



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:21 AM GMT

PDB ID : 3AH8
Title : Structure of heterotrimeric G protein Galpha-q beta gamma in complex with an inhibitor YM-254890
Authors : Nishimura, A.; Kitano, K.; Takasaki, J.; Taniguchi, M.; Mizuno, N.; Tago, K.; Hakoshima, T.; Itoh, H.
Deposited on : 2010-04-20
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 (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

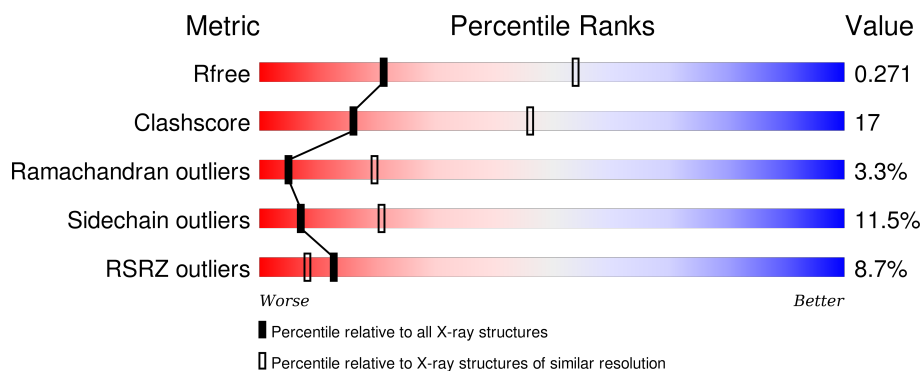
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	355	
2	B	340	
3	G	78	
4	Y	9	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	HF2	Y	6	-	-	X	-
4	MAA	Y	9	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5827 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 Guanine nucleotide-binding protein G(i) subunit alpha-1/Guanine nucleotide-binding protein G(q) subunit alpha chimeric protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2818	1788	483	534	13			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	GLY	-	EXPRESSION TAG	UNP P10824
A	6	ALA	-	EXPRESSION TAG	UNP P10824
A	7	MET	-	EXPRESSION TAG	UNP P10824
A	35	ARG	-	LINKER	UNP P10824
A	36	SER	-	LINKER	UNP P10824

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	330	Total	C	N	O	S	0	0	0
			2530	1562	454	493	21			

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	50	Total	C	N	O	S	0	0	0
			383	239	67	74	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1	GLY	-	EXPRESSION TAG	UNP P63212
G	2	ALA	-	EXPRESSION TAG	UNP P63212

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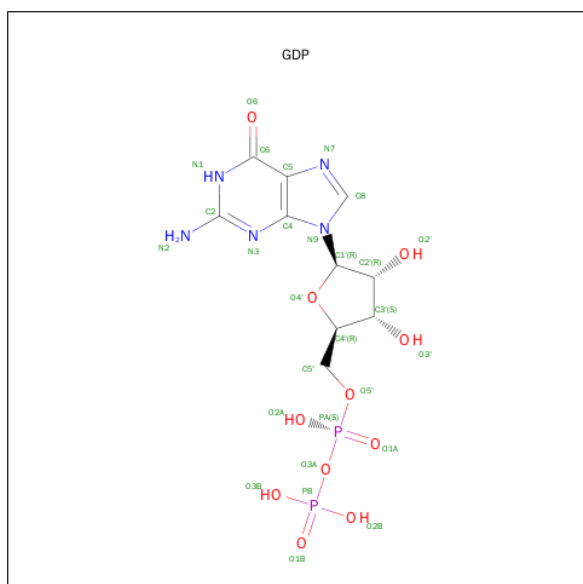
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Chain	Residue	Modelled	Actual	Comment	Reference
G	3	MET	-	EXPRESSION TAG	UNP P63212
G	4	ASP	-	EXPRESSION TAG	UNP P63212
G	5	PRO	-	EXPRESSION TAG	UNP P63212
G	6	GLU	-	EXPRESSION TAG	UNP P63212
G	7	PHE	-	EXPRESSION TAG	UNP P63212
G	75	SER	CYS	ENGINEERED MUTATION	UNP P63212

- Molecule 4 is a protein called YM-254890.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	Y	9	Total	C	N	O	0	0	0
			68	46	7	15			

