



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:15 AM GMT

PDB ID : 3H5C  
Title : X-Ray Structure of Protein Z-Protein Z Inhibitor Complex  
Authors : Dementiev, A.A.; Huang, X.; Olson, S.T.; Gettins, P.G.W.  
Deposited on : 2009-04-21  
Resolution : 3.26 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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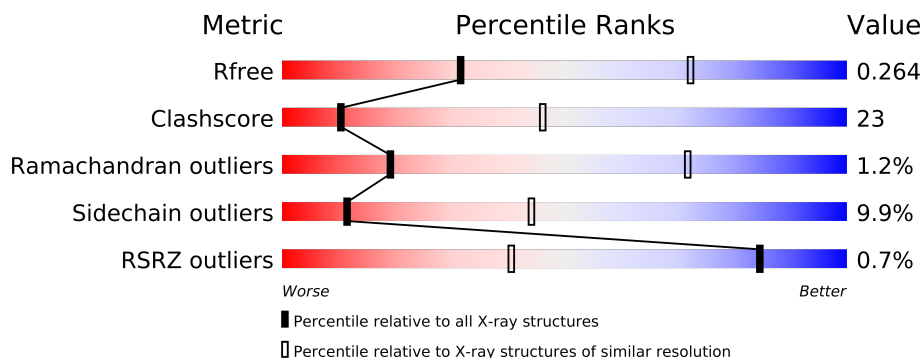
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.26 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))
$R_{free}$	66092	1085 (3.32-3.20)
Clashscore	79885	1374 (3.32-3.20)
Ramachandran outliers	78287	1348 (3.32-3.20)
Sidechain outliers	78261	1346 (3.32-3.20)
RSRZ outliers	66119	1086 (3.32-3.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	423	
2	B	317	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	NAG	A	502	-	X
3	NAG	B	403	-	X
3	NAG	B	405	-	X

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 5357 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Protein Z-dependent protease inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	0	0
			2930	1891	497	521	21			

- Molecule 2 is a protein called Vitamin K-dependent protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	312	Total	C	N	O	S	0	0	0
			2313	1436	413	439	25			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



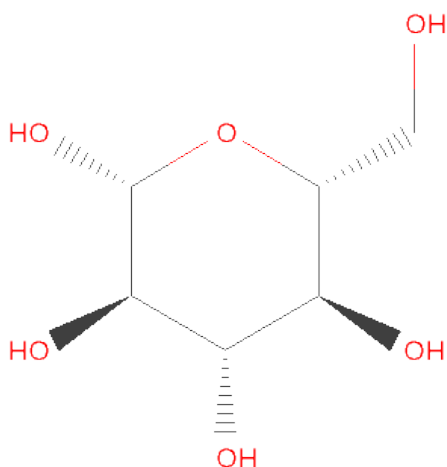
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 4 is SUGAR (BETA-D-GLUCOSE) (three-letter code: BGC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is water.

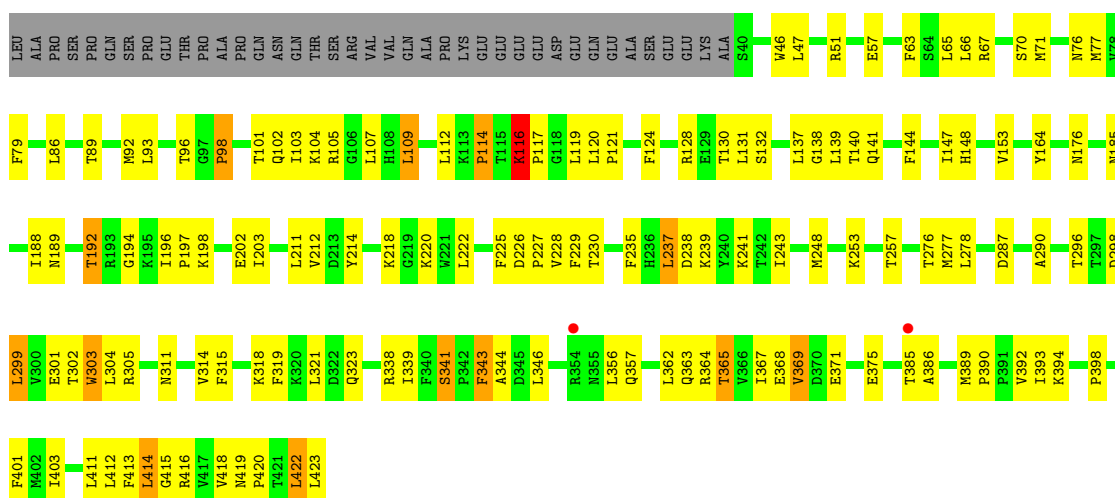
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total	O	0	0
			10	10		
5	B	9	Total	O	0	0
			9	9		

