



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2026 – 10:37 PM EDT

PDB ID : 1Z7S / pdb_00001z7s
Title : The crystal structure of coxsackievirus A21
Authors : Xiao, C.; Bator-Kelly, C.M.; Rieder, E.; Chipman, P.R.; Craig, A.; Kuhn, R.J.; Wimmer, E.; Rossmann, M.G.
Deposited on : 2005-03-28
Resolution : 3.20 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

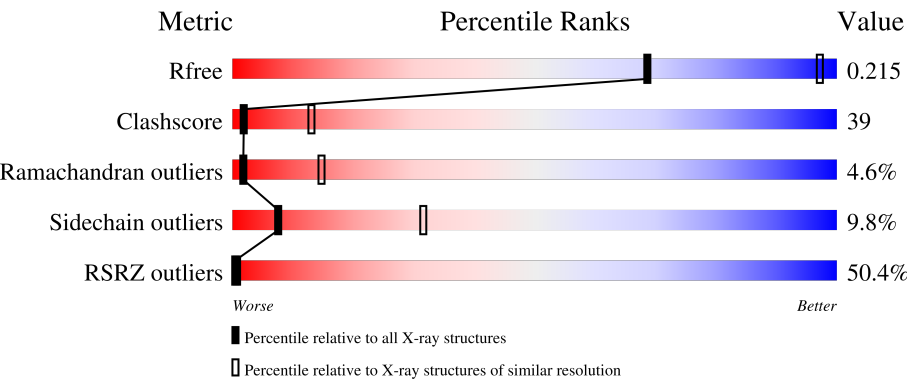
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	1	298	52% 34% 52% 9% 5%
2	2	272	50% 42% 46% 10% ••
3	3	240	44% 37% 51% 10% •
4	4	68	56% 46% 37% 15% •

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
6	MYR	1	300	-	-	X	-
7	5GP	2	273	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6765 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 Human COXSACKIEVIRUS A21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	283	Total	C	N	O	S	0	0	0
			2229	1411	380	428	10			

- Molecule 2 is a protein called Human COXSACKIEVIRUS A21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	267	Total	C	N	O	S	0	0	0
			2069	1314	349	394	12			

- Molecule 3 is a protein called Human coxsackievirus A21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	239	Total	C	N	O	S	0	0	0
			1846	1178	305	343	20			

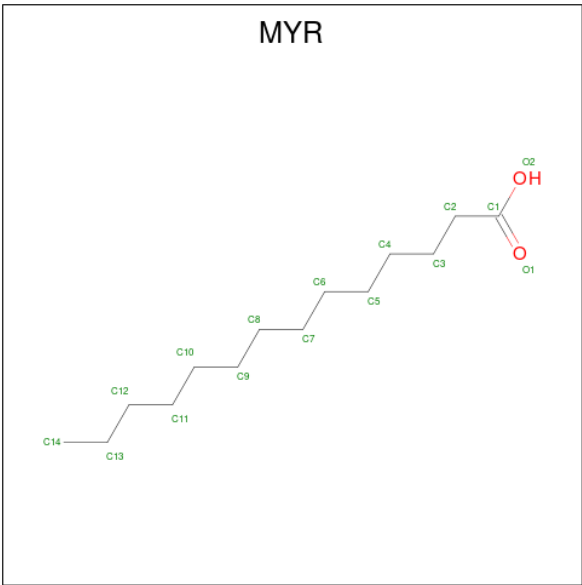
- Molecule 4 is a protein called Human coxsackievirus A21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	68	Total	C	N	O	S	0	0	0
			513	311	90	111	1			

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

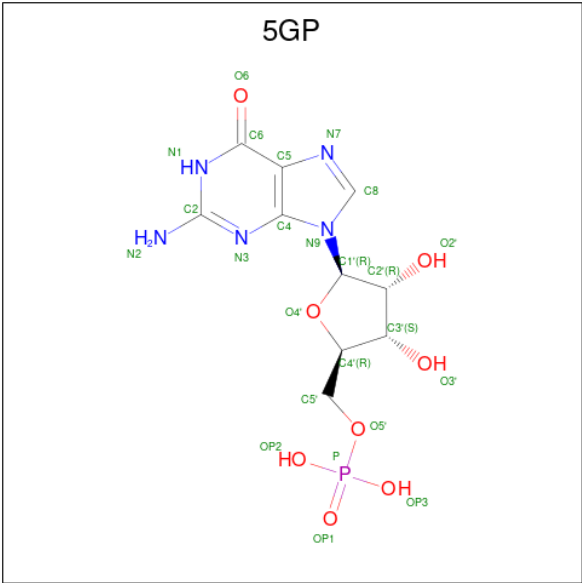
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	1	1	Total	Ca	0	0
			1	1		

- Molecule 6 is MYRISTIC ACID (CCD ID: MYR) (formula: C₁₄H₂₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	1	1	Total	C	O	0	0
			16	14	2		
6	4	1	Total	C	O	0	0
			15	14	1		

- Molecule 7 is GUANOSINE-5'-MONOPHOSPHATE (CCD ID: 5GP) (formula: C₁₀H₁₄N₅O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	2	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

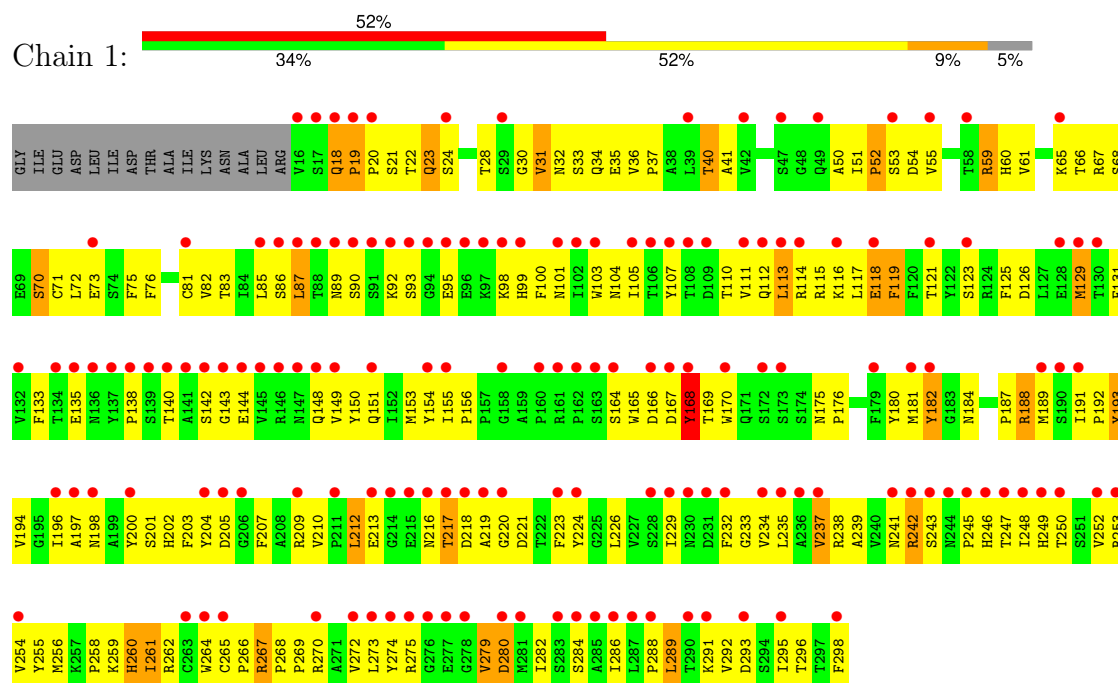
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	1	28	Total 28	O 28	0	0
8	2	9	Total 9	O 9	0	0
8	3	16	Total 16	O 16	0	0

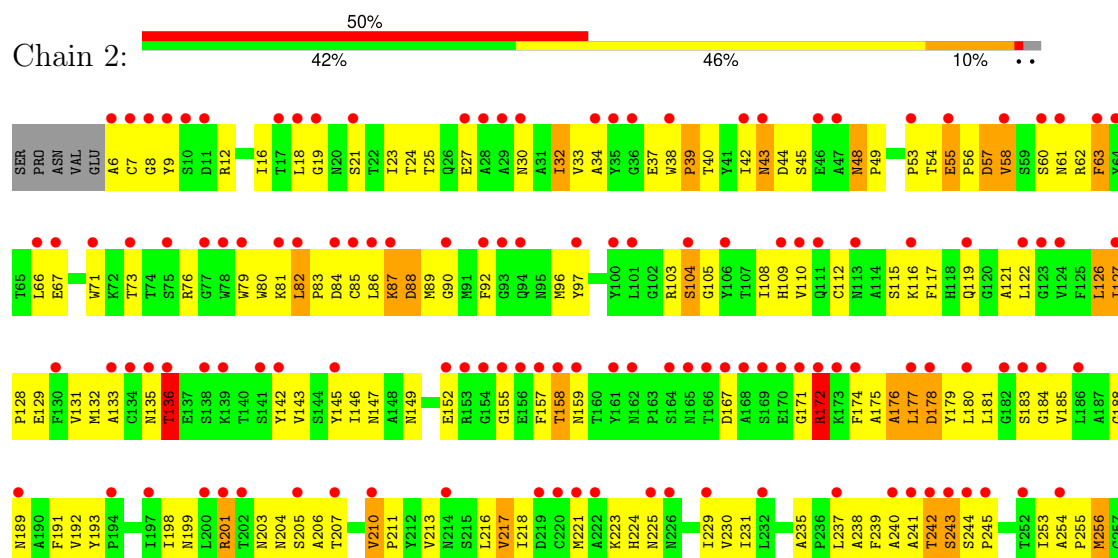
3 Residue-property plots

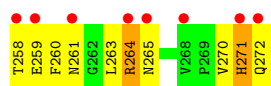
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Human COXSACKIEVIRUS A21

