:239:TYR:HB2	1:A:247:CYS:O	2.09	0.52
1:B:204:ASN:OD1	1:B:251:ARG:NH1	2.43	0.52
1:C:52:GLY:O	1:C:348:PRO:HB2	2.09	0.52
1:B:276:LEU:HD11	1:B:338:GLN:HG2	1.92	0.51
1:C:95:TRP:HD1	1:C:99:ASP:HB3	1.74	0.51
1:C:73:THR:OG1	1:C:91:TYR:O	2.26	0.51
1:A:54:GLN:HG2	1:A:343:LYS:C	2.31	0.51
1:B:95:TRP:HD1	1:B:99:ASP:HB3	1.76	0.51
1:B:237:CYS:O	1:B:238:ARG:NH1	2.45	0.50
1:A:38:ILE:HG21	1:A:360:MET:HG3	1.94	0.50
1:B:100:ILE:CD1	1:B:199:LEU:HD13	2.42	0.50
1:B:54:GLN:HG2	1:B:343:LYS:C	2.32	0.50
1:A:203:GLN:HB3	1:A:263:PHE:CZ	2.47	0.49
1:A:318:TYR:CG	1:C:319:ASN:HA	2.48	0.49
1:B:239:TYR:HB2	1:B:247:CYS:O	2.13	0.49
1:A:297:LEU:HD23	5:A:521:HOH:O	2.12	0.48
1:C:204:ASN:OD1	1:C:251:ARG:NH1	2.46	0.48
1:A:73:THR:OG1	1:A:91:TYR:O	2.32	0.48
1:B:123:GLU:HG3	1:B:125:LYS:HE3	1.94	0.48
1:B:130:ASP:OD1	5:B:503:HOH:O	2.20	0.48
1:B:196:THR:HG22	1:B:197:PRO:HD2	1.95	0.48
1:C:256:VAL:HG22	1:C:273:ILE:HD12	1.96	0.47
1:C:297:LEU:HD23	5:C:516:HOH:O	2.13	0.47
1:B:116:LEU:HD12	1:B:116:LEU:HA	1.64	0.47
1:B:214:GLU:HB3	5:B:501:HOH:O	2.14	0.47
1:A:228:ILE:HA	1:A:229:GLU:HA	1.59	0.47
1:B:34:ILE:HG21	1:B:366:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:LEU:HA	1:C:116:LEU:HD12	1.57	0.47
1:C:117:ILE:HB	1:C:327:LYS:HB3	1.97	0.47
1:C:97:ILE:HD12	1:C:98:ALA:N	2.30	0.47
1:C:140:SER:HA	1:C:175:HIS:CG	2.50	0.47
1:C:72:SER:OG	1:C:74:LYS:HG3	2.15	0.47
1:C:228:ILE:HA	1:C:229:GLU:HA	1.60	0.46
1:A:299:LEU:HD13	1:B:61:ALA:O	2.15	0.46
1:B:71:VAL:HG21	1:B:199:LEU:HD22	1.96	0.46
1:C:191:PRO:HD2	5:C:507:HOH:O	2.15	0.46
1:C:127:CYS:SG	1:C:184:PRO:HA	2.56	0.46
1:A:204:ASN:OD1	1:A:251:ARG:NH1	2.45	0.46
1:B:299:LEU:HB3	1:C:62:ALA:HB2	1.97	0.46
1:C:196:THR:HG22	1:C:197:PRO:HD2	1.97	0.46
1:A:317:TYR:CD1	1:B:316:LYS:HE3	2.51	0.45
1:C:311:ASN:HB3	1:C:329:TYR:CD2	2.52	0.45
1:A:319:ASN:HA	1:B:318:TYR:CG	2.51	0.45
1:B:182:TRP:HB2	5:C:513:HOH:O	2.16	0.45
1:C:73:THR:OG1	1:C:95:TRP:CZ3	2.66	0.45
1:B:122:GLN:NE2	5:B:507:HOH:O	2.43	0.45
1:A:95:TRP:HD1	1:A:99:ASP:CB	2.29	0.45
1:B:113:THR:HG21	1:B:116:LEU:HD13	1.99	0.45
1:A:196:THR:HG22	1:A:197:PRO:HD2	1.98	0.45
1:B:256:VAL:HG22	1:B:273:ILE:HD12	1.99	0.45
1:A:218:PHE:HB2	1:A:220:VAL:HG12	1.98	0.45
1:B:345:SER:O	1:B:349:ILE:HG13	2.17	0.45
1:C:164:CYS:SG	1:C:175:HIS:HB3	2.57	0.45
1:B:228:ILE:HA	1:B:229:GLU:HA	1.57	0.45
1:C:125:LYS:HG3	1:C:183:CYS:CB	2.47	0.44
1:A:143:ASP:OD2	1:A:146:SER:OG	2.36	0.44
1:A:208:LEU:HD22	4:C:401:ATP:C8	2.53	0.44
1:A:57:SER:H	1:A:341:ALA:HB3	1.83	0.44
1:C:239:TYR:HB2	1:C:247:CYS:O	2.17	0.44