### 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.

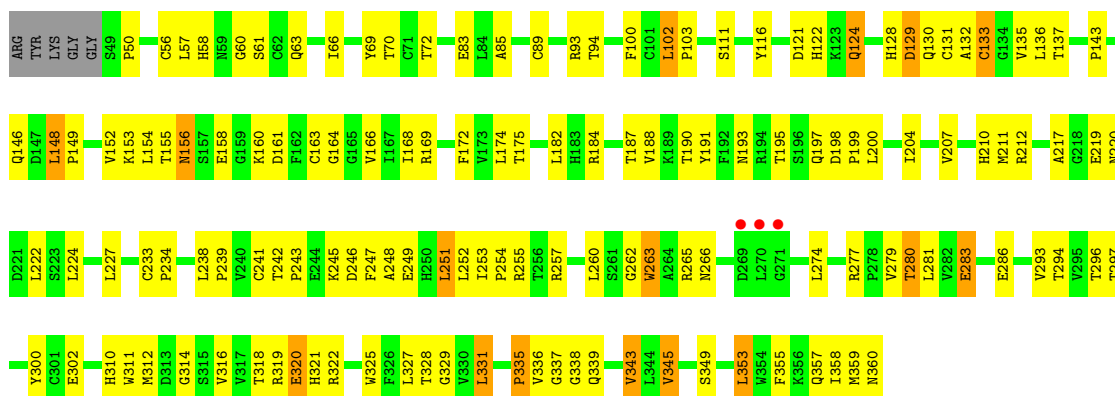
- Molecule 1: Protein Z-dependent protease inhibitor

Chain A:



- Molecule 2: Vitamin K-dependent protein Z

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.93Å 119.93Å 347.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.58 – 3.26 44.58 – 3.26	Depositor EDS
% Data completeness (in resolution range)	97.8 (44.58-3.26) 97.8 (44.58-3.26)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.201 , 0.269 0.214 , 0.264	Depositor DCC
$R_{free}$ test set	1703 reflections (7.82%)	DCC
Wilson B-factor (Å <sup>2</sup> )	83.6	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 59.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 23487 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5357	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.27	0/2994	0.50	0/4059
2	B	0.27	0/2364	0.54	0/3219
All	All	0.27	0/5358	0.52	0/7278

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2930	0	2845	125	0
2	B	2313	0	2098	123	0
3	A	28	0	26	0	0
3	B	56	0	52	0	0
4	B	11	0	10	8	0
5	A	10	0	0	2	0
5	B	9	0	0	0	0
All	All	5357	0	5031	242	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 23.