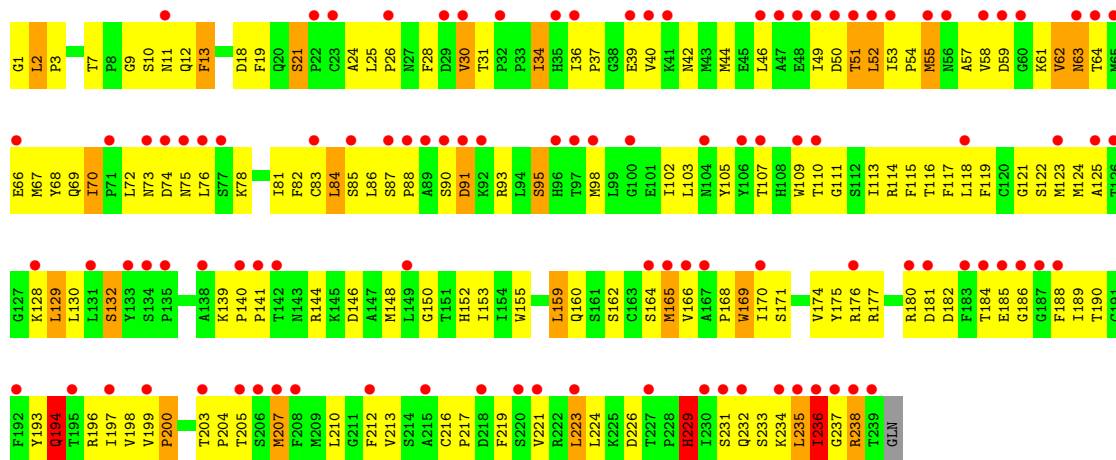


• Molecule 2: Human COXSACKIEVIRUS A21

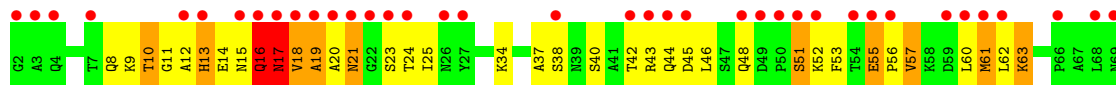




• Molecule 3: Human coxsackievirus A21



• Molecule 4: Human coxsackievirus A21



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 3 2	Depositor
Cell constants a, b, c, α , β , γ	348.01Å 348.01Å 348.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.72 – 3.20 49.72 – 3.20	Depositor EDS
% Data completeness (in resolution range)	94.3 (49.72-3.20) 94.3 (49.72-3.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.81 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.224 , 0.235 0.203 , 0.215	Depositor DCC
R_{free} test set	8790 reflections (7.90%)	wwPDB-VP
Wilson B-factor (Å ²)	59.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.34	EDS
Total number of atoms	6765	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.18% 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, 0.333 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: CA, 5GP, MYR

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	1	0.46	0/2291	1.00	14/3124 (0.4%)
2	2	0.48	0/2126	1.00	11/2908 (0.4%)
3	3	0.48	0/1895	1.03	12/2579 (0.5%)
4	4	0.56	0/520	1.04	4/705 (0.6%)
All	All	0.48	0/6832	1.01	41/9316 (0.4%)

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	16	GLN	N-CA-C	-9.78	96.45	110.24
2	2	55	GLU	CA-C-N	7.77	128.48	119.47
2	2	55	GLU	C-N-CA	7.77	128.48	119.47
1	1	210	VAL	N-CA-C	7.37	114.85	107.55
2	2	105	GLY	N-CA-C	-6.72	101.32	111.14
3	3	87	SER	CA-C-N	6.65	128.16	119.84
3	3	87	SER	C-N-CA	6.65	128.16	119.84
1	1	55	VAL	N-CA-C	6.61	117.95	111.67
1	1	289	LEU	N-CA-C	6.30	118.00	110.19
2	2	127	ILE	N-CA-C	6.22	115.39	108.05
3	3	73	ASN	N-CA-C	6.13	117.20	108.74
1	1	125	PHE	N-CA-C	5.88	117.08	108.14
1	1	34	GLN	N-CA-C	-5.85	105.72	112.92
2	2	178	ASP	N-CA-C	5.84	118.14	111.02
3	3	194	GLN	N-CA-C	-5.84	104.51	111.69
4	4	23	SER	N-CA-C	-5.83	105.93	113.16
1	1	239	ALA	N-CA-C	-5.79	100.26	109.76
1	1	260	HIS	N-CA-C	-5.78	103.43	111.52
2	2	243	SER	N-CA-C	-5.77	105.55	112.59
3	3	188	PHE	N-CA-C	5.58	117.49	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	51	SER	N-CA-C	5.58	118.12	111.71
3	3	25	LEU	CA-C-N	5.54	125.47	119.76
3	3	25	LEU	C-N-CA	5.54	125.47	119.76
3	3	78	LYS	N-CA-C	-5.41	105.38	112.41
1	1	193	TYR	N-CA-C	-5.40	100.31	108.67
3	3	70	ILE	CA-C-N	5.39	125.56	119.90
3	3	70	ILE	C-N-CA	5.39	125.56	119.90
1	1	261	ILE	N-CA-C	5.36	116.85	109.46
2	2	104	SER	N-CA-C	5.33	116.63	108.42
2	2	224	HIS	N-CA-C	5.29	117.52	108.90
1	1	126	ASP	N-CA-C	-5.28	102.23	110.42
2	2	58	VAL	N-CA-C	5.25	116.60	110.62
1	1	19	PRO	CA-C-N	5.22	126.03	119.98
1	1	19	PRO	C-N-CA	5.22	126.03	119.98
1	1	212	LEU	N-CA-C	5.12	118.10	110.52
3	3	229	HIS	N-CA-C	5.11	121.69	110.80
1	1	217	THR	N-CA-C	-5.11	107.07	113.15
4	4	21	ASN	N-CA-C	5.10	115.73	107.32
3	3	132	SER	N-CA-C	5.08	117.44	108.75
2	2	57	ASP	CB-CA-C	-5.04	110.78	116.63
2	2	63	PHE	N-CA-C	5.03	116.85	107.99

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	1	2229	0	2148	217	0
2	2	2069	0	1988	163	0
3	3	1846	0	1836	177	0
4	4	513	0	493	55	0
5	1	1	0	0	0	0
6	1	16	0	27	11	0
6	4	15	0	27	0	0
7	2	23	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	1	28	0	0	2	0
8	2	9	0	0	0	0
8	3	16	0	0	1	0
All	All	6765	0	6531	523	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 39.