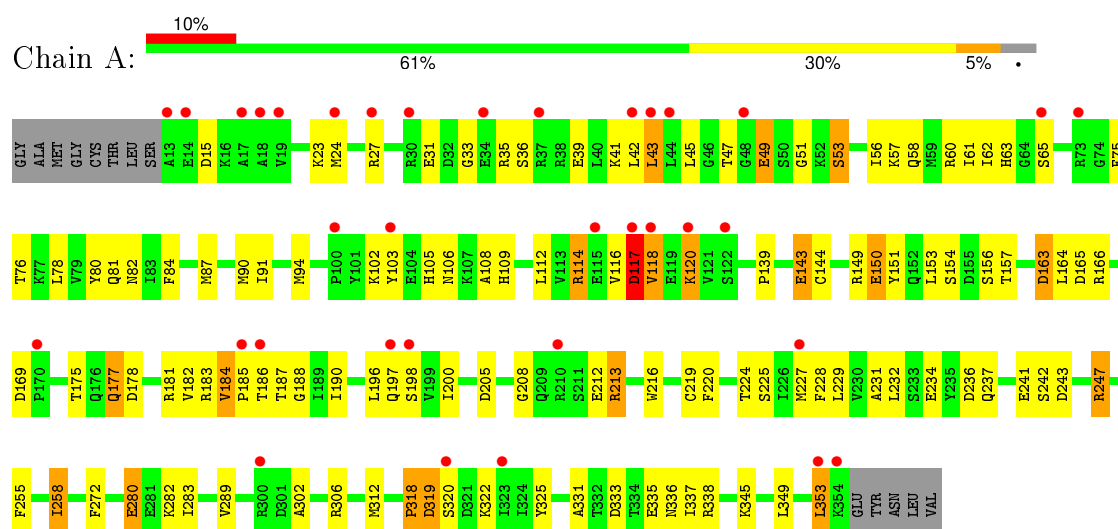
- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



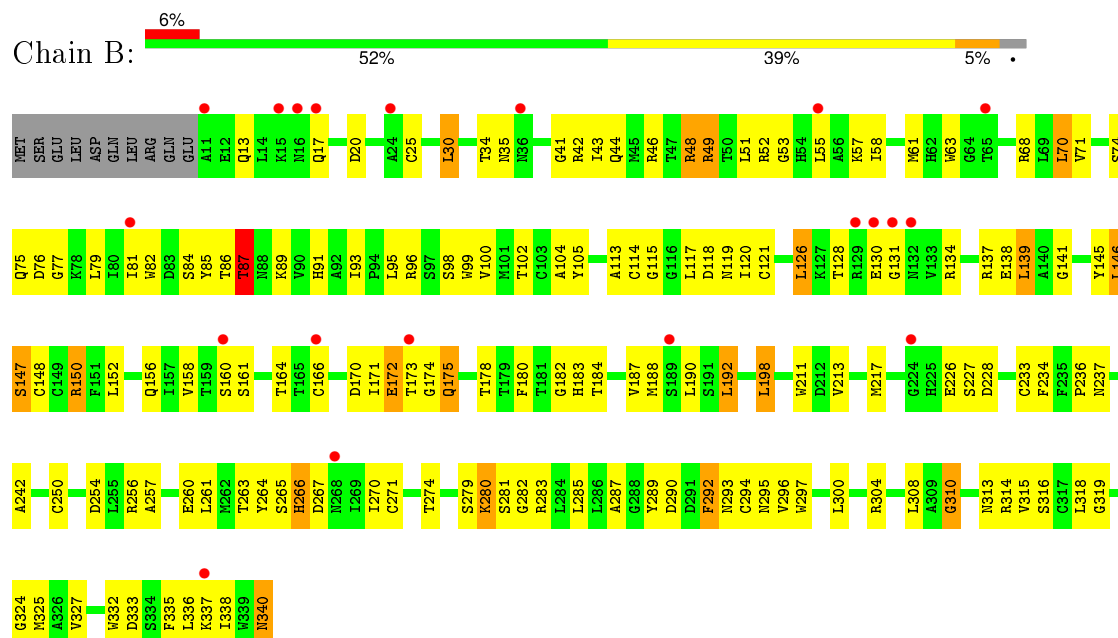
3 Residue-property plots

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.

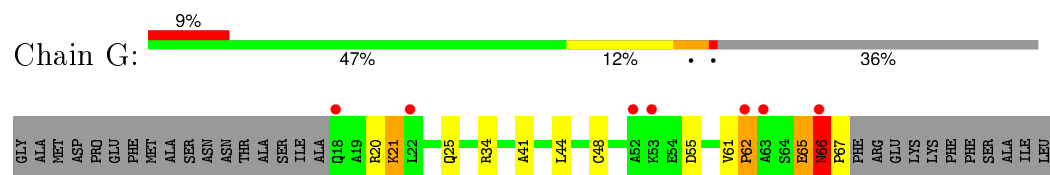
- Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-1/Guanine nucleotide-binding protein G(q) subunit alpha chimeric protein



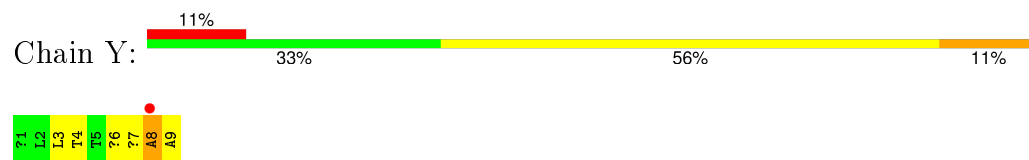
- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