All (242) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:116:LYS:HB3	1:A:117:PRO:CD	1.53	1.37
1:A:116:LYS:CB	1:A:117:PRO:CD	2.22	1.15
1:A:116:LYS:CG	1:A:117:PRO:HD3	1.75	1.14
1:A:422:LEU:O	1:A:423:LEU:HB2	1.48	1.13
1:A:116:LYS:HB3	1:A:117:PRO:HD2	1.06	1.04
1:A:298:ASP:O	1:A:302:THR:HG23	1.64	0.98
1:A:89:THR:HG22	1:A:120:LEU:HG	1.44	0.96
1:A:116:LYS:HG3	1:A:117:PRO:HD3	1.47	0.95
1:A:116:LYS:CB	1:A:117:PRO:HD3	1.93	0.94
2:B:129:ASP:CB	2:B:130:GLN:HA	1.99	0.91
1:A:131:LEU:HB3	1:A:141:GLN:HE21	1.38	0.85
1:A:321:LEU:HD22	1:A:423:LEU:HG	1.57	0.84
2:B:148:LEU:H	2:B:148:LEU:HD23	1.43	0.84
1:A:403:ILE:HB	1:A:413:PHE:HB2	1.61	0.83
1:A:76:ASN:HD22	1:A:423:LEU:HD23	1.49	0.78
1:A:296:THR:HG23	1:A:299:LEU:H	1.49	0.78
2:B:128:HIS:O	2:B:128:HIS:CG	2.37	0.76
1:A:76:ASN:HB2	1:A:423:LEU:HD21	1.70	0.72
2:B:116:TYR:CE1	2:B:132:ALA:HB1	2.23	0.72
1:A:185:ASN:HD22	1:A:198:LYS:HA	1.53	0.72
2:B:69:TYR:CE2	4:B:401:BGC:C6	2.74	0.71
2:B:338:GLY:HA2	2:B:339:GLN:HB2	1.71	0.71
2:B:262:GLY:O	2:B:274:LEU:HD12	1.91	0.71
1:A:46:TRP:CH2	1:A:114:PRO:HB3	2.26	0.70
1:A:116:LYS:HD3	1:A:116:LYS:C	2.11	0.70
1:A:117:PRO:O	1:A:121:PRO:HD2	1.91	0.69
2:B:318:THR:HG22	2:B:327:LEU:HA	1.74	0.69
2:B:238:LEU:HD12	2:B:239:PRO:HD2	1.75	0.69
1:A:228:VAL:HG12	5:A:433:HOH:O	1.93	0.69
1:A:124:PHE:CD2	1:A:164:TYR:HB3	2.28	0.68
2:B:156:ASN:C	2:B:156:ASN:HD22	1.97	0.68
2:B:57:LEU:HD23	2:B:57:LEU:H	1.59	0.68
1:A:116:LYS:CD	1:A:117:PRO:HD3	2.23	0.67
1:A:93:LEU:HD12	1:A:120:LEU:HD22	1.76	0.67
2:B:257:ARG:HG2	2:B:280:THR:HG23	1.76	0.67
2:B:56:CYS:HB3	2:B:60:GLY:HA3	1.77	0.66
2:B:190:THR:HG22	2:B:200:LEU:HB3	1.77	0.66
2:B:153:LYS:HD3	2:B:161:ASP:OD2	1.96	0.66
1:A:192:THR:HG21	1:A:196:ILE:H	1.61	0.66
2:B:148:LEU:N	2:B:148:LEU:HD23	2.10	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:76:ASN:HD22	1:A:423:LEU:CD2	2.09	0.65
2:B:129:ASP:HB3	2:B:130:GLN:HA	1.78	0.65
1:A:229:PHE:CZ	5:A:432:HOH:O	2.50	0.65
1:A:76:ASN:ND2	1:A:423:LEU:HD23	2.11	0.64
1:A:144:PHE:HB2	1:A:212:VAL:HG22	1.79	0.64
1:A:92:MET:HE1	1:A:119:LEU:HD23	1.80	0.64
2:B:319:ARG:HH21	2:B:328:THR:HG21	1.62	0.64
1:A:131:LEU:HD12	1:A:132:SER:N	2.14	0.63
2:B:191:TYR:CE2	2:B:199:PRO:HG3	2.34	0.63
2:B:164:GLY:C	2:B:314:GLY:HA3	2.19	0.62
1:A:128:ARG:HD3	1:A:128:ARG:C	2.19	0.62
1:A:93:LEU:HB2	1:A:120:LEU:HD21	1.82	0.62
2:B:319:ARG:NH2	2:B:328:THR:HG21	2.15	0.62