1:C:100:ILE:CD1	1:C:199:LEU:HD13	2.48	0.44
1:A:279:TRP:CE2	1:A:292:PRO:HB3	2.52	0.44
1:A:255:MET:HE3	1:A:255:MET:HB2	1.73	0.44
1:A:202:VAL:HA	1:A:205:PHE:CD1	2.53	0.43
1:A:72:SER:OG	1:A:74:LYS:HG3	2.17	0.43
1:C:239:TYR:CE1	1:C:245:PRO:HA	2.52	0.43
1:B:124:ILE:HA	1:B:181:GLY:O	2.18	0.43
1:B:347:ILE:H	1:B:347:ILE:HG13	1.53	0.43
1:A:311:ASN:HB3	1:A:329:TYR:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:SER:OG	1:B:74:LYS:HG3	2.18	0.43
1:A:310:TRP:HH2	1:B:105:GLU:HG3	1.83	0.43
1:C:141:GLU:OE1	1:C:175:HIS:NE2	2.52	0.43
1:B:239:TYR:CE1	1:B:245:PRO:HA	2.54	0.43
1:A:276:LEU:HD11	1:A:338:GLN:HG2	2.01	0.43
1:B:240:HIS:O	1:B:244:ASP:N	2.51	0.43
1:C:93:ARG:NH1	1:C:94:VAL:O	2.36	0.43
1:C:203:GLN:HB3	1:C:263:PHE:CZ	2.53	0.43
1:B:279:TRP:CZ3	1:B:292:PRO:HD3	2.53	0.43
1:A:116:LEU:HA	1:A:116:LEU:HD12	1.65	0.42
1:B:95:TRP:HD1	1:B:99:ASP:CB	2.32	0.42
1:A:240:HIS:O	1:A:244:ASP:N	2.52	0.42
1:B:319:ASN:HA	1:C:318:TYR:CG	2.54	0.42
1:A:111:PHE:CZ	1:A:330:GLY:HA3	2.54	0.42
1:B:57:SER:H	1:B:341:ALA:HB3	1.83	0.42
1:A:34:ILE:HA	1:A:37:LEU:HB2	2.02	0.42
1:B:58:THR:OG1	1:B:59:PHE:N	2.53	0.42
1:C:345:SER:O	1:C:349:ILE:HG13	2.20	0.42
1:A:105:GLU:HG3	1:C:310:TRP:HH2	1.85	0.42
1:C:255:MET:HE3	1:C:255:MET:HB2	1.79	0.42
1:C:126:THR:HA	1:C:179:ILE:O	2.19	0.42
1:A:279:TRP:CD2	1:A:292:PRO:HB3	2.54	0.42
1:A:345:SER:O	1:A:349:ILE:HG13	2.20	0.42
1:A:237:CYS:O	1:A:238:ARG:NH1	2.52	0.42
1:B:286:ASP:OD1	1:B:287:VAL:N	2.52	0.42
1:A:194:ASP:O	1:A:196:THR:OG1	2.38	0.42
1:B:73:THR:OG1	1:B:91:TYR:O	2.35	0.42
1:C:240:HIS:O	1:C:244:ASP:N	2.52	0.42
1:B:299:LEU:HD13	1:C:61:ALA:O	2.20	0.41
1:C:113:THR:HG21	1:C:116:LEU:HD13	2.01	0.41
1:B:203:GLN:HB3	1:B:263:PHE:CZ	2.54	0.41
1:A:239:TYR:CE1	1:A:245:PRO:HA	2.55	0.41
1:C:57:SER:H	1:C:341:ALA:HB3	1.85	0.41
1:A:280:ASP:OD1	1:A:340:ARG:NH1	2.54	0.41
1:C:347:ILE:H	1:C:347:ILE:HG13	1.58	0.41
1:A:113:THR:HG21	1:A:116:LEU:HD13	2.03	0.41
1:A:238:ARG:HA	1:A:238:ARG:HD3	1.90	0.40
1:A:73:THR:OG1	1:A:95:TRP:CZ3	2.68	0.40
1:B:129:GLU:OE1	1:B:130:ASP:N	2.37	0.40
1:A:68:LYS:HD3	4:C:401:ATP:C5	2.56	0.40
1:B:127:CYS:SG	1:B:184:PRO:HA	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:GLY:HA2	1:B:20:SER:HA	1.84	0.40
1:A:131:PRO:HG2	1:A:171:GLN:HG3	2.02	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	341/358 (95%)	327 (96%)	14 (4%)	0	100	100
1	B	353/358 (99%)	339 (96%)	14 (4%)	0	100	100
1	C	342/358 (96%)	328 (96%)	14 (4%)	0	100	100