- Molecule 4: YM-254890



4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	173.34Å 173.34Å 60.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 19.65 – 2.90	Depositor EDS
% Data completeness (in resolution range)	94.1 (20.00-2.90) 94.1 (19.65-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.93Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.259 , 0.315 0.284 , 0.271	Depositor DCC
R_{free} test set	975 reflections (5.41%)	DCC
Wilson B-factor (Å ²)	77.9	Xtriage
Anisotropy	1.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.5	EDS
Estimated twinning fraction	0.026 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 19009 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5827	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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: OTH, GDP, ACE, DAM, HF2, HL2, MAA, THC

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	0.45	1/2874 (0.0%)	0.60	1/3878 (0.0%)
2	B	0.39	0/2577	0.61	0/3494
3	G	1.20	4/388 (1.0%)	0.68	1/524 (0.2%)
4	Y	0.35	0/4	0.67	0/4
All	All	0.51	5/5843 (0.1%)	0.61	2/7900 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	66	ASN	CG-ND2	15.97	1.72	1.32
3	G	65	GLU	CD-OE2	-9.09	1.15	1.25
1	A	15	ASP	CG-OD2	8.86	1.45	1.25
3	G	66	ASN	CB-CG	6.79	1.66	1.51
3	G	65	GLU	CG-CD	6.30	1.61	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	ASP	CB-CG-OD2	-8.25	110.88	118.30
3	G	66	ASN	CB-CG-ND2	-5.26	104.07	116.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2818	0	2785	88	0
2	B	2530	0	2438	89	0
3	G	383	0	393	15	0
4	Y	68	0	68	14	0
5	A	28	0	12	4	0
All	All	5827	0	5696	195	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 17.