1:A:192:THR:CG2	1:A:196:ILE:H	2.14	0.61
2:B:69:TYR:CD2	4:B:401:BGC:H6C2	2.36	0.61
2:B:337:GLY:O	2:B:339:GLN:HB2	2.00	0.61
1:A:120:LEU:N	1:A:120:LEU:HD12	2.16	0.61
2:B:129:ASP:CB	2:B:130:GLN:CA	2.78	0.61
1:A:76:ASN:HB2	1:A:423:LEU:CD2	2.32	0.60
2:B:172:PHE:CG	2:B:359:MET:HE3	2.37	0.60
1:A:225:PHE:HB2	1:A:371:GLU:HB2	1.83	0.59
2:B:129:ASP:HB3	2:B:131:CYS:N	2.18	0.59
2:B:69:TYR:CE2	4:B:401:BGC:H6C1	2.36	0.59
1:A:124:PHE:HD2	1:A:164:TYR:HB3	1.67	0.58
1:A:112:LEU:O	1:A:114:PRO:HD3	2.02	0.58
2:B:129:ASP:HB3	2:B:130:GLN:CA	2.32	0.58
2:B:174:LEU:HD11	2:B:222:LEU:HG	1.85	0.58
2:B:355:PHE:O	2:B:359:MET:HG3	2.04	0.57
2:B:164:GLY:O	2:B:314:GLY:HA3	2.04	0.57
2:B:243:PRO:HB2	2:B:248:ALA:HB2	1.85	0.57
1:A:117:PRO:O	1:A:121:PRO:CD	2.53	0.57
2:B:69:TYR:HE2	4:B:401:BGC:C6	2.18	0.57
2:B:166:VAL:CG2	2:B:316:VAL:HG11	2.35	0.57
1:A:338:ARG:O	1:A:344:ALA:HB2	2.04	0.57
2:B:353:LEU:HD22	2:B:357:GLN:HG2	1.86	0.57
2:B:300:TYR:OH	2:B:328:THR:HG23	2.05	0.56
2:B:128:HIS:O	2:B:128:HIS:CD2	2.57	0.56
2:B:69:TYR:CD2	4:B:401:BGC:C6	2.89	0.56
2:B:166:VAL:HG21	2:B:316:VAL:HG11	1.88	0.56
1:A:225:PHE:HB2	1:A:371:GLU:CB	2.36	0.56
2:B:191:TYR:HE2	2:B:199:PRO:HG3	1.71	0.55
1:A:341:SER:C	1:A:357:GLN:OE1	2.44	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:70:SER:O	2:B:297:THR:HG21	2.07	0.54
1:A:185:ASN:HD22	1:A:198:LYS:CA	2.18	0.54
1:A:89:THR:CG2	1:A:120:LEU:HG	2.29	0.54
2:B:129:ASP:N	2:B:130:GLN:HA	2.21	0.53
2:B:241:CYS:HB2	2:B:325:TRP:O	2.08	0.53
2:B:263:TRP:CD1	2:B:263:TRP:N	2.76	0.53
2:B:63:GLN:HB2	2:B:70:THR:HB	1.89	0.53
1:A:218:LYS:HD2	1:A:368:GLU:HG2	1.90	0.53
2:B:188:VAL:HG23	2:B:204:ILE:HD11	1.91	0.53
1:A:419:ASN:ND2	1:A:422:LEU:HG	2.24	0.53
2:B:129:ASP:HB2	2:B:130:GLN:HA	1.88	0.53
2:B:121:ASP:OD1	2:B:124:GLN:NE2	2.42	0.52
1:A:76:ASN:HD22	1:A:423:LEU:CG	2.23	0.52
2:B:129:ASP:HB3	2:B:131:CYS:H	1.74	0.52
2:B:121:ASP:O	2:B:122:HIS:HB2	2.09	0.52
1:A:107:LEU:HB2	1:A:109:LEU:CD2	2.40	0.52
2:B:156:ASN:HD22	2:B:158:GLU:H	1.56	0.52
2:B:132:ALA:C	2:B:133:CYS:SG	2.88	0.52
1:A:124:PHE:HD2	1:A:164:TYR:C	2.13	0.51
2:B:69:TYR:HE2	4:B:401:BGC:H6C1	1.75	0.51
2:B:338:GLY:CA	2:B:339:GLN:HB2	2.40	0.51
2:B:169:ARG:HD3	2:B:359:MET:HE2	1.92	0.51
1:A:301:GLU:HA	1:A:304:LEU:HB2	1.91	0.51
1:A:220:LYS:HG2	1:A:375:GLU:HG3	1.93	0.51
1:A:314:VAL:HG22	1:A:393:ILE:HG23	1.93	0.51