All	All	1036/1074 (96%)	994 (96%)	42 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	265/317 (84%)	225 (85%)	40 (15%)	3	11
1	B	278/317 (88%)	231 (83%)	47 (17%)	2	8
1	C	262/317 (83%)	215 (82%)	47 (18%)	2	6
All	All	805/951 (85%)	671 (83%)	134 (17%)	3	8

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	37	LEU
1	A	39	LEU
1	A	63	THR
1	A	72	SER
1	A	74	LYS
1	A	78	ASP
1	A	90	VAL
1	A	93	ARG
1	A	95	TRP
1	A	107	SER
1	A	109	GLN
1	A	125	LYS
1	A	129	GLU
1	A	144	THR
1	A	146	SER
1	A	159	VAL
1	A	171	GLN
1	A	176	VAL
1	A	180	SER
1	A	196	THR
1	A	200	SER
1	A	221	ARG
1	A	223	SER
1	A	225	LEU
1	A	230	ASN
1	A	238	ARG
1	A	247	CYS
1	A	265	ASP
1	A	278	SER
1	A	297	LEU
1	A	301	ASP
1	A	304	THR
1	A	305	VAL
1	A	316	LYS
1	A	321	LYS
1	A	324	SER
1	A	340	ARG
1	A	366	LEU
1	A	370	VAL
1	B	25	GLN
1	B	30	LEU

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Mol	Chain	Res	Type
1	B	33	LEU
1	B	37	LEU
1	B	39	LEU
1	B	63	THR
1	B	71	VAL
1	B	74	LYS
1	B	78	ASP
1	B	90	VAL
1	B	93	ARG
1	B	95	TRP
1	B	107	SER
1	B	109	GLN
1	B	125	LYS
1	B	129	GLU
1	B	144	THR
1	B	146	SER
1	B	159	VAL
1	B	171	GLN
1	B	172	GLU
1	B	176	VAL
1	B	180	SER
1	B	187	GLN
1	B	188	ASP
1	B	196	THR
1	B	200	SER
1	B	221	ARG
1	B	223	SER
1	B	225	LEU
1	B	230	ASN
1	B	237	CYS
1	B	238	ARG
1	B	247	CYS
1	B	257	ASP
1	B	265	ASP
1	B	278	SER
1	B	297	LEU
1	B	304	THR
1	B	305	VAL
1	B	310	TRP
1	B	316	LYS
1	B	321	LYS
1	B	340	ARG

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Mol	Chain	Res	Type
1	B	352	ASN
1	B	366	LEU
1	B	370	VAL
1	C	29	VAL
1	C	30	LEU
1	C	33	LEU
1	C	34	ILE
1	C	37	LEU
1	C	39	LEU
1	C	63	THR
1	C	72	SER
1	C	74	LYS
1	C	78	ASP
1	C	90	VAL
1	C	93	ARG
1	C	95	TRP
1	C	107	SER
1	C	109	GLN
1	C	125	LYS
1	C	129	GLU
1	C	144	THR
1	C	146	SER
1	C	159	VAL
1	C	172	GLU
1	C	176	VAL
1	C	180	SER
1	C	187	GLN
1	C	196	THR
1	C	200	SER
1	C	216	SER
1	C	221	ARG
1	C	223	SER
1	C	225	LEU
1	C	230	ASN
1	C	237	CYS
1	C	238	ARG
1	C	247	CYS
1	C	257	ASP
1	C	265	ASP
1	C	278	SER
1	C	297	LEU
1	C	301	ASP

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Mol	Chain	Res	Type
1	C	304	THR
1	C	310	TRP
1	C	316	LYS
1	C	321	LYS
1	C	324	SER
1	C	340	ARG
1	C	361	VAL
1	C	370	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	166	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 21 ligands modelled in this entry, 13 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	NAG	A	401	1	14,14,15	0.63	0	15,19,21	2.72	6 (40%)
2	NAG	A	402	1	14,14,15	0.71	0	15,19,21	1.21	1 (6%)
4	ATP	A	409	3	26,33,33	1.13	2 (7%)	26,52,52	1.89	9 (34%)
2	NAG	B	401	1	14,14,15	0.69	0	15,19,21	1.39	2 (13%)