All (195) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:4:OTH:OG1	4:Y:4:OTH:C22	1.67	1.40
3:G:66:ASN:CG	3:G:66:ASN:ND2	1.72	1.39
1:A:186:THR:HB	1:A:190:ILE:HD11	1.34	1.04
1:A:335:GLU:HG2	1:A:338:ARG:HH21	1.20	1.02
2:B:48:ARG:HD2	2:B:340:ASN:HB2	1.48	0.95
2:B:44:GLN:HE21	2:B:46:ARG:HH12	1.04	0.94
4:Y:4:OTH:CB	4:Y:4:OTH:C22	2.50	0.88
2:B:86:THR:O	2:B:87:THR:HB	1.76	0.85
2:B:294:CYS:HB3	2:B:308:LEU:HB2	1.61	0.82
2:B:198:LEU:HA	2:B:213:VAL:HG23	1.63	0.79
1:A:335:GLU:HG2	1:A:338:ARG:NH2	1.98	0.79
2:B:81:ILE:HD13	2:B:91:HIS:HB2	1.65	0.77
1:A:23:LYS:HE2	1:A:27:ARG:HH22	1.49	0.77
2:B:147:SER:OG	2:B:188:MET:HA	1.86	0.76
1:A:255:PHE:HA	1:A:258:ILE:HG22	1.67	0.76
4:Y:6:HF2:CG	4:Y:7:DAM:HM1	2.16	0.75
2:B:48:ARG:HD2	2:B:340:ASN:CB	2.17	0.74
1:A:177:GLN:O	1:A:181:ARG:HG3	1.86	0.74
2:B:95:LEU:HD13	2:B:100:VAL:HG11	1.69	0.73
1:A:53:SER:O	1:A:57:LYS:HG3	1.90	0.72
1:A:190:ILE:HB	1:A:205:ASP:HB3	1.73	0.71
2:B:44:GLN:HE21	2:B:46:ARG:NH1	1.85	0.70
1:A:280:GLU:HA	1:A:283:ILE:HG22	1.73	0.70
1:A:318:PRO:O	1:A:319:ASP:HB3	1.91	0.69
1:A:36:SER:O	1:A:39:GLU:HG2	1.93	0.68
4:Y:6:HF2:CD2	4:Y:7:DAM:HM1	2.23	0.68
1:A:33:GLY:HA3	2:B:55:LEU:HD13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:LEU:HB2	2:B:336:LEU:HB2	1.75	0.67
1:A:75:PHE:HA	1:A:78:LEU:HD12	1.77	0.67
1:A:103:TYR:HB2	1:A:106:ASN:HD22	1.60	0.66
1:A:229:LEU:HG	1:A:272:PHE:HB2	1.78	0.66
1:A:45:LEU:HD13	1:A:258:ILE:HD11	1.77	0.66
1:A:280:GLU:CB	1:A:302:ALA:HB2	2.26	0.66
2:B:44:GLN:NE2	2:B:46:ARG:HH12	1.87	0.66
4:Y:8:ALA:N	4:Y:9:MAA:HA	2.11	0.65
1:A:280:GLU:HB3	1:A:302:ALA:HB2	1.78	0.65
2:B:25:CYS:SG	3:G:34:ARG:HG2	2.39	0.62
2:B:271:CYS:HB2	2:B:290:ASP:HB2	1.80	0.61
2:B:237:ASN:HD21	3:G:44:LEU:HD22	1.65	0.61
1:A:87:MET:O	1:A:91:ILE:HG12	2.00	0.61
2:B:48:ARG:HH11	2:B:340:ASN:HB3	1.64	0.60
1:A:62:ILE:HB	1:A:63:HIS:HD2	1.65	0.60
4:Y:4:OTH:C22	4:Y:4:OTH:HB	2.30	0.60
2:B:198:LEU:HB2	2:B:211:TRP:O	2.01	0.60
2:B:233:CYS:HB3	2:B:242:ALA:HB3	1.82	0.60
1:A:255:PHE:O	1:A:258:ILE:HG22	2.03	0.59
2:B:265:SER:O	2:B:266:HIS:HB2	2.03	0.59
2:B:30:LEU:HD23	3:G:41:ALA:HB1	1.85	0.59
2:B:115:GLY:HA3	2:B:146:LEU:HD13	1.85	0.59
2:B:283:ARG:HD3	2:B:300:LEU:HD12	1.85	0.58
3:G:66:ASN:CB	3:G:66:ASN:ND2	2.67	0.58
1:A:60:ARG:HG2	1:A:65:SER:O	2.04	0.58
2:B:117:LEU:HD23	2:B:145:TYR:HB3	1.84	0.58
2:B:289:TYR:HB2	2:B:293:ASN:O	2.04	0.58
1:A:213:ARG:HD3	1:A:216:TRP:CZ2	2.38	0.58
1:A:151:TYR:CE2	1:A:153:LEU:HB2	2.39	0.58
1:A:31:GLU:HB3	1:A:35:ARG:NH2	2.19	0.57
1:A:102:LYS:HB3	1:A:139:PRO:HD2	1.86	0.57
1:A:318:PRO:O	1:A:319:ASP:CB	2.53	0.56
1:A:237:GLN:HB3	1:A:247:ARG:HG3	1.87	0.56
4:Y:6:HF2:O	4:Y:7:DAM:C	2.50	0.56
1:A:186:THR:OG1	1:A:208:GLY:HA3	2.06	0.56
1:A:213:ARG:HA	1:A:216:TRP:CE2	2.40	0.56
1:A:149:ARG:O	1:A:237:GLN:HA	2.06	0.56
2:B:254:ASP:HB2	2:B:261:LEU:HD11	1.87	0.56
1:A:219:CYS:O	2:B:99:TRP:HZ3	1.88	0.55
1:A:103:TYR:HB2	1:A:106:ASN:ND2	2.21	0.55