2:B:102:LEU:HD23	2:B:103:PRO:HD2	1.92	0.51
2:B:136:LEU:HD12	2:B:137:THR:H	1.76	0.51
1:A:101:THR:O	1:A:105:ARG:HG3	2.11	0.51
2:B:217:ALA:HB3	2:B:219:GLU:HG2	1.93	0.50
1:A:77:MET:HA	1:A:323:GLN:HE22	1.76	0.50
2:B:135:VAL:HG11	2:B:325:TRP:HE1	1.76	0.50
2:B:57:LEU:HG	2:B:58:HIS:ND1	2.26	0.50
2:B:283:GLU:HG3	2:B:286:GLU:OE2	2.12	0.50
1:A:116:LYS:CG	1:A:117:PRO:CD	2.58	0.50
2:B:155:THR:HG22	2:B:161:ASP:OD1	2.12	0.50
2:B:311:TRP:O	2:B:312:MET:C	2.50	0.50
2:B:69:TYR:CE2	4:B:401:BGC:H6C2	2.46	0.50
2:B:168:ILE:HG22	2:B:359:MET:HE1	1.94	0.50
1:A:214:TYR:HA	1:A:364:ARG:O	2.12	0.49
1:A:124:PHE:N	1:A:124:PHE:CD1	2.79	0.49
2:B:156:ASN:ND2	2:B:158:GLU:H	2.10	0.49
2:B:85:ALA:O	2:B:93:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:343:PHE:N	1:A:343:PHE:CD1	2.80	0.49
1:A:121:PRO:HG3	1:A:164:TYR:CE2	2.47	0.49
2:B:129:ASP:CB	2:B:131:CYS:H	2.25	0.49
1:A:389:MET:N	1:A:390:PRO:CD	2.76	0.49
1:A:147:ILE:HG12	1:A:148:HIS:N	2.28	0.49
1:A:318:LYS:HE2	1:A:371:GLU:OE2	2.11	0.49
2:B:210:HIS:CE1	2:B:212:ARG:HB2	2.48	0.49
2:B:359:MET:O	2:B:360:ASN:HB2	2.13	0.49
1:A:202:GLU:O	1:A:203:ILE:HG13	2.13	0.49
2:B:204:ILE:CD1	2:B:227:LEU:HD23	2.43	0.49
2:B:172:PHE:CB	2:B:359:MET:HE3	2.42	0.48
1:A:276:THR:HG22	1:A:277:MET:N	2.28	0.48
1:A:401:PHE:CZ	1:A:415:GLY:HA3	2.48	0.48
2:B:149:PRO:HB2	2:B:238:LEU:HB3	1.95	0.48
1:A:235:PHE:CE1	1:A:420:PRO:HD3	2.48	0.48
1:A:296:THR:HG22	1:A:299:LEU:HB2	1.94	0.48
1:A:385:THR:CB	1:A:386:ALA:HA	2.42	0.48
2:B:251:LEU:O	2:B:255:ARG:HB2	2.14	0.48
1:A:290:ALA:HB1	2:B:353:LEU:HB2	1.95	0.48
2:B:61:SER:HB2	2:B:72:THR:HB	1.95	0.48
2:B:331:LEU:HD11	2:B:343:VAL:CG2	2.44	0.48
2:B:335:PRO:CB	2:B:336:VAL:HA	2.43	0.48
1:A:124:PHE:N	1:A:124:PHE:HD1	2.12	0.47
1:A:225:PHE:CD2	1:A:248:MET:HE3	2.49	0.47
1:A:369:VAL:HG22	1:A:369:VAL:O	2.13	0.47
1:A:363:GLN:HG2	1:A:365:THR:HG22	1.95	0.47
2:B:283:GLU:H	2:B:283:GLU:HG2	1.46	0.47
1:A:92:MET:CE	1:A:119:LEU:HD23	2.44	0.47
1:A:319:PHE:CE2	1:A:369:VAL:HG11	2.49	0.47
1:A:315:PHE:CD2	1:A:394:LYS:HG2	2.49	0.47
2:B:129:ASP:H	2:B:130:GLN:HA	1.80	0.46
1:A:67:ARG:NH2	2:B:212:ARG:HH21	2.13	0.46
1:A:278:LEU:O	1:A:401:PHE:HA	2.15	0.46
2:B:154:LEU:HD12	2:B:163:CYS:HB3	1.98	0.46
2:B:57:LEU:CD2	2:B:57:LEU:H	2.26	0.46
2:B:100:PHE:HB2	2:B:111:SER:HB3	1.96	0.46
2:B:198:ASP:HA	2:B:199:PRO:HD3	1.82	0.46
1:A:314:VAL:HG22	1:A:393:ILE:CG2	2.45	0.46