All (523) 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)
1:1:275:ARG:HD3	1:1:282:ILE:HG22	1.28	1.07
4:4:11:GLY:H	4:4:14:GLU:HG3	1.20	1.04
1:1:110:THR:HA	3:3:232:GLN:HE22	1.18	1.04
4:4:34:LYS:H	4:4:34:LYS:HD2	1.14	1.03
1:1:129:MET:HE1	1:1:256:MET:HG2	1.42	1.02
3:3:61:LYS:O	3:3:64:THR:HG22	1.60	1.01
2:2:116:LYS:HD3	3:3:123:MET:HE3	1.48	0.91
1:1:85:LEU:HD11	1:1:103:TRP:HB2	1.52	0.90
3:3:55:MET:HG3	3:3:70:ILE:HD11	1.53	0.89
1:1:131:PHE:HE1	1:1:254:VAL:HG22	1.35	0.88
2:2:48:ASN:HB3	2:2:49:PRO:HD3	1.56	0.88
4:4:62:LEU:HD23	4:4:62:LEU:H	1.39	0.87
1:1:92:LYS:HB2	1:1:95:GLU:HG3	1.54	0.87
2:2:108:ILE:HG13	2:2:126:LEU:HD11	1.56	0.86
2:2:135:ASN:O	2:2:171:GLY:HA2	1.77	0.83
1:1:202:HIS:C	1:1:203:PHE:HD2	1.87	0.83
1:1:90:SER:HB3	1:1:95:GLU:HB3	1.60	0.83
1:1:131:PHE:CE1	1:1:254:VAL:HG22	2.15	0.82
2:2:27:GLU:HB2	2:2:204:ASN:OD1	1.81	0.81
1:1:110:THR:HA	3:3:232:GLN:NE2	1.94	0.80
2:2:12:ARG:HH21	3:3:159:LEU:HD21	1.46	0.80
4:4:11:GLY:N	4:4:14:GLU:HG3	1.96	0.79
3:3:51:THR:HG21	3:3:98:MET:HB2	1.61	0.79
1:1:275:ARG:CD	1:1:282:ILE:HG22	2.12	0.79
4:4:34:LYS:HD2	4:4:34:LYS:N	1.97	0.78
2:2:198:ILE:HA	2:2:203:ASN:HD21	1.47	0.78
1:1:275:ARG:HD3	1:1:282:ILE:CG2	2.12	0.77
3:3:44:MET:HA	3:3:44:MET:HE2	1.67	0.77
2:2:63:PHE:CD1	2:2:254:ALA:HB2	2.20	0.77
2:2:43:ASN:H	2:2:43:ASN:ND2	1.82	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:116:LYS:HD3	3:3:123:MET:CE	2.15	0.76
3:3:166:VAL:O	3:3:168:PRO:HD3	1.86	0.75
1:1:168:TYR:CD1	1:1:169:THR:N	2.55	0.74
3:3:9:GLY:O	3:3:12:GLN:HG2	1.86	0.74
1:1:129:MET:CE	1:1:256:MET:HG2	2.16	0.74
2:2:38:TRP:CD1	2:2:39:PRO:HD2	2.22	0.74
4:4:15:ASN:CG	4:4:21:ASN:HB2	2.13	0.74
4:4:16:GLN:O	4:4:18:VAL:N	2.20	0.74
2:2:103:ARG:HB2	2:2:218:ILE:HG13	1.70	0.73
1:1:216:ASN:HB3	1:1:218:ASP:OD1	1.88	0.73
1:1:105:ILE:CD1	1:1:235:LEU:HG	2.19	0.73
2:2:127:ILE:HG23	2:2:193:TYR:CE2	2.24	0.73
3:3:235:LEU:HD23	3:3:235:LEU:H	1.53	0.73
1:1:154:TYR:HB2	6:1:300:MYR:H122	1.69	0.72
1:1:280:ASP:HA	2:2:133:ALA:HB1	1.71	0.72
1:1:70:SER:HB2	3:3:42:ASN:OD1	1.90	0.72
1:1:98:LYS:HA	3:3:238:ARG:NH2	2.05	0.71
1:1:104:ASN:HA	1:1:234:VAL:HG12	1.72	0.71
1:1:65:LYS:NZ	3:3:110:THR:HG21	2.06	0.71
1:1:105:ILE:HD11	1:1:235:LEU:HG	1.70	0.71
2:2:96:MET:HE3	2:2:221:MET:HB3	1.72	0.71
1:1:270:ARG:NH1	2:2:184:GLY:HA3	2.06	0.71
2:2:244:SER:N	2:2:245:PRO:HD3	2.06	0.69
3:3:55:MET:HE1	3:3:84:LEU:HG	1.73	0.69
1:1:73:GLU:OE1	1:1:260:HIS:N	2.25	0.68
1:1:261:ILE:HG12	1:1:262:ARG:N	2.08	0.68
3:3:128:LYS:O	3:3:194:GLN:HB2	1.93	0.68
3:3:193:TYR:HD2	3:3:196:ARG:HA	1.58	0.67
3:3:236:ILE:HG12	3:3:237:GLY:N	2.09	0.67
1:1:207:PHE:CE2	1:1:224:TYR:HB2	2.29	0.67
1:1:85:LEU:HB2	1:1:252:VAL:CG1	2.25	0.67
1:1:168:TYR:HD1	1:1:169:THR:N	1.93	0.67
2:2:86:LEU:HD23	2:2:89:MET:HG3	1.75	0.67
3:3:18:ASP:C	3:3:19:PHE:HD2	2.02	0.67
3:3:236:ILE:HG23	3:3:237:GLY:H	1.58	0.67
2:2:23:ILE:HG21	2:2:109:HIS:CD2	2.30	0.66
1:1:68:SER:HB2	4:4:44:GLN:NE2	2.10	0.66
2:2:12:ARG:HH21	3:3:159:LEU:CD2	2.07	0.66
1:1:209:ARG:HA	2:2:223:LYS:HE2	1.78	0.66
1:1:116:LYS:O	1:1:119:PHE:HB2	1.97	0.65
1:1:168:TYR:HD1	1:1:169:THR:H	1.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:154:TYR:HB3	1:1:176:PRO:HG2	1.78	0.65
1:1:37:PRO:HB2	1:1:54:ASP:HB3	1.79	0.65
3:3:51:THR:HG21	3:3:98:MET:CB	2.27	0.65
1:1:291:LYS:HD3	3:3:59:ASP:HB2	1.79	0.65
1:1:170:TRP:CE3	1:1:238:ARG:HD3	2.32	0.65
1:1:191:ILE:HD11	6:1:300:MYR:H112	1.79	0.65
2:2:42:ILE:HG22	2:2:217:VAL:HG12	1.78	0.64
2:2:108:ILE:HG23	2:2:253:ILE:CD1	2.27	0.64
3:3:30:VAL:HG12	3:3:31:THR:N	2.13	0.64
2:2:242:THR:HG22	2:2:243:SER:H	1.61	0.64
4:4:16:GLN:CD	4:4:16:GLN:H	2.05	0.64
1:1:280:ASP:HA	2:2:133:ALA:CB	2.28	0.63
1:1:85:LEU:HD11	1:1:103:TRP:CB	2.26	0.63
1:1:82:VAL:O	1:1:110:THR:HG23	1.97	0.63
1:1:86:SER:OG	1:1:249:HIS:HE1	1.81	0.62
1:1:90:SER:HB3	1:1:95:GLU:CB	2.28	0.62
1:1:40:THR:OG1	1:1:41:ALA:N	2.32	0.62
1:1:168:TYR:CE1	1:1:169:THR:HG23	2.34	0.62
1:1:291:LYS:HA	3:3:62:VAL:HG21	1.82	0.62
1:1:107:TYR:HB3	1:1:256:MET:HE1	1.81	0.62
1:1:217:THR:CG2	2:2:272:GLN:HE21	2.13	0.62
3:3:30:VAL:CG1	3:3:31:THR:N	2.62	0.62
1:1:217:THR:HG21	2:2:272:GLN:HE21	1.65	0.62
4:4:24:THR:C	4:4:25:ILE:HD13	2.25	0.62
1:1:110:THR:CA	3:3:232:GLN:HE22	2.05	0.62
1:1:85:LEU:HB2	1:1:252:VAL:HG12	1.82	0.62
2:2:198:ILE:HA	2:2:203:ASN:ND2	2.14	0.61
3:3:62:VAL:HG12	3:3:63:ASN:H	1.65	0.61
3:3:13:PHE:C	3:3:13:PHE:CD2	2.78	0.61
1:1:36:VAL:HG23	1:1:36:VAL:O	2.00	0.61
1:1:264:TRP:CD1	3:3:36:ILE:HB	2.36	0.61
2:2:199:ASN:HD22	3:3:118:LEU:HD11	1.66	0.60
1:1:83:THR:HG22	1:1:254:VAL:HB	1.83	0.60
2:2:108:ILE:HG13	2:2:126:LEU:CD1	2.31	0.60
3:3:39:GLU:HG2	3:3:40:VAL:N	2.16	0.60
3:3:55:MET:HE2	3:3:55:MET:HA	1.84	0.60
1:1:129:MET:HE2	1:1:129:MET:HA	1.83	0.60
2:2:192:VAL:HG11	3:3:98:MET:CE	2.32	0.60
4:4:34:LYS:H	4:4:34:LYS:CD	1.98	0.60
3:3:9:GLY:HA2	3:3:12:GLN:OE1	2.01	0.59
2:2:21:SER:HB2	2:2:63:PHE:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:204:TYR:CD2	1:1:229:ILE:HD13	2.38	0.59
1:1:267:ARG:HB3	2:2:193:TYR:OH	2.03	0.59
4:4:13:HIS:CG	4:4:13:HIS:O	2.53	0.59
1:1:207:PHE:CZ	2:2:145:TYR:HA	2.38	0.59
3:3:130:LEU:C	3:3:130:LEU:HD23	2.28	0.58
2:2:104:SER:HB2	2:2:258:THR:HG22	1.84	0.58
2:2:119:GLN:OE1	3:3:204:PRO:HB2	2.03	0.58
3:3:174:VAL:HG13	3:3:175:TYR:HD2	1.67	0.58
3:3:53:ILE:HD11	3:3:213:VAL:HB	1.84	0.58
3:3:66:GLU:HA	3:3:69:GLN:NE2	2.18	0.58
3:3:76:LEU:HD23	3:3:76:LEU:H	1.69	0.58
2:2:192:VAL:HG11	3:3:98:MET:HE3	1.86	0.58
2:2:237:LEU:HD12	2:2:238:ALA:H	1.67	0.58
3:3:182:ASP:O	3:3:185:GLU:HG3	2.04	0.58
2:2:56:PRO:HG2	2:2:260:PHE:HE2	1.68	0.58
1:1:253:ARG:HG3	1:1:253:ARG:HH11	1.68	0.58
2:2:48:ASN:HB3	2:2:49:PRO:CD	2.33	0.58
4:4:62:LEU:HD23	4:4:62:LEU:N	2.14	0.58
1:1:119:PHE:CE1	1:1:269:PRO:HG3	2.39	0.57
2:2:116:LYS:CD	3:3:123:MET:HE3	2.27	0.57
3:3:58:VAL:HG12	3:3:59:ASP:N	2.18	0.57
3:3:62:VAL:HG12	3:3:63:ASN:N	2.18	0.57
1:1:82:VAL:HG21	1:1:256:MET:HG3	1.86	0.57
1:1:140:THR:C	1:1:142:SER:H	2.11	0.57
1:1:202:HIS:C	1:1:203:PHE:CD2	2.77	0.57
1:1:268:PRO:HD3	2:2:193:TYR:CE1	2.39	0.57
2:2:84:ASP:C	2:2:86:LEU:H	2.13	0.57
3:3:10:SER:O	3:3:11:ASN:HB2	2.04	0.57
1:1:70:SER:HB2	3:3:42:ASN:CG	2.29	0.57
1:1:168:TYR:HE1	1:1:169:THR:HG23	1.68	0.56
1:1:298:PHE:CD1	3:3:83:CYS:HB3	2.41	0.56
2:2:62:ARG:O	2:2:254:ALA:HA	2.06	0.56
3:3:57:ALA:C	3:3:62:VAL:HG22	2.31	0.56
1:1:298:PHE:CE1	3:3:83:CYS:HB3	2.40	0.56
3:3:75:ASN:HA	8:3:251:HOH:O	2.04	0.56
1:1:82:VAL:HG13	1:1:107:TYR:HA	1.87	0.56
1:1:181:MET:HB3	1:1:184:ASN:HD22	1.70	0.56
1:1:207:PHE:CD2	1:1:224:TYR:HB2	2.41	0.56
1:1:153:MET:HE2	1:1:155:ILE:HG12	1.88	0.55
3:3:233:SER:O	3:3:234:LYS:C	2.49	0.55
4:4:15:ASN:O	4:4:16:GLN:C	2.49	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:12:ARG:NH1	2:2:12:ARG:HG2	2.20	0.55
1:1:65:LYS:HZ1	3:3:110:THR:HG21	1.71	0.55
1:1:221:ASP:OD2	2:2:172:ARG:HD3	2.05	0.55
2:2:76:ARG:HE	2:2:159:ASN:HB3	1.71	0.55
1:1:82:VAL:CG1	1:1:107:TYR:HA	2.37	0.55
2:2:53:PRO:HG3	2:2:261:ASN:HD21	1.70	0.55
1:1:82:VAL:HG21	1:1:256:MET:HE2	1.89	0.55
1:1:99:HIS:HB3	1:1:165:TRP:HB3	1.89	0.55
2:2:191:PHE:C	2:2:193:TYR:H	2.14	0.55
3:3:103:LEU:HD21	3:3:219:PHE:HZ	1.72	0.55
1:1:90:SER:HB2	1:1:247:THR:HG23	1.89	0.54
1:1:98:LYS:HA	3:3:238:ARG:HH21	1.71	0.54
1:1:181:MET:HB3	1:1:184:ASN:ND2	2.23	0.54
2:2:23:ILE:HG22	2:2:24:THR:N	2.21	0.54
2:2:34:ALA:HB2	2:2:210:VAL:HG23	1.89	0.54
2:2:80:TRP:O	2:2:81:LYS:HD3	2.08	0.54
2:2:82:LEU:HD21	2:2:229:ILE:HD11	1.90	0.54
3:3:84:LEU:HD23	3:3:85:SER:H	1.73	0.54
3:3:235:LEU:H	3:3:235:LEU:CD2	2.21	0.54
1:1:204:TYR:CE2	1:1:229:ILE:HD13	2.43	0.53
2:2:142:TYR:CE2	2:2:172:ARG:HG2	2.43	0.53