1:A:84:PHE:CD1	1:A:116:VAL:HG11	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:ARG:HG3	2:B:192:LEU:HD22	1.89	0.54
2:B:52:ARG:HG3	2:B:335:PHE:HE1	1.73	0.54
1:A:151:TYR:HE2	1:A:153:LEU:HB2	1.72	0.54
1:A:43:LEU:HD13	1:A:45:LEU:HD11	1.90	0.54
1:A:49:GLU:HG3	5:A:1:GDP:H5"	1.90	0.53
1:A:49:GLU:N	5:A:1:GDP:O2B	2.40	0.53
1:A:94:MET:HE3	1:A:144:CYS:HB2	1.91	0.53
1:A:42:LEU:HB3	1:A:227:MET:CE	2.39	0.53
2:B:274:THR:OG1	2:B:315:VAL:O	2.18	0.53
2:B:325:MET:O	2:B:340:ASN:ND2	2.39	0.52
1:A:57:LYS:O	1:A:61:ILE:HG13	2.08	0.52
2:B:102:THR:HG21	2:B:148:CYS:HA	1.91	0.52
2:B:254:ASP:HB3	2:B:257:ALA:HB3	1.92	0.52
3:G:62:PRO:HB2	3:G:65:GLU:OE1	2.09	0.52
1:A:60:ARG:NH1	4:Y:6:HF2:O	2.44	0.51
2:B:160:SER:HB2	2:B:187:VAL:CG1	2.41	0.50
2:B:180:PHE:HB3	2:B:211:TRP:CE3	2.46	0.50
2:B:77:GLY:HA2	2:B:98:SER:HA	1.93	0.50
1:A:302:ALA:O	1:A:306:ARG:HG3	2.12	0.50
1:A:349:LEU:O	1:A:353:LEU:HB2	2.11	0.50
2:B:260:GLU:OE2	2:B:263:THR:OG1	2.30	0.50
2:B:121:CYS:HB3	2:B:139:LEU:HB2	1.93	0.50
1:A:186:THR:HB	1:A:190:ILE:CD1	2.24	0.50
2:B:327:VAL:O	2:B:338:ILE:HA	2.12	0.50
2:B:290:ASP:O	2:B:314:ARG:HB3	2.12	0.49
2:B:43:ILE:HG21	2:B:296:VAL:HG11	1.93	0.49
2:B:71:VAL:HG12	2:B:81:ILE:HG13	1.92	0.49
1:A:187:THR:HG22	4:Y:3:HL2:HD1	1.94	0.49
2:B:310:GLY:O	2:B:337:LYS:NZ	2.39	0.49
2:B:152:LEU:HD11	2:B:158:VAL:HG23	1.94	0.49
2:B:270:ILE:HG22	2:B:270:ILE:O	2.13	0.49
3:G:20:ARG:O	3:G:21:LYS:HB2	2.13	0.49
1:A:325:TYR:N	1:A:325:TYR:CD2	2.81	0.49
1:A:255:PHE:HA	1:A:258:ILE:CG2	2.40	0.49
1:A:280:GLU:HB2	1:A:302:ALA:HB2	1.95	0.48
1:A:31:GLU:HB3	1:A:35:ARG:HH21	1.78	0.48
2:B:63:TRP:HE1	2:B:319:GLY:C	2.17	0.48
1:A:196:LEU:HD22	1:A:345:LYS:HD2	1.94	0.48
2:B:250:CYS:HB2	2:B:264:TYR:HB2	1.94	0.47
1:A:186:THR:CB	1:A:190:ILE:HD11	2.24	0.47
2:B:237:ASN:ND2	3:G:44:LEU:HD22	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ALA:HB3	1:A:234:GLU:HB2	1.96	0.47
2:B:173:THR:HG23	2:B:175:GLN:HB2	1.97	0.47
2:B:166:CYS:SG	2:B:187:VAL:HG11	2.55	0.47
2:B:79:LEU:HB3	2:B:93:ILE:HB	1.96	0.47
2:B:120:ILE:HG23	2:B:138:GLU:O	2.15	0.47
2:B:285:LEU:HB3	2:B:297:TRP:HB2	1.97	0.47
1:A:236:ASP:OD2	1:A:282:LYS:NZ	2.47	0.47
1:A:42:LEU:HB3	1:A:227:MET:HE1	1.97	0.46
2:B:126:LEU:O	2:B:128:THR:HG23	2.15	0.46
1:A:23:LYS:HE2	1:A:27:ARG:NH2	2.24	0.46
2:B:281:SER:HB3	3:G:55:ASP:HB2	1.97	0.46
2:B:104:ALA:HB3	2:B:113:ALA:HB3	1.97	0.46
2:B:171:ILE:O	2:B:172:GLU:C	2.54	0.46
1:A:232:LEU:C	1:A:234:GLU:H	2.18	0.46
3:G:66:ASN:O	3:G:67:PRO:O	2.34	0.46
2:B:48:ARG:NH1	2:B:340:ASN:HB3	2.29	0.46
4:Y:9:MAA:HM3	4:Y:9:MAA:O	2.16	0.46
1:A:280:GLU:HA	1:A:283:ILE:CG2	2.42	0.46
2:B:121:CYS:HB2	2:B:146:LEU:HD11	1.98	0.46
3:G:61:VAL:O	3:G:62:PRO:O	2.34	0.46
2:B:74:SER:C	2:B:76:ASP:H	2.18	0.46
1:A:43:LEU:HD22	1:A:45:LEU:HG	1.96	0.45
2:B:266:HIS:ND1	2:B:267:ASP:O	2.44	0.45
2:B:333:ASP:OD1	2:B:335:PHE:HB2	2.16	0.45
2:B:226:GLU:O	2:B:227:SER:HB2	2.16	0.45