2	NAG	B	402	1	14,14,15	1.00	2 (14%)	15,19,21	1.51	3 (20%)
4	ATP	B	407	3	26,33,33	1.14	2 (7%)	26,52,52	2.07	7 (26%)
4	ATP	C	401	3	26,33,33	1.20	3 (11%)	26,52,52	2.04	6 (23%)
2	NAG	C	402	1	14,14,15	0.55	0	15,19,21	1.38	2 (13%)

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	NAG	A	401	1	-	0/6/23/26	0/1/1/1
2	NAG	A	402	1	-	0/6/23/26	0/1/1/1
4	ATP	A	409	3	-	0/18/38/38	0/3/3/3
2	NAG	B	401	1	-	0/6/23/26	0/1/1/1
2	NAG	B	402	1	-	0/6/23/26	0/1/1/1
4	ATP	B	407	3	-	0/18/38/38	0/3/3/3
4	ATP	C	401	3	-	0/18/38/38	0/3/3/3
2	NAG	C	402	1	-	0/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	401	ATP	C2'-C1'	-2.07	1.50	1.53
4	C	401	ATP	O4'-C4'	-2.03	1.40	1.45
2	B	402	NAG	C3-C2	2.02	1.57	1.52
4	B	407	ATP	C2-N3	2.09	1.35	1.32
4	A	409	ATP	C8-N7	2.13	1.38	1.34
2	B	402	NAG	C1-C2	2.28	1.55	1.52
4	A	409	ATP	C5-C4	3.59	1.48	1.40
4	B	407	ATP	C5-C4	3.64	1.48	1.40
4	C	401	ATP	C5-C4	3.75	1.49	1.40

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAG	C2-N2-C7	-7.18	113.77	123.11
4	B	407	ATP	N3-C2-N1	-6.58	123.70	128.87
4	C	401	ATP	N3-C2-N1	-5.90	124.23	128.87
4	A	409	ATP	N3-C2-N1	-5.36	124.66	128.87
4	C	401	ATP	O4'-C1'-N9	-3.29	101.89	108.11
4	B	407	ATP	O3'-C3'-C2'	-3.00	102.14	111.86
2	B	401	NAG	C4-C3-C2	-2.81	106.98	111.34
4	B	407	ATP	C2'-C1'-N9	-2.80	105.97	113.47
4	A	409	ATP	O3'-C3'-C4'	-2.66	103.06	111.01
2	A	401	NAG	C6-C5-C4	-2.40	106.97	112.99
4	A	409	ATP	C1'-N9-C4	-2.35	124.18	126.81
2	B	402	NAG	O7-C7-C8	-2.24	117.94	122.07
2	A	401	NAG	O3-C3-C4	-2.18	105.44	110.36
2	B	402	NAG	C2-N2-C7	-2.01	120.49	123.11
4	B	407	ATP	C2'-C3'-C4'	2.05	106.82	102.64
4	A	409	ATP	C2'-C3'-C4'	2.06	106.86	102.64
4	A	409	ATP	O2B-PB-O3A	2.07	114.12	105.27
4	A	409	ATP	O3G-PG-O1G	2.07	117.38	110.63
2	A	401	NAG	O3-C3-C2	2.07	113.81	109.37
2	C	402	NAG	O5-C5-C6	2.07	111.78	107.34
4	C	401	ATP	O2G-PG-O1G	2.28	118.08	110.63
2	C	402	NAG	C1-O5-C5	2.39	115.66	112.14
2	A	401	NAG	O5-C5-C4	2.47	114.22	110.13
4	A	409	ATP	O3G-PG-O2G	2.50	116.63	107.44
2	B	401	NAG	C1-O5-C5	2.56	115.90	112.14
2	A	402	NAG	C1-O5-C5	2.60	115.96	112.14
4	B	407	ATP	C2-N1-C6	2.61	123.42	118.77
4	C	401	ATP	C2'-C3'-C4'	2.72	108.21	102.64
4	A	409	ATP	O2A-PA-O3A	2.81	117.31	105.27
4	B	407	ATP	N6-C6-N1	2.90	123.38	118.52
2	B	402	NAG	C4-C3-C2	3.11	116.16	111.34
4	A	409	ATP	C4'-O4'-C1'	3.11	112.94	109.64
4	C	401	ATP	O2B-PB-O3A	3.34	119.57	105.27
4	B	407	ATP	O2A-PA-O3A	3.44	119.99	105.27
4	C	401	ATP	C4'-O4'-C1'	3.52	113.38	109.64