3:3:86:LEU:O	3:3:186:GLY:HA3	2.08	0.53
2:2:181:LEU:HD12	2:2:185:VAL:HG23	1.90	0.53
1:1:65:LYS:HZ2	3:3:110:THR:HG21	1.72	0.53
3:3:111:GLY:O	3:3:169:TRP:HB2	2.08	0.53
3:3:54:PRO:HG3	3:3:68:TYR:HE2	1.73	0.53
1:1:259:LYS:HE3	4:4:37:ALA:O	2.09	0.53
3:3:110:THR:HA	3:3:169:TRP:CZ3	2.43	0.53
2:2:119:GLN:HB2	2:2:238:ALA:HB3	1.90	0.53
1:1:66:THR:C	1:1:68:SER:H	2.17	0.53
3:3:168:PRO:O	3:3:170:ILE:HG13	2.09	0.52
4:4:24:THR:O	4:4:25:ILE:HD13	2.09	0.52
2:2:23:ILE:HG12	2:2:63:PHE:CE2	2.44	0.52
2:2:242:THR:HG22	2:2:243:SER:N	2.25	0.52
2:2:12:ARG:HG2	2:2:12:ARG:HH11	1.75	0.52
2:2:271:HIS:N	2:2:271:HIS:CD2	2.77	0.52
3:3:181:ASP:OD2	3:3:182:ASP:N	2.43	0.52
1:1:143:GLY:HA3	1:1:246:HIS:CD2	2.44	0.52
1:1:155:ILE:HA	1:1:175:ASN:ND2	2.25	0.52
1:1:253:ARG:HG3	1:1:253:ARG:NH1	2.25	0.52
1:1:261:ILE:HG12	1:1:262:ARG:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:275:ARG:HB2	1:1:282:ILE:CG2	2.40	0.52
2:2:57:ASP:HA	2:2:61:ASN:HD22	1.75	0.52
3:3:125:ALA:HB2	3:3:199:VAL:HG12	1.92	0.52
1:1:40:THR:HG23	3:3:162:SER:HB2	1.90	0.52
1:1:220:GLY:HA2	1:1:223:PHE:CE1	2.44	0.52
2:2:60:SER:HB3	2:2:92:PHE:HA	1.91	0.51
3:3:61:LYS:O	3:3:64:THR:CG2	2.49	0.51
2:2:21:SER:CB	2:2:63:PHE:HB2	2.40	0.51
3:3:72:LEU:O	3:3:207:MET:HE2	2.11	0.51
1:1:28:THR:HG21	1:1:53:SER:HB3	1.91	0.51
1:1:218:ASP:HB2	2:2:172:ARG:NE	2.26	0.51
1:1:232:PHE:CD1	6:1:300:MYR:H41	2.46	0.51
2:2:175:ALA:O	2:2:177:LEU:N	2.42	0.51
1:1:282:ILE:HG13	1:1:282:ILE:O	2.10	0.51
2:2:117:PHE:CZ	3:3:124:MET:HE3	2.46	0.51
2:2:240:ALA:HB2	3:3:204:PRO:HD3	1.92	0.51
1:1:221:ASP:HA	2:2:143:VAL:O	2.11	0.51
4:4:16:GLN:O	4:4:17:ASN:C	2.54	0.51
4:4:16:GLN:O	4:4:18:VAL:HG12	2.11	0.51
1:1:264:TRP:NE1	3:3:36:ILE:HB	2.26	0.51
1:1:85:LEU:CD1	1:1:103:TRP:HB2	2.34	0.51
1:1:67:ARG:HD3	3:3:44:MET:CB	2.41	0.50
1:1:189:MET:SD	6:1:300:MYR:H132	2.51	0.50
1:1:242:ARG:HB2	1:1:242:ARG:HH11	1.77	0.50
2:2:84:ASP:O	2:2:86:LEU:N	2.41	0.50
3:3:174:VAL:HG13	3:3:175:TYR:CD2	2.46	0.50
4:4:16:GLN:C	4:4:18:VAL:N	2.68	0.50
2:2:43:ASN:ND2	2:2:43:ASN:N	2.56	0.50
3:3:52:LEU:HD11	3:3:210:LEU:HB3	1.93	0.50
3:3:129:LEU:N	3:3:129:LEU:HD23	2.26	0.50
3:3:150:GLY:O	3:3:152:HIS:HD2	1.94	0.50
2:2:183:SER:HB2	2:2:185:VAL:HG22	1.93	0.50
3:3:132:SER:O	3:3:189:ILE:HA	2.12	0.50
4:4:18:VAL:HG22	4:4:18:VAL:O	2.12	0.50
3:3:58:VAL:O	3:3:62:VAL:HG23	2.11	0.49
3:3:116:THR:HG23	3:3:164:SER:OG	2.11	0.49
4:4:18:VAL:HG22	4:4:20:ALA:HB3	1.94	0.49
1:1:194:VAL:HA	3:3:28:PHE:HE2	1.77	0.49
3:3:88:PRO:HB3	3:3:103:LEU:HD13	1.93	0.49
2:2:79:TRP:CE2	2:2:155:GLY:HA3	2.47	0.49
4:4:14:GLU:HA	4:4:14:GLU:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:198:ASN:CB	3:3:34:ILE:HD12	2.43	0.49
2:2:66:LEU:HD23	2:2:89:MET:HE2	1.94	0.49
3:3:57:ALA:O	3:3:62:VAL:HG22	2.12	0.49
3:3:90:SER:O	3:3:91:ASP:C	2.56	0.49
1:1:154:TYR:CB	6:1:300:MYR:H122	2.41	0.49
3:3:21:SER:O	4:4:38:SER:HB3	2.12	0.49
4:4:44:GLN:OE1	4:4:46:LEU:HD11	2.13	0.49
1:1:67:ARG:NH1	4:4:48:GLN:HE22	2.10	0.49
1:1:135:GLU:OE1	1:1:150:TYR:OH	2.28	0.49
1:1:181:MET:O	1:1:182:TYR:C	2.56	0.49
1:1:59:ARG:HD3	1:1:60:HIS:O	2.13	0.49
2:2:157:PHE:HA	2:2:176:ALA:HB1	1.93	0.49
3:3:176:ARG:HG2	3:3:184:THR:HB	1.94	0.49
1:1:131:PHE:HB2	1:1:187:PRO:HG2	1.95	0.48
1:1:202:HIS:O	1:1:203:PHE:HD2	1.96	0.48
4:4:20:ALA:C	4:4:21:ASN:OD1	2.56	0.48
1:1:121:THR:O	1:1:202:HIS:HB2	2.13	0.48
1:1:221:ASP:HB2	2:2:142:TYR:CE1	2.48	0.48
2:2:128:PRO:HD2	2:2:193:TYR:CD2	2.47	0.48
3:3:55:MET:HE3	3:3:84:LEU:HD12	1.95	0.48
3:3:84:LEU:HD23	3:3:85:SER:N	2.28	0.48
1:1:67:ARG:HD3	3:3:44:MET:HB2	1.94	0.48
1:1:272:VAL:HG12	1:1:288:PRO:HG3	1.95	0.48
2:2:76:ARG:NH2	3:3:66:GLU:OE2	2.36	0.48
3:3:139:LYS:HD2	3:3:140:PRO:O	2.14	0.48
3:3:189:ILE:N	3:3:189:ILE:HD12	2.28	0.48
1:1:114:ARG:O	1:1:118:GLU:HB2	2.13	0.48
1:1:168:TYR:CD1	1:1:168:TYR:C	2.89	0.48
1:1:288:PRO:HD2	3:3:63:ASN:OD1	2.14	0.48
3:3:155:TRP:CD1	3:3:155:TRP:C	2.89	0.48
1:1:107:TYR:HB3	1:1:256:MET:CE	2.44	0.48
1:1:221:ASP:HB2	2:2:142:TYR:CD1	2.48	0.48
2:2:104:SER:CB	2:2:258:THR:HG22	2.44	0.48
2:2:108:ILE:HG23	2:2:253:ILE:HD12	1.94	0.48
1:1:23:GLN:OE1	3:3:217:PRO:HG2	2.13	0.48
1:1:261:ILE:CG1	1:1:262:ARG:N	2.76	0.48
2:2:32:ILE:C	2:2:32:ILE:HD12	2.38	0.48
3:3:46:LEU:HA	3:3:49:ILE:CD1	2.43	0.48
3:3:110:THR:HG22	3:3:111:GLY:N	2.29	0.48
1:1:19:PRO:HA	1:1:20:PRO:HD3	1.75	0.48
1:1:76:PHE:HB3	1:1:258:PRO:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:76:LEU:HG	3:3:76:LEU:O	2.14	0.48
4:4:8:GLN:HB2	4:4:25:ILE:HG22	1.96	0.48
3:3:165:MET:C	3:3:165:MET:HE2	2.38	0.47
1:1:189:MET:CE	6:1:300:MYR:H132	2.44	0.47
2:2:43:ASN:H	2:2:43:ASN:HD22	1.58	0.47
3:3:115:PHE:CE1	3:3:189:ILE:HG12	2.49	0.47
1:1:22:THR:O	1:1:23:GLN:C	2.58	0.47
1:1:270:ARG:HH21	1:1:274:TYR:HA	1.79	0.47
2:2:158:THR:OG1	2:2:159:ASN:N	2.48	0.47
4:4:17:ASN:OD1	4:4:17:ASN:N	2.48	0.47
4:4:55:GLU:C	4:4:57:VAL:H	2.23	0.47
1:1:203:PHE:CD2	1:1:203:PHE:N	2.82	0.47
2:2:37:GLU:OE1	3:3:37:PRO:HA	2.14	0.47
2:2:84:ASP:OD1	2:2:149:ASN:HB3	2.14	0.47
2:2:178:ASP:OD1	2:2:179:TYR:N	2.47	0.47
2:2:263:LEU:C	2:2:264:ARG:HG3	2.38	0.47
1:1:194:VAL:HA	3:3:28:PHE:CE2	2.50	0.47
2:2:43:ASN:O	2:2:45:SER:N	2.48	0.47
2:2:115:SER:C	2:2:117:PHE:H	2.22	0.47
1:1:164:SER:C	1:1:166:ASP:H	2.23	0.47
2:2:108:ILE:HD12	2:2:253:ILE:HD12	1.96	0.47
1:1:232:PHE:CE1	6:1:300:MYR:H22	2.50	0.47
2:2:12:ARG:NH2	3:3:159:LEU:HD21	2.23	0.47
3:3:76:LEU:HB3	3:3:196:ARG:CD	2.45	0.47
3:3:203:THR:O	3:3:204:PRO:C	2.58	0.47
1:1:21:SER:HA	1:1:66:THR:HG22	1.97	0.47
1:1:33:SER:OG	1:1:35:GLU:HB2	2.14	0.47
1:1:204:TYR:HB3	1:1:226:LEU:HA	1.97	0.47
2:2:42:ILE:HG12	2:2:259:GLU:CD	2.40	0.47
3:3:88:PRO:CB	3:3:103:LEU:HD13	2.45	0.47
3:3:95:SER:O	3:3:229:HIS:HE1	1.97	0.47
3:3:98:MET:O	3:3:102:ILE:HG13	2.15	0.47
4:4:55:GLU:O	4:4:57:VAL:N	2.43	0.47
1:1:191:ILE:HD13	6:1:300:MYR:H92	1.96	0.46
1:1:289:LEU:HD12	3:3:67:MET:SD	2.54	0.46
1:1:155:ILE:HA	1:1:175:ASN:HD22	1.80	0.46
1:1:170:TRP:CZ3	1:1:238:ARG:HD3	2.51	0.46
3:3:18:ASP:O	3:3:19:PHE:HD2	1.98	0.46
4:4:9:LYS:O	4:4:10:THR:C	2.58	0.46
1:1:71:CYS:O	1:1:72:LEU:C	2.57	0.46
1:1:70:SER:HB2	3:3:42:ASN:ND2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:189:ASN:HA	3:3:51:THR:HG22	1.96	0.46
1:1:100:PHE:CD2	1:1:165:TRP:HA	2.50	0.46
1:1:135:GLU:HG2	1:1:182:TYR:CZ	2.50	0.46
1:1:266:PRO:HG3	3:3:40:VAL:HG21	1.97	0.46
1:1:115:ARG:HD3	3:3:105:TYR:OH	2.15	0.46
3:3:7:THR:O	3:3:10:SER:HB2	2.14	0.46
1:1:149:VAL:HG22	1:1:181:MET:SD	2.55	0.46
3:3:107:THR:HB	3:3:223:LEU:HB3	1.97	0.46
4:4:45:ASP:OD2	4:4:45:ASP:C	2.58	0.46
1:1:140:THR:HG22	1:1:140:THR:O	2.15	0.46
1:1:151:GLN:HE21	1:1:153:MET:HB2	1.81	0.46
1:1:197:ALA:HA	2:2:216:LEU:HD21	1.97	0.46
2:2:76:ARG:HB3	2:2:157:PHE:O	2.15	0.46
1:1:129:MET:HG3	1:1:189:MET:HE2	1.97	0.46
1:1:289:LEU:CD1	3:3:67:MET:SD	3.04	0.46
2:2:239:PHE:HD2	2:2:240:ALA:H	1.64	0.46
3:3:121:GLY:CA	3:3:207:MET:HG3	2.46	0.46
1:1:100:PHE:CD1	1:1:100:PHE:C	2.94	0.46
4:4:18:VAL:HG13	4:4:21:ASN:OD1	2.15	0.46
1:1:68:SER:HB2	4:4:44:GLN:HE22	1.80	0.45
1:1:203:PHE:HD2	1:1:203:PHE:N	2.12	0.45
3:3:18:ASP:OD2	4:4:40:SER:HB3	2.15	0.45
3:3:74:ASP:HB2	3:3:205:THR:OG1	2.16	0.45
1:1:298:PHE:CZ	3:3:190:THR:HG22	2.51	0.45
2:2:16:ILE:HD11	2:2:207:THR:HG21	1.98	0.45
3:3:110:THR:HG23	3:3:169:TRP:CE2	2.51	0.45
1:1:292:VAL:O	1:1:293:ASP:C	2.57	0.45
3:3:55:MET:HE1	3:3:84:LEU:CG	2.43	0.45
3:3:91:ASP:OD2	3:3:93:ARG:HB2	2.16	0.45
2:2:6:ALA:C	2:2:8:GLY:H	2.24	0.45
2:2:61:ASN:HA	2:2:255:PRO:HG2	1.97	0.45
3:3:1:GLY:O	3:3:3:PRO:HD3	2.16	0.45
4:4:62:LEU:O	4:4:63:LYS:C	2.59	0.45
2:2:33:VAL:HG21	2:2:38:TRP:CZ3	2.51	0.45
2:2:30:ASN:CG	4:4:57:VAL:CG2	2.90	0.45