1:A:183:ARG:O	1:A:185:PRO:HD3	2.16	0.45
1:A:117:ASP:O	1:A:118:VAL:C	2.55	0.45
2:B:52:ARG:CG	2:B:335:PHE:HE1	2.29	0.45
1:A:78:LEU:HD22	1:A:184:VAL:HA	1.98	0.45
2:B:280:LYS:CG	2:B:324:GLY:HA3	2.46	0.45
1:A:156:SER:HB3	1:A:181:ARG:HE	1.82	0.45
2:B:150:ARG:HG2	2:B:190:LEU:HD11	1.97	0.45
1:A:109:HIS:HA	1:A:112:LEU:HD22	1.98	0.45
2:B:292:PHE:CD1	2:B:313:ASN:C	2.90	0.45
2:B:152:LEU:HD13	2:B:156:GLN:HB3	1.98	0.44
5:A:1:GDP:O3B	5:A:1:GDP:O1A	2.36	0.44
3:G:66:ASN:N	3:G:67:PRO:CD	2.81	0.44
1:A:51:GLY:HA2	5:A:1:GDP:O2A	2.17	0.44
2:B:256:ARG:HH12	3:G:44:LEU:HD21	1.83	0.44
1:A:149:ARG:HA	1:A:237:GLN:NE2	2.32	0.44
2:B:183:HIS:CD2	2:B:187:VAL:HG22	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:340:ASN:HD22	2:B:340:ASN:HA	1.55	0.44
4:Y:8:ALA:H	4:Y:9:MAA:HA	1.83	0.43
2:B:158:VAL:HG12	2:B:190:LEU:HD22	1.99	0.43
1:A:331:ALA:HA	1:A:337:ILE:HD11	1.99	0.43
2:B:160:SER:HB2	2:B:187:VAL:HG11	2.00	0.43
1:A:56:ILE:HD11	1:A:205:ASP:HB2	1.98	0.43
1:A:163:ASP:O	1:A:164:LEU:C	2.56	0.43
2:B:82:TRP:CZ3	2:B:89:LYS:HE3	2.53	0.43
2:B:138:GLU:O	2:B:139:LEU:C	2.57	0.43
1:A:333:ASP:HB3	1:A:336:ASN:HB3	2.01	0.43
2:B:49:ARG:HD2	2:B:84:SER:O	2.18	0.43
1:A:108:ALA:O	1:A:112:LEU:HD13	2.19	0.42
1:A:114:ARG:HH11	1:A:114:ARG:HB2	1.85	0.42
1:A:196:LEU:O	1:A:198:SER:N	2.53	0.42
1:A:82:ASN:HD21	1:A:183:ARG:H	1.67	0.42
1:A:154:SER:O	1:A:157:THR:HG23	2.20	0.42
4:Y:4:OTH:H24	4:Y:6:HF2:HD2	2.02	0.42
2:B:283:ARG:HA	2:B:283:ARG:HD2	1.91	0.42
2:B:79:LEU:HD22	2:B:93:ILE:HG13	2.01	0.42
4:Y:9:MAA:CM	4:Y:9:MAA:O	2.67	0.41
2:B:34:THR:HG21	2:B:300:LEU:HD22	2.02	0.41
4:Y:6:HF2:HA	4:Y:6:HF2:HD2	1.67	0.41
1:A:75:PHE:O	1:A:76:THR:C	2.58	0.41
1:A:139:PRO:O	1:A:143:GLU:HB3	2.20	0.41
1:A:82:ASN:HD21	1:A:183:ARG:N	2.18	0.41
1:A:241:GLU:C	1:A:243:ASP:H	2.23	0.41
2:B:170:ASP:O	2:B:174:GLY:N	2.48	0.41
2:B:295:ASN:HD21	2:B:304:ARG:HH21	1.68	0.41
2:B:58:ILE:O	2:B:316:SER:OG	2.29	0.41
1:A:228:PHE:CE1	1:A:255:PHE:HB2	2.55	0.41
2:B:30:LEU:HD23	3:G:41:ALA:CB	2.50	0.41
2:B:279:SER:O	2:B:282:GLY:N	2.48	0.41
1:A:94:MET:CE	1:A:144:CYS:HB2	2.51	0.41
2:B:57:LYS:HB2	2:B:332:TRP:HA	2.03	0.41
2:B:287:ALA:C	2:B:318:LEU:HD11	2.41	0.41
2:B:61:MET:HE3	2:B:70:LEU:HD13	2.03	0.41
1:A:42:LEU:HB3	1:A:227:MET:HE2	2.03	0.41
1:A:80:TYR:O	1:A:84:PHE:HD2	2.03	0.40
2:B:137:ARG:HG3	2:B:171:ILE:HG23	2.03	0.40
2:B:85:TYR:CE1	3:G:67:PRO:HB3	2.57	0.40
1:A:255:PHE:CA	1:A:258:ILE:HG22	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:TRP:CE3	1:A:220:PHE:HE2	2.38	0.40
1:A:333:ASP:HB3	1:A:336:ASN:CB	2.51	0.40
1:A:166:ARG:NH2	1:A:178:ASP:OD1	2.54	0.40
1:A:322:LYS:HD2	1:A:322:LYS:HA	1.87	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	340/355 (96%)	298 (88%)	33 (10%)	9 (3%)	7	26
2	B	328/340 (96%)	269 (82%)	47 (14%)	12 (4%)	4	17
3	G	48/78 (62%)	40 (83%)	6 (12%)	2 (4%)	3	13
4	Y	1/9 (11%)	0	0	1 (100%)	0	0
All	All	717/782 (92%)	607 (85%)	86 (12%)	24 (3%)	5	20