2	A	401	NAG	C1-O5-C5	5.28	119.90	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	409	ATP	2	0
4	B	407	ATP	2	0
4	C	401	ATP	3	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	343/358 (95%)	0.01	17 (4%)	32 26	30, 61, 111, 145	0
1	B	355/358 (99%)	0.06	11 (3%)	52 45	29, 60, 108, 143	0
1	C	344/358 (96%)	0.31	30 (8%)	13 8	32, 64, 110, 144	0
All	All	1042/1074 (97%)	0.13	58 (5%)	28 21	29, 61, 110, 145	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	241	PRO	5.4
1	A	36	LEU	4.8
1	B	231	SER	4.5
1	C	246	HIS	4.3
1	C	239	TYR	3.9
1	A	32	ARG	3.9
1	B	230	ASN	3.8
1	A	33	LEU	3.7
1	C	163	ARG	3.6
1	C	362	VAL	3.6
1	C	173	THR	3.5
1	C	49	TYR	3.4
1	A	49	TYR	3.4
1	B	342	GLY	3.3
1	A	367	CYS	3.2
1	C	31	ASN	3.2
1	A	242	GLU	3.1
1	C	242	GLU	3.0
1	B	227	ASP	3.0
1	C	144	THR	2.9
1	C	240	HIS	2.9
1	C	137	HIS	2.7
1	C	161	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	37	LEU	2.5
1	C	30	LEU	2.5
1	C	165	VAL	2.4
1	B	285	TYR	2.4
1	C	174	LEU	2.4
1	C	370	VAL	2.3
1	A	76	LEU	2.3
1	C	178	GLU	2.3
1	C	220	VAL	2.3
1	B	341	ALA	2.3
1	A	370	VAL	2.3
1	C	86	SER	2.3
1	C	287	VAL	2.2
1	A	240	HIS	2.2
1	B	49	TYR	2.2
1	B	229	GLU	2.2
1	C	302	PRO	2.2
1	B	288	LYS	2.2
1	C	226	HIS	2.2
1	A	55	GLN	2.2
1	C	151	LYS	2.2
1	C	241	PRO	2.2
1	A	45	TYR	2.2
1	C	247	CYS	2.2
1	A	305	VAL	2.2
1	B	103	PRO	2.1
1	C	236	TYR	2.1
1	C	164	CYS	2.1
1	C	142	ASN	2.1
1	A	56	PHE	2.0
1	A	218	PHE	2.0
1	C	33	LEU	2.0
1	A	212	TYR	2.0
1	C	285	TYR	2.0
1	B	284	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
2	NAG	B	402	14/15	0.93	0.29	3.11	38,60,82,87	0
2	NAG	C	402	14/15	0.95	0.24	1.60	42,55,65,69	0
2	NAG	A	401	14/15	0.93	0.20	1.27	45,87,112,133	0
3	ZN	A	406	1/1	0.99	0.23	-0.34	70,70,70,70	0
4	ATP	A	409	31/31	0.97	0.15	-0.67	27,34,44,54	0
3	ZN	B	404	1/1	0.98	0.21	-0.75	66,66,66,66	0
2	NAG	B	401	14/15	0.96	0.15	-0.87	28,45,60,72	0
4	ATP	C	401	31/31	0.97	0.15	-0.90	30,55,65,80	0
3	ZN	A	407	1/1	0.96	0.21	-1.00	66,66,66,66	0
4	ATP	B	407	31/31	0.98	0.14	-1.22	27,36,44,52	0
3	ZN	A	403	1/1	0.98	0.21	-	52,52,52,52	0
3	ZN	B	405	1/1	0.89	0.05	-	126,126,126,126	0
3	ZN	B	403	1/1	0.99	0.18	-	50,50,50,50	0
2	NAG	A	402	14/15	0.74	0.36	-	65,98,122,123	0
3	ZN	A	404	1/1	1.00	0.10	-	38,38,38,38	0
3	ZN	A	408	1/1	0.93	0.05	-	125,125,125,125	0
3	ZN	C	404	1/1	0.88	0.07	-	105,105,105,105	0
3	ZN	B	406	1/1	0.99	0.14	-	58,58,58,58	0
3	ZN	C	405	1/1	0.96	0.07	-	115,115,115,115	0
3	ZN	A	405	1/1	0.99	0.17	-	38,38,38,38	0
3	ZN	C	403	1/1	0.98	0.20	-	65,65,65,65	0

6.5 Other polymers ⓘ

There are no such residues in this entry.