2:2:136:THR:HG23	2:2:136:THR:O	2.17	0.45
1:1:198:ASN:HB3	3:3:34:ILE:HD12	1.99	0.45
1:1:273:LEU:HD23	8:1:320:HOH:O	2.17	0.45
2:2:244:SER:N	2:2:245:PRO:CD	2.77	0.45
3:3:207:MET:HE2	3:3:207:MET:H	1.82	0.45
2:2:34:ALA:HB3	2:2:211:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:99:HIS:CE1	1:1:165:TRP:CE3	3.04	0.44
1:1:117:LEU:C	1:1:119:PHE:H	2.25	0.44
1:1:87:LEU:HD11	1:1:250:THR:HB	1.98	0.44
2:2:79:TRP:CE2	2:2:132:MET:HE1	2.52	0.44
2:2:121:ALA:HB3	2:2:235:ALA:HB3	1.99	0.44
1:1:117:LEU:HB3	1:1:202:HIS:CE1	2.52	0.44
1:1:205:ASP:HA	2:2:131:VAL:HG22	2.00	0.44
3:3:76:LEU:HB3	3:3:196:ARG:HD3	2.00	0.44
3:3:199:VAL:HB	3:3:203:THR:HB	1.99	0.44
3:3:216:CYS:HB3	3:3:217:PRO:HD2	1.99	0.44
1:1:105:ILE:HG12	1:1:233:GLY:O	2.17	0.44
2:2:86:LEU:CD2	2:2:89:MET:HG3	2.44	0.44
2:2:201:ARG:HB2	3:3:123:MET:HA	2.00	0.44
3:3:18:ASP:C	3:3:19:PHE:CD2	2.90	0.44
3:3:39:GLU:HG2	3:3:40:VAL:H	1.81	0.44
3:3:193:TYR:CD2	3:3:196:ARG:HA	2.46	0.44
4:4:15:ASN:OD1	4:4:21:ASN:HB2	2.17	0.44
1:1:212:LEU:O	2:2:270:VAL:HG12	2.17	0.44
1:1:81:CYS:HB2	1:1:255:TYR:CE1	2.53	0.44
3:3:24:ALA:C	3:3:26:PRO:HD3	2.42	0.44
3:3:81:ILE:HD11	3:3:193:TYR:CE1	2.52	0.44
4:4:16:GLN:C	4:4:18:VAL:H	2.25	0.44
4:4:55:GLU:N	4:4:56:PRO:CD	2.81	0.44
1:1:111:VAL:HG21	3:3:232:GLN:HB2	2.00	0.44
1:1:202:HIS:O	1:1:203:PHE:CD2	2.71	0.44
3:3:114:ARG:NH2	3:3:216:CYS:HA	2.33	0.44
2:2:57:ASP:CG	2:2:58:VAL:H	2.26	0.44
2:2:132:MET:HB2	2:2:174:PHE:CD1	2.53	0.44
2:2:55:GLU:HG2	2:2:259:GLU:HB3	1.99	0.44
3:3:117:PHE:HB2	3:3:155:TRP:CZ3	2.53	0.44
2:2:7:CYS:HB2	2:2:9:TYR:HE2	1.83	0.43
2:2:128:PRO:HD2	2:2:193:TYR:CE2	2.53	0.43
2:2:147:ASN:ND2	2:2:172:ARG:O	2.50	0.43
2:2:87:LYS:HB2	2:2:97:TYR:CE2	2.52	0.43
2:2:191:PHE:CZ	3:3:52:LEU:HD22	2.53	0.43
4:4:16:GLN:CD	4:4:16:GLN:N	2.71	0.43
1:1:86:SER:OG	1:1:249:HIS:CE1	2.68	0.43
1:1:133:PHE:HB2	1:1:180:TYR:HE2	1.83	0.43
1:1:216:ASN:HA	8:1:312:HOH:O	2.18	0.43
1:1:218:ASP:O	1:1:219:ALA:C	2.61	0.43
1:1:226:LEU:O	1:1:229:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:18:LEU:HD11	2:2:256:MET:CE	2.48	0.43
2:2:86:LEU:C	2:2:88:ASP:N	2.77	0.43
1:1:89:ASN:OD1	1:1:243:SER:HA	2.19	0.43
2:2:239:PHE:CD2	2:2:240:ALA:N	2.86	0.43
3:3:111:GLY:C	3:3:169:TRP:HB2	2.44	0.43
1:1:143:GLY:HA3	1:1:246:HIS:NE2	2.33	0.43
1:1:168:TYR:CE1	1:1:169:THR:CG2	3.01	0.43
1:1:260:HIS:HA	4:4:42:THR:HG23	2.01	0.43
2:2:18:LEU:O	2:2:19:GLY:C	2.62	0.43
2:2:34:ALA:HB3	2:2:211:PRO:CD	2.48	0.43
3:3:30:VAL:CG1	3:3:31:THR:H	2.31	0.43
3:3:199:VAL:HB	3:3:203:THR:CG2	2.49	0.43
1:1:112:GLN:HE22	3:3:226:ASP:CG	2.27	0.43
1:1:298:PHE:HZ	3:3:190:THR:HG22	1.84	0.43
2:2:239:PHE:HD2	2:2:240:ALA:N	2.15	0.43
1:1:267:ARG:NH1	2:2:193:TYR:OH	2.52	0.43
3:3:110:THR:HG23	3:3:169:TRP:CZ2	2.53	0.43
4:4:60:LEU:HD12	4:4:61:MET:H	1.83	0.43
1:1:167:ASP:O	1:1:169:THR:N	2.52	0.43
2:2:30:ASN:ND2	4:4:57:VAL:HG21	2.33	0.43
2:2:76:ARG:HA	2:2:76:ARG:HD2	1.70	0.43
2:2:83:PRO:HG3	2:2:221:MET:HB3	2.00	0.43
3:3:171:SER:HB2	3:3:176:ARG:CZ	2.49	0.43
1:1:87:LEU:CD1	1:1:250:THR:HB	2.49	0.43
1:1:154:TYR:O	1:1:156:PRO:HD3	2.19	0.43
1:1:268:PRO:HG3	2:2:189:ASN:O	2.19	0.43
1:1:279:VAL:O	1:1:280:ASP:O	2.35	0.43
2:2:71:TRP:CE2	2:2:237:LEU:HB2	2.54	0.43
4:4:15:ASN:ND2	4:4:25:ILE:HG13	2.33	0.43
2:2:146:ILE:HD11	2:2:270:VAL:HG23	2.01	0.42
3:3:55:MET:CE	3:3:84:LEU:HG	2.45	0.42
4:4:55:GLU:O	4:4:57:VAL:HG12	2.19	0.42
1:1:154:TYR:CE1	6:1:300:MYR:H102	2.54	0.42
1:1:286:ILE:O	2:2:179:TYR:OH	2.36	0.42
2:2:96:MET:HE3	2:2:221:MET:CB	2.44	0.42
3:3:197:ILE:CD1	3:3:207:MET:HE3	2.49	0.42
1:1:188:ARG:HD2	3:3:21:SER:HB3	2.01	0.42
1:1:273:LEU:HD11	3:3:231:SER:HB2	2.01	0.42
2:2:110:VAL:HB	2:2:206:ALA:HB3	2.02	0.42
1:1:140:THR:C	1:1:142:SER:N	2.75	0.42
2:2:86:LEU:HA	2:2:89:MET:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:242:THR:HG21	2:2:244:SER:OG	2.20	0.42
2:2:67:GLU:HG3	2:2:152:GLU:OE1	2.19	0.42
2:2:201:ARG:HH21	3:3:119:PHE:HE1	1.67	0.42
3:3:51:THR:O	3:3:212:PHE:HA	2.18	0.42
2:2:42:ILE:HG12	2:2:259:GLU:OE2	2.19	0.42
2:2:67:GLU:HG3	2:2:152:GLU:CD	2.45	0.42
2:2:271:HIS:H	2:2:271:HIS:HD2	1.68	0.42
3:3:2:LEU:C	3:3:2:LEU:CD2	2.93	0.42
4:4:15:ASN:C	4:4:16:GLN:O	2.57	0.42
1:1:216:ASN:C	1:1:218:ASP:H	2.26	0.42
3:3:177:ARG:HG3	3:3:184:THR:HG21	2.01	0.42
4:4:14:GLU:O	4:4:15:ASN:C	2.63	0.42
1:1:99:HIS:HB3	1:1:165:TRP:CB	2.50	0.42
1:1:193:TYR:CD1	1:1:193:TYR:C	2.97	0.42
3:3:42:ASN:OD1	3:3:44:MET:HB2	2.19	0.42
3:3:177:ARG:H	3:3:184:THR:HG21	1.85	0.42
2:2:86:LEU:O	2:2:88:ASP:N	2.53	0.42
3:3:54:PRO:HG3	3:3:68:TYR:CE2	2.52	0.42
3:3:141:PRO:HG2	3:3:190:THR:HG21	2.01	0.42
1:1:113:LEU:O	1:1:113:LEU:HD12	2.20	0.41
2:2:119:GLN:HG2	3:3:122:SER:N	2.35	0.41
1:1:100:PHE:HD1	1:1:101:ASN:N	2.18	0.41
1:1:170:TRP:CG	1:1:238:ARG:NH1	2.88	0.41
2:2:109:HIS:CE1	2:2:205:SER:HB3	2.54	0.41
3:3:40:VAL:HG22	4:4:53:PHE:CE1	2.55	0.41
3:3:103:LEU:HD21	3:3:219:PHE:CZ	2.53	0.41
1:1:270:ARG:HG2	1:1:274:TYR:CZ	2.56	0.41
3:3:119:PHE:CZ	3:3:121:GLY:HA3	2.55	0.41
1:1:148:GLN:HE22	1:1:241:ASN:HB2	1.85	0.41
1:1:191:ILE:HA	1:1:192:PRO:HD3	1.82	0.41
1:1:51:ILE:O	1:1:52:PRO:C	2.63	0.41
1:1:164:SER:C	1:1:166:ASP:N	2.78	0.41
1:1:282:ILE:O	1:1:282:ILE:CG1	2.68	0.41
3:3:219:PHE:HE1	3:3:221:VAL:CG1	2.34	0.41
1:1:24:SER:HB3	1:1:61:VAL:O	2.21	0.41
1:1:273:LEU:N	1:1:273:LEU:HD22	2.36	0.41
2:2:115:SER:C	2:2:117:PHE:N	2.78	0.41
4:4:16:GLN:NE2	4:4:16:GLN:CA	2.83	0.41
1:1:18:GLN:OE1	1:1:18:GLN:HA	2.21	0.41
2:2:191:PHE:C	2:2:193:TYR:N	2.78	0.41
2:2:192:VAL:HG11	3:3:98:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:58:VAL:CG1	3:3:59:ASP:N	2.82	0.41
3:3:81:ILE:HD11	3:3:193:TYR:CD1	2.56	0.41
4:4:16:GLN:CA	4:4:16:GLN:HE21	2.33	0.41
4:4:18:VAL:C	4:4:20:ALA:N	2.78	0.41
1:1:218:ASP:HB2	2:2:172:ARG:CD	2.51	0.41
1:1:261:ILE:CG1	1:1:262:ARG:H	2.33	0.41
1:1:279:VAL:O	1:1:280:ASP:C	2.64	0.41
2:2:122:LEU:HD22	2:2:231:ILE:HG22	2.02	0.41
2:2:237:LEU:HD12	2:2:238:ALA:N	2.34	0.41
1:1:30:GLY:O	1:1:31:VAL:HB	2.21	0.41
1:1:154:TYR:CD1	6:1:300:MYR:H102	2.56	0.41
1:1:154:TYR:CG	6:1:300:MYR:H122	2.56	0.41
2:2:23:ILE:CG2	2:2:109:HIS:CD2	3.03	0.41
2:2:121:ALA:N	2:2:235:ALA:HB3	2.36	0.41
2:2:178:ASP:C	2:2:180:LEU:H	2.29	0.41
2:2:191:PHE:CE1	3:3:52:LEU:HD22	2.56	0.41
3:3:46:LEU:HA	3:3:49:ILE:HD12	2.02	0.41
3:3:144:ARG:C	3:3:146:ASP:H	2.28	0.41
3:3:165:MET:HE2	3:3:165:MET:O	2.21	0.41
3:3:196:ARG:O	3:3:198:VAL:HG23	2.19	0.41
4:4:18:VAL:O	4:4:20:ALA:N	2.54	0.41
1:1:82:VAL:HG21	1:1:256:MET:CG	2.51	0.41
2:2:188:GLY:HA3	3:3:68:TYR:CZ	2.56	0.41
3:3:109:TRP:CZ3	3:3:113:ILE:HD11	2.56	0.41
1:1:75:PHE:HD2	1:1:76:PHE:CE1	2.39	0.40
1:1:123:SER:O	1:1:200:TYR:HB2	2.21	0.40
1:1:282:ILE:CD1	1:1:284:SER:HB3	2.51	0.40
2:2:84:ASP:HB2	2:2:225:ASN:OD1	2.21	0.40
2:2:211:PRO:O	2:2:213:VAL:HG23	2.22	0.40
3:3:82:PHE:CD1	3:3:82:PHE:C	3.00	0.40
4:4:51:SER:C	4:4:53:PHE:N	2.78	0.40
2:2:62:ARG:O	2:2:255:PRO:HD2	2.22	0.40
4:4:18:VAL:O	4:4:19:ALA:C	2.64	0.40
1:1:170:TRP:CD2	1:1:238:ARG:HD3	2.57	0.40
1:1:237:VAL:HG12	1:1:238:ARG:H	1.85	0.40
2:2:83:PRO:HB3	2:2:221:MET:HE2	2.03	0.40
1:1:89:ASN:HB3	1:1:248:ILE:HG22	2.03	0.40
1:1:295:ILE:HG23	1:1:296:THR:HG23	2.04	0.40
2:2:79:TRP:HB3	2:2:157:PHE:CE1	2.56	0.40
2:2:271:HIS:CD2	2:2:271:HIS:H	2.39	0.40
2:2:23:ILE:CG2	2:2:24:THR:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:54:THR:O	2:2:259:GLU:HA	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	1	281/298 (94%)	233 (83%)	36 (13%)	12 (4%)	2	16
2	2	265/272 (97%)	226 (85%)	28 (11%)	11 (4%)	2	16
3	3	237/240 (99%)	203 (86%)	24 (10%)	10 (4%)	2	16
4	4	66/68 (97%)	52 (79%)	8 (12%)	6 (9%)	0	3
All	All	849/878 (97%)	714 (84%)	96 (11%)	39 (5%)	2	15