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	GLN
1	A	319	ASP
2	B	87	THR
2	B	139	LEU
2	B	266	HIS
3	G	21	LYS
3	G	62	PRO
1	A	120	LYS
1	A	150	GLU
2	B	126	LEU
2	B	228	ASP

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Mol	Chain	Res	Type
4	Y	8	ALA
1	A	118	VAL
1	A	165	ASP
2	B	41	GLY
2	B	310	GLY
1	A	117	ASP
1	A	318	PRO
2	B	53	GLY
2	B	182	GLY
2	B	131	GLY
2	B	236	PRO
1	A	188	GLY
2	B	141	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	311/321 (97%)	277 (89%)	34 (11%)	8	23
2	B	273/283 (96%)	238 (87%)	35 (13%)	5	16
3	G	41/63 (65%)	38 (93%)	3 (7%)	17	45
All	All	625/667 (94%)	553 (88%)	72 (12%)	7	21

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	MET
1	A	41	LYS
1	A	43	LEU
1	A	47	THR
1	A	49	GLU
1	A	53	SER
1	A	58	GLN
1	A	81	GLN
1	A	90	MET

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Mol	Chain	Res	Type
1	A	105	HIS
1	A	114	ARG
1	A	117	ASP
1	A	120	LYS
1	A	143	GLU
1	A	150	GLU
1	A	163	ASP
1	A	169	ASP
1	A	175	THR
1	A	177	GLN
1	A	182	VAL
1	A	184	VAL
1	A	200	ILE
1	A	212	GLU
1	A	213	ARG
1	A	224	THR
1	A	225	SER
1	A	242	SER
1	A	247	ARG
1	A	258	ILE
1	A	280	GLU
1	A	289	VAL
1	A	312	MET
1	A	320	SER
1	A	353	LEU
2	B	13	GLN
2	B	17	GLN
2	B	20	ASP
2	B	30	LEU
2	B	35	ASN
2	B	42	ARG
2	B	48	ARG
2	B	49	ARG
2	B	68	ARG
2	B	70	LEU
2	B	75	GLN
2	B	87	THR
2	B	96	ARG
2	B	105	TYR
2	B	114	CYS
2	B	118	ASP
2	B	119	ASN

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Mol	Chain	Res	Type
2	B	130	GLU
2	B	134	ARG
2	B	146	LEU
2	B	147	SER
2	B	150	ARG
2	B	161	SER
2	B	164	THR
2	B	172	GLU
2	B	175	GLN
2	B	178	THR
2	B	184	THR
2	B	192	LEU
2	B	198	LEU
2	B	217	MET
2	B	234	PHE
2	B	280	LYS
2	B	292	PHE
2	B	340	ASN
3	G	25	GLN
3	G	48	CYS
3	G	66	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	63	HIS
1	A	106	ASN
1	A	152	GLN
1	A	197	GLN
2	B	13	GLN
2	B	44	GLN
2	B	75	GLN
2	B	239	ASN
2	B	293	ASN
3	G	25	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	HL2	Y	2	4	7,8,9	0.65	0	8,10,12	1.47	1 (12%)
4	HL2	Y	3	4	7,8,9	0.38	0	8,10,12	2.26	5 (62%)
4	OTH	Y	4	4	6,8,9	3.05	2 (33%)	4,9,11	1.60	1 (25%)
4	THC	Y	5	4	8,9,10	0.27	0	8,11,13	1.16	1 (12%)
4	HF2	Y	6	4	11,11,12	0.59	0	13,13,15	1.60	2 (15%)
4	DAM	Y	7	4	5,5,6	0.64	0	3,5,7	2.54	2 (66%)
4	MAA	Y	9	4	4,5,6	0.38	0	2,5,7	0.97	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HL2	Y	2	4	-	0/8/10/12	0/0/0/0
4	HL2	Y	3	4	-	0/8/10/12	0/0/0/0
4	OTH	Y	4	4	-	0/7/10/12	0/0/0/0
4	THC	Y	5	4	-	0/8/10/12	0/0/0/0
4	HF2	Y	6	4	-	0/4/6/8	0/1/1/1
4	DAM	Y	7	4	-	0/0/4/6	0/0/0/0
4	MAA	Y	9	4	-	0/1/4/6	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Y	4	OTH	CG2-CB	3.28	1.59	1.51
4	Y	4	OTH	OG1-C22	6.67	1.67	1.42