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	168	TYR
1	1	280	ASP
2	2	176	ALA
2	2	241	ALA
3	3	236	ILE
4	4	17	ASN
1	1	93	SER
1	1	138	PRO
2	2	44	ASP
2	2	85	CYS
2	2	167	ASP
3	3	62	VAL
3	3	63	ASN
3	3	229	HIS

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Mol	Chain	Res	Type
3	3	238	ARG
4	4	12	ALA
4	4	18	VAL
1	1	23	GLN
1	1	32	ASN
1	1	50	ALA
1	1	182	TYR
1	1	213	GLU
2	2	48	ASN
2	2	87	LYS
2	2	136	THR
3	3	200	PRO
2	2	112	CYS
3	3	30	VAL
3	3	91	ASP
4	4	63	LYS
1	1	31	VAL
1	1	265	CYS
2	2	172	ARG
3	3	95	SER
4	4	19	ALA
2	2	90	GLY
3	3	169	TRP
1	1	245	PRO
4	4	55	GLU

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	1	249/261 (95%)	230 (92%)	19 (8%)	12	42
2	2	225/230 (98%)	202 (90%)	23 (10%)	7	29
3	3	212/213 (100%)	189 (89%)	23 (11%)	6	27
4	4	57/57 (100%)	49 (86%)	8 (14%)	3	17
All	All	743/761 (98%)	670 (90%)	73 (10%)	7	31

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	18	GLN
1	1	40	THR
1	1	52	PRO
1	1	59	ARG
1	1	70	SER
1	1	87	LEU
1	1	113	LEU
1	1	118	GLU
1	1	119	PHE
1	1	129	MET
1	1	144	GLU
1	1	168	TYR
1	1	188	ARG
1	1	196	ILE
1	1	201	SER
1	1	237	VAL
1	1	242	ARG
1	1	267	ARG
1	1	279	VAL
2	2	25	THR
2	2	32	ILE
2	2	39	PRO
2	2	40	THR
2	2	43	ASN
2	2	73	THR
2	2	82	LEU
2	2	88	ASP
2	2	126	LEU
2	2	129	GLU
2	2	136	THR
2	2	158	THR
2	2	172	ARG
2	2	177	LEU
2	2	201	ARG
2	2	210	VAL
2	2	217	VAL
2	2	230	VAL
2	2	242	THR
2	2	256	MET
2	2	264	ARG
2	2	265	ASN
2	2	271	HIS

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Mol	Chain	Res	Type
3	3	2	LEU
3	3	13	PHE
3	3	21	SER
3	3	34	ILE
3	3	50	ASP
3	3	51	THR
3	3	52	LEU
3	3	55	MET
3	3	84	LEU
3	3	129	LEU
3	3	148	MET
3	3	153	ILE
3	3	159	LEU
3	3	160	GLN
3	3	165	MET
3	3	180	ARG
3	3	194	GLN
3	3	200	PRO
3	3	207	MET
3	3	223	LEU
3	3	224	LEU
3	3	235	LEU
3	3	236	ILE
4	4	10	THR
4	4	13	HIS
4	4	16	GLN
4	4	17	ASN
4	4	43	ARG
4	4	52	LYS
4	4	57	VAL
4	4	61	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	104	ASN
1	1	112	GLN
1	1	148	GLN
1	1	151	GLN
1	1	184	ASN
1	1	198	ASN
1	1	249	HIS

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Mol	Chain	Res	Type
2	2	43	ASN
2	2	48	ASN
2	2	94	GLN
2	2	109	HIS
2	2	147	ASN
2	2	199	ASN
2	2	214	ASN
2	2	226	ASN
2	2	246	GLN
2	2	261	ASN
2	2	272	GLN
3	3	56	ASN
3	3	152	HIS
3	3	160	GLN
3	3	229	HIS
3	3	232	GLN
4	4	4	GLN
4	4	15	ASN
4	4	16	GLN
4	4	31	ASN
4	4	39	ASN
4	4	48	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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
7	5GP	2	273	-	22,25,26	0.30	0	32,37,40	0.30	0
6	MYR	1	300	-	15,15,15	0.68	0	15,15,15	0.71	0
6	MYR	4	1	4	13,14,15	0.39	0	12,13,15	0.48	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
7	5GP	2	273	-	-	2/7/25/26	0/3/3/3
6	MYR	1	300	-	-	7/13/13/13	-
6	MYR	4	1	4	-	5/12/12/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