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Y	6	HF2	O-C-CA	-3.90	115.49	125.35
4	Y	6	HF2	CG-CB-CA	-3.75	107.06	113.23
4	Y	7	DAM	CB-CA-N	-3.55	118.14	126.25
4	Y	3	HL2	O-C-CA	-2.94	117.66	125.44
4	Y	4	OTH	CG2-CB-CA	-2.60	107.88	113.17
4	Y	7	DAM	O-C-CA	-2.58	122.30	125.27
4	Y	5	THC	O-C-CA	-2.34	118.56	125.74
4	Y	3	HL2	OH-CB-CG	-2.27	105.59	109.90
4	Y	3	HL2	CD2-CG-CB	-2.10	107.75	111.26
4	Y	2	HL2	OH-CB-CG	2.40	114.44	109.90
4	Y	3	HL2	CG-CB-CA	2.77	119.72	113.55
4	Y	3	HL2	CD1-CG-CB	3.62	117.31	111.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Y	3	HL2	1	0
4	Y	4	OTH	4	0
4	Y	6	HF2	6	0
4	Y	7	DAM	3	0
4	Y	9	MAA	4	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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
5	GDP	A	1	-	23,30,30	1.27	2 (8%)	30,47,47	1.86	7 (23%)

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
5	GDP	A	1	-	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1	GDP	C5-C4	2.95	1.47	1.40
5	A	1	GDP	C6-C5	4.11	1.49	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1	GDP	C5-C6-N1	-4.34	117.66	123.59
5	A	1	GDP	C4-C5-N7	-4.26	105.56	109.48
5	A	1	GDP	PA-O3A-PB	-3.41	121.24	132.67
5	A	1	GDP	N3-C2-N1	-2.78	123.22	127.44
5	A	1	GDP	C2'-C1'-N9	-2.74	110.11	114.29
5	A	1	GDP	C6-C5-C4	-2.55	117.84	120.90
5	A	1	GDP	C6-N1-C2	4.24	121.83	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1	GDP	4	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	342/355 (96%)	0.63	35 (10%) 9 5	83, 91, 99, 107	0
2	B	330/340 (97%)	0.58	20 (6%) 25 18	83, 91, 98, 102	0
3	G	50/78 (64%)	0.83	7 (14%) 4 2	91, 93, 96, 98	0
4	Y	1/9 (11%)	2.92	1 (100%) 0 0	104, 104, 104, 104	0
All	All	723/782 (92%)	0.62	63 (8%) 13 8	83, 91, 98, 107	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	17	ALA	7.3
3	G	22	LEU	5.9
1	A	353	LEU	5.3
1	A	197	GLN	4.8
2	B	130	GLU	4.8
2	B	129	ARG	4.5
1	A	198	SER	4.4
1	A	18	ALA	4.2
1	A	117	ASP	4.2
2	B	131	GLY	4.1
2	B	132	ASN	3.9
1	A	30	ARG	3.9
2	B	36	ASN	3.8
1	A	24	MET	3.7
2	B	268	ASN	3.5
1	A	27	ARG	3.5
1	A	170	PRO	3.4
1	A	320	SER	3.2
2	B	55	LEU	3.2
2	B	65	THR	3.1
1	A	354	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
3	G	18	GLN	3.1
2	B	15	LYS	3.0
4	Y	8	ALA	2.9
2	B	16	ASN	2.9
3	G	52	ALA	2.8
1	A	19	VAL	2.8
1	A	34	GLU	2.7
3	G	53	LYS	2.7
1	A	65	SER	2.7
1	A	103	TYR	2.7
3	G	63	ALA	2.6
1	A	13	ALA	2.6
1	A	14	GLU	2.5
2	B	24	ALA	2.5
1	A	44	LEU	2.5
1	A	115	GLU	2.5
1	A	186	THR	2.5
3	G	62	PRO	2.5
2	B	224	GLY	2.5
1	A	73	ARG	2.4
1	A	210	ARG	2.4
2	B	160	SER	2.4
2	B	166	CYS	2.4
1	A	300	ARG	2.4
1	A	120	LYS	2.4
1	A	323	ILE	2.4
1	A	118	VAL	2.3
2	B	189	SER	2.3
3	G	66	ASN	2.3
2	B	17	GLN	2.3
1	A	122	SER	2.3
1	A	48	GLY	2.3
2	B	173	THR	2.2
1	A	37	ARG	2.1
1	A	42	LEU	2.1
1	A	100	PRO	2.1
2	B	81	ILE	2.1
1	A	43	LEU	2.1
1	A	227	MET	2.1
2	B	337	LYS	2.1
2	B	11	ALA	2.0
1	A	185	PRO	2.0

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

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
4	HL2	Y	2	9/10	0.92	0.20	-	98,99,100,102	0
4	HL2	Y	3	9/10	0.86	0.22	-	100,102,103,105	0
4	THC	Y	5	10/11	0.90	0.22	-	98,99,100,100	0
4	DAM	Y	7	6/7	0.82	0.23	-	103,104,104,104	0
4	HF2	Y	6	11/12	0.82	0.34	-	101,101,103,104	0
4	MAA	Y	9	6/7	0.91	0.14	-	102,102,103,103	0
4	OTH	Y	4	9/10	0.87	0.24	-	100,102,103,103	0

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
5	GDP	A	1	28/28	0.93	0.15	-1.10	89,91,92,92	0

6.5 Other polymers ⓘ

There are no such residues in this entry.