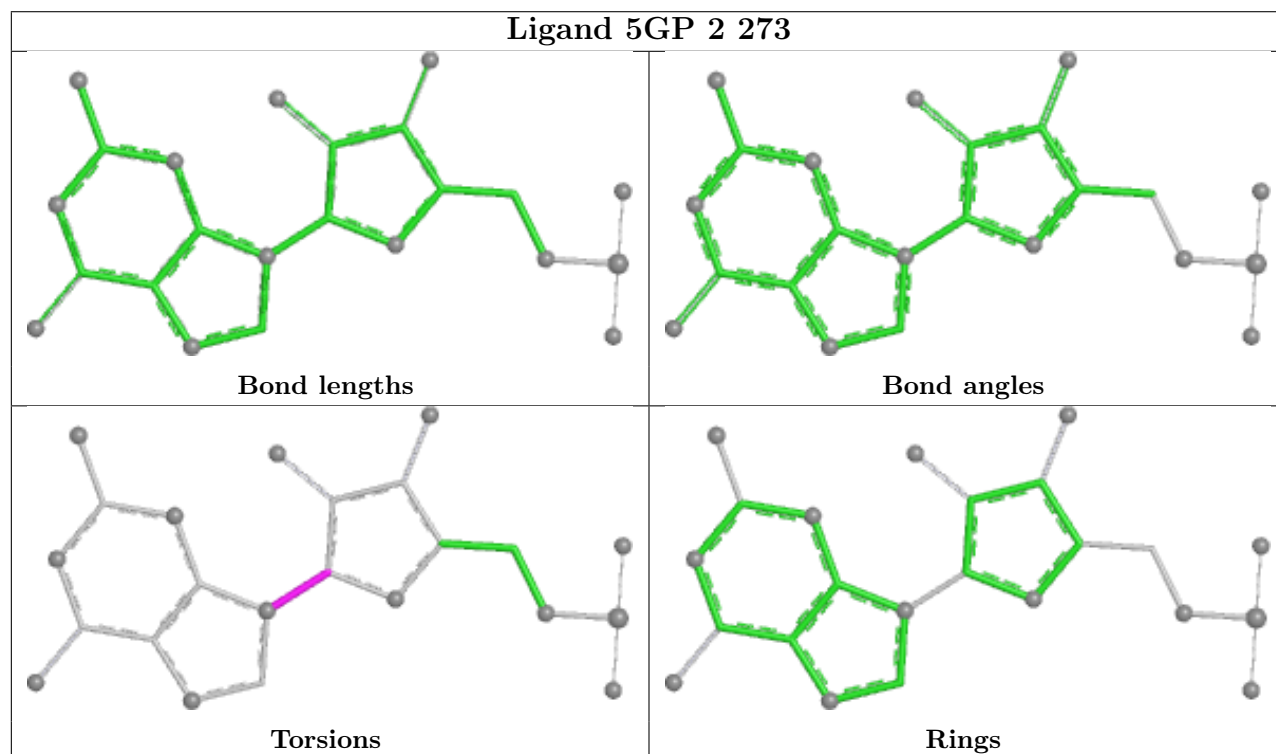
Mol	Chain	Res	Type	Atoms
6	4	1	MYR	O1-C1-C2-C3
7	2	273	5GP	O4'-C1'-N9-C8
7	2	273	5GP	O4'-C1'-N9-C4
6	1	300	MYR	C1-C2-C3-C4
6	1	300	MYR	C4-C5-C6-C7
6	4	1	MYR	C4-C5-C6-C7
6	1	300	MYR	C6-C7-C8-C9
6	4	1	MYR	C11-C10-C9-C8
6	1	300	MYR	C7-C8-C9-C10
6	4	1	MYR	C6-C7-C8-C9
6	1	300	MYR	O2-C1-C2-C3
6	1	300	MYR	O1-C1-C2-C3
6	4	1	MYR	C1-C2-C3-C4
6	1	300	MYR	C2-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	1	300	MYR	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	1	283/298 (94%)	2.34	154 (54%) 0 0	5, 51, 91, 105	4 (1%)
2	2	267/272 (98%)	2.24	135 (50%) 0 1	32, 46, 79, 119	0
3	3	239/240 (99%)	1.95	105 (43%) 0 1	32, 44, 69, 135	0
4	4	68/68 (100%)	2.49	38 (55%) 0 0	32, 50, 93, 108	0
All	All	857/878 (97%)	2.21	432 (50%) 0 1	5, 47, 86, 135	4 (0%)

All (432) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	4	17	ASN	11.9
4	4	2	GLY	9.9
1	1	287	LEU	9.1
1	1	274	TYR	8.2
1	1	277	GLU	7.7
2	2	222	ALA	7.4
2	2	168	ALA	7.3
1	1	144	GLU	7.1
1	1	93	SER	7.1
3	3	238	ARG	6.6
2	2	9	TYR	6.6
2	2	6	ALA	6.5
1	1	18	GLN	6.4
2	2	7	CYS	6.3
1	1	276	GLY	6.2
1	1	285	ALA	6.1
1	1	143	GLY	5.8
3	3	237	GLY	5.8
2	2	152	GLU	5.7
1	1	141	ALA	5.7
1	1	228	SER	5.6

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Mol	Chain	Res	Type	RSRZ
1	1	140	THR	5.6
1	1	214	GLY	5.4
1	1	97	LYS	5.4
2	2	8	GLY	5.4
4	4	18	VAL	5.3
2	2	141	SER	5.1
3	3	239	THR	5.0
1	1	249	HIS	4.9
1	1	142	SER	4.8
3	3	89	ALA	4.8
1	1	89	ASN	4.7
2	2	242	THR	4.7
1	1	241	ASN	4.7
2	2	219	ASP	4.7
1	1	219	ALA	4.7
4	4	43	ARG	4.7
1	1	139	SER	4.7
4	4	15	ASN	4.6
4	4	55	GLU	4.6
1	1	160	PRO	4.6
3	3	206	SER	4.6
4	4	60	LEU	4.6
3	3	65	MET	4.5
1	1	94	GLY	4.5
1	1	213	GLU	4.5
4	4	16	GLN	4.5
2	2	92	PHE	4.4
3	3	11	ASN	4.4
1	1	181	MET	4.4
2	2	145	TYR	4.4
2	2	189	ASN	4.3
2	2	272	GLN	4.3
2	2	243	SER	4.2
4	4	44	GLN	4.2
3	3	88	PRO	4.1
1	1	234	VAL	4.1
1	1	91	SER	4.1
2	2	42	ILE	4.1
2	2	116	LYS	4.1
2	2	214	ASN	4.1
2	2	183	SER	4.0
3	3	104	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
3	3	232	GLN	4.0
1	1	16	VAL	3.9
3	3	142	THR	3.9
1	1	129	MET	3.9
2	2	225	ASN	3.9
1	1	243	SER	3.9
1	1	284	SER	3.9
1	1	113	LEU	3.9
2	2	133	ALA	3.9
3	3	231	SER	3.9
3	3	236	ILE	3.9
1	1	288	PRO	3.8
1	1	218	ASP	3.8
1	1	246	HIS	3.8
3	3	203	THR	3.8
1	1	230	ASN	3.8
1	1	242	ARG	3.8
2	2	244	SER	3.8
1	1	231	ASP	3.8
2	2	258	THR	3.8
2	2	29	ALA	3.8
2	2	130	PHE	3.7
2	2	71	TRP	3.7
1	1	151	GLN	3.7
3	3	63	ASN	3.7
1	1	20	PRO	3.7
1	1	263	CYS	3.7
2	2	162	ASN	3.6
3	3	100	GLY	3.6
1	1	217	THR	3.6
3	3	212	PHE	3.6
1	1	146	ARG	3.6
2	2	113	ASN	3.6
4	4	19	ALA	3.6
1	1	95	GLU	3.6
4	4	45	ASP	3.6
3	3	205	THR	3.6
1	1	73	GLU	3.6
1	1	88	THR	3.6
1	1	179	PHE	3.6
1	1	147	ASN	3.6
1	1	244	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	1	135	GLU	3.5
2	2	166	THR	3.5
4	4	69	ASN	3.5
1	1	99	HIS	3.5
1	1	96	GLU	3.5
2	2	170	GLU	3.5
1	1	111	VAL	3.5
4	4	22	GLY	3.5
2	2	60	SER	3.5
4	4	49	ASP	3.5
3	3	49	ILE	3.4
3	3	227	THR	3.4
4	4	56	PRO	3.4
1	1	291	LYS	3.4
2	2	245	PRO	3.4
2	2	21	SER	3.4
2	2	75	SER	3.4
2	2	46	GLU	3.4
4	4	13	HIS	3.4
1	1	136	ASN	3.3
4	4	3	ALA	3.3
4	4	48	GLN	3.3
1	1	65	LYS	3.3
3	3	73	ASN	3.3
2	2	226	ASN	3.3
4	4	61	MET	3.3
1	1	92	LYS	3.2
1	1	245	PRO	3.2
2	2	167	ASP	3.2
1	1	134	THR	3.2
1	1	137	TYR	3.2
3	3	30	VAL	3.2
4	4	59	ASP	3.2
2	2	90	GLY	3.2
1	1	198	ASN	3.2
2	2	135	ASN	3.2
1	1	86	SER	3.2
2	2	205	SER	3.2
3	3	23	CYS	3.1
2	2	79	TRP	3.1
3	3	56	ASN	3.1
3	3	166	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
2	2	153	ARG	3.1
1	1	229	ILE	3.1
2	2	87	LYS	3.1
3	3	92	LYS	3.1
2	2	252	THR	3.1
2	2	19	GLY	3.1
2	2	67	GLU	3.1
2	2	220	CYS	3.1
2	2	43	ASN	3.1
3	3	75	ASN	3.1
2	2	81	LYS	3.1
2	2	158	THR	3.1
3	3	90	SER	3.1
3	3	208	PHE	3.1
3	3	59	ASP	3.1
2	2	155	GLY	3.0
1	1	128	GLU	3.0
1	1	155	ILE	3.0
2	2	127	ILE	3.0
3	3	29	ASP	3.0
2	2	134	CYS	3.0
1	1	281	MET	3.0
3	3	32	PRO	3.0
1	1	275	ARG	3.0
2	2	111	GLN	3.0
1	1	248	ILE	3.0
2	2	186	LEU	2.9
1	1	154	TYR	2.9
2	2	109	HIS	2.9
3	3	197	ILE	2.9
2	2	106	TYR	2.9
4	4	52	LYS	2.9
1	1	215	GLU	2.9
3	3	185	GLU	2.9
2	2	58	VAL	2.9
2	2	184	GLY	2.9
3	3	128	LYS	2.9
1	1	103	TRP	2.9
1	1	132	VAL	2.9
1	1	149	VAL	2.9
3	3	180	ARG	2.9
1	1	90	SER	2.9

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Mol	Chain	Res	Type	RSRZ
3	3	35	HIS	2.9
4	4	38	SER	2.9
1	1	19	PRO	2.9
1	1	290	THR	2.9
3	3	64	THR	2.9
2	2	159	ASN	2.9
2	2	261	ASN	2.9
1	1	81	CYS	2.9
3	3	83	CYS	2.9
3	3	106	TYR	2.9
3	3	183	PHE	2.9
2	2	11	ASP	2.8
3	3	218	ASP	2.8
2	2	27	GLU	2.8
1	1	216	ASN	2.8
1	1	253	ARG	2.8
1	1	189	MET	2.8
1	1	106	THR	2.8
2	2	177	LEU	2.8
3	3	170	ILE	2.8
2	2	28	ALA	2.8
1	1	161	ARG	2.8
1	1	98	LYS	2.8
1	1	247	THR	2.8
2	2	157	PHE	2.8
3	3	123	MET	2.8
1	1	114	ARG	2.8
2	2	34	ALA	2.8
1	1	55	VAL	2.8
1	1	53	SER	2.8
2	2	122	LEU	2.8
1	1	205	ASP	2.7
1	1	206	GLY	2.7
3	3	181	ASP	2.7
2	2	97	TYR	2.7
4	4	27	TYR	2.7
1	1	116	LYS	2.7
2	2	64	TYR	2.7
1	1	148	GLN	2.7
3	3	192	PHE	2.7
3	3	48	GLU	2.7
2	2	17	THR	2.7

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Mol	Chain	Res	Type	RSRZ
3	3	234	LYS	2.7
4	4	26	ASN	2.7
1	1	162	PRO	2.7
2	2	241	ALA	2.7
2	2	86	LEU	2.7
3	3	221	VAL	2.7
3	3	235	LEU	2.7
1	1	232	PHE	2.7
3	3	207	MET	2.7
1	1	158	GLY	2.7
1	1	47	SER	2.7
1	1	283	SER	2.7
2	2	268	VAL	2.7
3	3	71	PRO	2.6
1	1	209	ARG	2.6
1	1	173	SER	2.6
2	2	254	ALA	2.6
2	2	61	ASN	2.6
3	3	187	GLY	2.6
2	2	164	SER	2.6
1	1	182	TYR	2.6
3	3	133	TYR	2.6
2	2	139	LYS	2.6
3	3	165	MET	2.6
1	1	112	GLN	2.6
1	1	58	THR	2.6
3	3	109	TRP	2.6
4	4	12	ALA	2.6
1	1	278	GLY	2.6
2	2	82	LEU	2.6
4	4	20	ALA	2.6
2	2	172	ARG	2.6
2	2	229	ILE	2.6
1	1	138	PRO	2.6
1	1	280	ASP	2.6
2	2	84	ASP	2.6
2	2	154	GLY	2.6
3	3	76	LEU	2.6
1	1	108	THR	2.6
4	4	7	THR	2.6
4	4	24	THR	2.5
2	2	161	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
2	2	138	SER	2.5
4	4	4	GLN	2.5
3	3	36	ILE	2.5
2	2	142	TYR	2.5
2	2	173	LYS	2.5
2	2	200	LEU	2.5
1	1	163	SER	2.5
2	2	240	ALA	2.5
2	2	197	ILE	2.5
2	2	221	MET	2.5
1	1	264	TRP	2.5
1	1	49	GLN	2.5
2	2	47	ALA	2.5
1	1	118	GLU	2.5
4	4	21	ASN	2.5
2	2	78	TRP	2.5
3	3	126	THR	2.5
3	3	96	HIS	2.5
3	3	58	VAL	2.5
1	1	172	SER	2.4
2	2	10	SER	2.4
3	3	52	LEU	2.4
2	2	271	HIS	2.4
2	2	182	GLY	2.4
3	3	167	ALA	2.4
4	4	54	THR	2.4
1	1	145	VAL	2.4
2	2	124	VAL	2.4
3	3	186	GLY	2.4
3	3	199	VAL	2.4
3	3	53	ILE	2.4
3	3	164	SER	2.4
2	2	180	LEU	2.4
2	2	38	TRP	2.4
3	3	141	PRO	2.4
3	3	184	THR	2.4
1	1	167	ASP	2.4
3	3	60	GLY	2.4
1	1	85	LEU	2.4
2	2	101	LEU	2.4
2	2	136	THR	2.4
2	2	94	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
3	3	118	LEU	2.4
1	1	204	TYR	2.3
1	1	298	PHE	2.3
1	1	196	ILE	2.3
3	3	51	THR	2.3
3	3	176	ARG	2.3
2	2	100	TYR	2.3
3	3	50	ASP	2.3
3	3	39	GLU	2.3
3	3	140	PRO	2.3
4	4	50	PRO	2.3
1	1	17	SER	2.3
1	1	170	TRP	2.3
1	1	273	LEU	2.3
2	2	63	PHE	2.3
3	3	188	PHE	2.3
2	2	178	ASP	2.3
3	3	91	ASP	2.3
1	1	102	ILE	2.3
1	1	286	ILE	2.3
3	3	135	PRO	2.3
3	3	125	ALA	2.3
2	2	207	THR	2.3
3	3	195	THR	2.3
1	1	39	LEU	2.3
3	3	40	VAL	2.3
2	2	194	PRO	2.3
3	3	230	ILE	2.3
3	3	149	LEU	2.3
3	3	77	SER	2.3
1	1	200	TYR	2.3
2	2	30	ASN	2.3
2	2	201	ARG	2.3
1	1	237	VAL	2.3
2	2	93	GLY	2.2
4	4	66	PRO	2.2
3	3	215	ALA	2.2
1	1	168	TYR	2.2
3	3	87	SER	2.2
2	2	232	LEU	2.2
1	1	252	VAL	2.2
2	2	259	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	1	235	LEU	2.2
2	2	53	PRO	2.2
3	3	41	LYS	2.2
3	3	110	THR	2.2
1	1	29	SER	2.2
2	2	237	LEU	2.2
3	3	131	LEU	2.2
1	1	265	CYS	2.2
2	2	171	GLY	2.2
3	3	22	PRO	2.2
1	1	24	SER	2.2
2	2	104	SER	2.2
2	2	119	GLN	2.2
2	2	169	SER	2.2
2	2	66	LEU	2.2
3	3	223	LEU	2.2
2	2	55	GLU	2.2
2	2	165	ASN	2.2
1	1	220	GLY	2.2
1	1	293	ASP	2.2
1	1	107	TYR	2.1
2	2	35	TYR	2.1
1	1	164	SER	2.1
3	3	85	SER	2.1
3	3	138	ALA	2.1
4	4	51	SER	2.1
2	2	264	ARG	2.1
1	1	224	TYR	2.1
1	1	295	ILE	2.1
3	3	134	SER	2.1
2	2	265	ASN	2.1
2	2	85	CYS	2.1
1	1	270	ARG	2.1
3	3	55	MET	2.1
3	3	98	MET	2.1
1	1	211	PRO	2.1
2	2	77	GLY	2.1
1	1	123	SER	2.1
1	1	101	ASN	2.1
1	1	42	VAL	2.1
1	1	254	VAL	2.1
1	1	272	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	2	110	VAL	2.1
2	2	210	VAL	2.1
1	1	87	LEU	2.1
4	4	68	LEU	2.1
2	2	202	THR	2.1
3	3	97	THR	2.1
2	2	36	GLY	2.1
2	2	123	GLY	2.1
4	4	23	SER	2.1
1	1	105	ILE	2.1
2	2	18	LEU	2.1
3	3	46	LEU	2.1
4	4	62	LEU	2.1
1	1	109	ASP	2.1
1	1	121	THR	2.1
1	1	130	THR	2.1
3	3	107	THR	2.1
4	4	42	THR	2.1
1	1	197	ALA	2.1
1	1	236	ALA	2.1
3	3	47	ALA	2.1
2	2	156	GLU	2.1
3	3	26	PRO	2.1
3	3	220	SER	2.0
1	1	166	ASP	2.0
1	1	250	THR	2.0
2	2	73	THR	2.0
3	3	74	ASP	2.0
1	1	190	SER	2.0
1	1	223	PHE	2.0
2	2	174	PHE	2.0
3	3	66	GLU	2.0
1	1	191	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

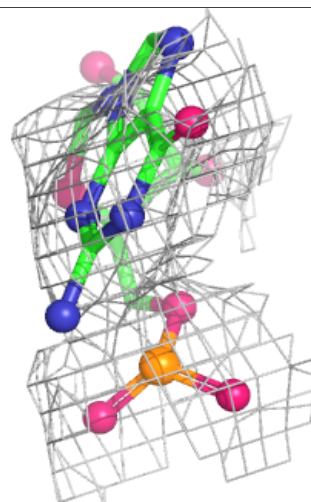
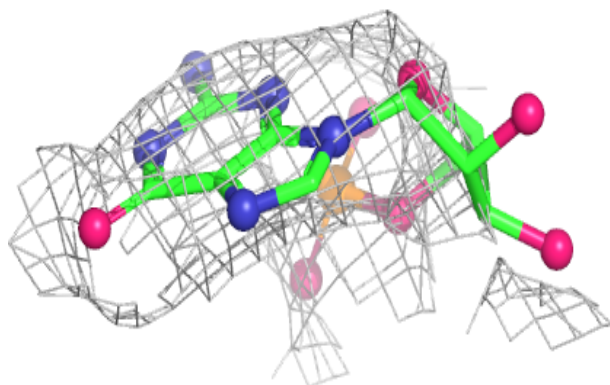
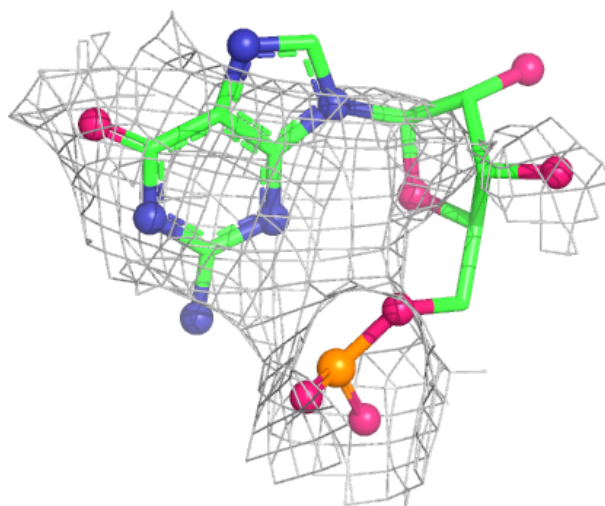
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	5GP	2	273	23/24	0.66	0.45	94,98,113,114	23
6	MYR	4	1	15/16	0.76	0.39	58,70,82,83	0
6	MYR	1	300	16/16	0.84	0.28	36,41,71,72	0
5	CA	1	299	1/1	0.86	0.09	58,58,58,58	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 5GP 2 273:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.