1:A:185:ASN:O	1:A:189:ASN:HB2	2.15	0.46
2:B:190:THR:CG2	2:B:200:LEU:HB3	2.45	0.46
2:B:253:ILE:N	2:B:254:PRO:CD	2.79	0.46
1:A:104:LYS:O	1:A:109:LEU:HD23	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:422:LEU:O	1:A:423:LEU:CB	2.36	0.45
1:A:57:GLU:HA	1:A:57:GLU:OE1	2.16	0.45
1:A:239:LYS:HG3	2:B:246:ASP:OD2	2.16	0.45
1:A:323:GLN:OE1	1:A:423:LEU:HD11	2.15	0.45
2:B:245:LYS:O	2:B:249:GLU:HG3	2.16	0.45
2:B:188:VAL:HG21	2:B:227:LEU:HD21	1.99	0.45
2:B:191:TYR:CE2	2:B:199:PRO:HB3	2.52	0.45
2:B:152:VAL:HG11	2:B:188:VAL:HG13	1.97	0.45
1:A:392:VAL:HG12	1:A:393:ILE:N	2.32	0.45
2:B:251:LEU:HD12	2:B:252:LEU:N	2.31	0.45
2:B:265:ARG:CB	2:B:266:ASN:HA	2.46	0.45
1:A:71:MET:HG3	2:B:296:THR:HB	1.99	0.45
1:A:362:LEU:HD23	1:A:362:LEU:N	2.32	0.45
2:B:338:GLY:HA2	2:B:339:GLN:C	2.36	0.45
2:B:224:LEU:HD12	2:B:358:ILE:HD12	1.98	0.45
2:B:148:LEU:CD2	2:B:148:LEU:N	2.79	0.44
2:B:156:ASN:C	2:B:156:ASN:ND2	2.68	0.44
2:B:245:LYS:HA	2:B:349:SER:HB2	1.99	0.44
2:B:210:HIS:HE1	2:B:212:ARG:HB2	1.83	0.44
2:B:279:VAL:HB	2:B:302:GLU:HB3	2.00	0.44
1:A:46:TRP:CE3	1:A:47:LEU:HD23	2.52	0.44
1:A:66:LEU:C	1:A:66:LEU:HD23	2.38	0.44
2:B:155:THR:HA	2:B:160:LYS:O	2.18	0.44
1:A:147:ILE:HG12	1:A:148:HIS:H	1.83	0.44
1:A:131:LEU:HB3	1:A:141:GLN:NE2	2.19	0.44
2:B:89:CYS:HA	2:B:93:ARG:HH12	1.83	0.43
2:B:242:THR:HA	2:B:243:PRO:HD3	1.79	0.43
2:B:152:VAL:CG1	2:B:188:VAL:HG13	2.49	0.43
2:B:212:ARG:HB3	2:B:220:ASN:HD22	1.83	0.43
1:A:346:LEU:HB2	1:A:356:LEU:HD22	2.00	0.43
2:B:247:PHE:CE2	2:B:251:LEU:HD11	2.53	0.43
1:A:107:LEU:HB2	1:A:109:LEU:HD22	2.01	0.43
2:B:252:LEU:HD21	2:B:321:HIS:HB2	2.00	0.43
2:B:233:CYS:HB2	2:B:234:PRO:HA	2.00	0.43
1:A:120:LEU:N	1:A:120:LEU:CD1	2.81	0.43
1:A:131:LEU:HD12	1:A:131:LEU:C	2.39	0.43
1:A:227:PRO:HA	1:A:230:THR:HG23	2.01	0.43
2:B:320:GLU:HB3	2:B:325:TRP:CD2	2.53	0.43
1:A:103:ILE:HD11	1:A:339:ILE:HD12	2.00	0.42
1:A:63:PHE:CD1	1:A:414:LEU:HD11	2.54	0.42
1:A:116:LYS:CD	1:A:117:PRO:CD	2.94	0.42
2:B:293:VAL:HG12	2:B:294:THR:N	2.34	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:230:THR:HG21	1:A:371:GLU:OE1	2.19	0.42
1:A:339:ILE:HG12	1:A:339:ILE:O	2.20	0.42
2:B:195:THR:HG22	2:B:197:GLN:H	1.84	0.42
1:A:77:MET:HE3	1:A:416:ARG:CZ	2.50	0.42
1:A:137:LEU:O	1:A:137:LEU:HD12	2.20	0.42
2:B:321:HIS:NE2	2:B:322:ARG:HD2	2.35	0.42
1:A:79:PHE:HA	1:A:365:THR:HG21	2.01	0.42
1:A:86:LEU:C	1:A:86:LEU:HD23	2.40	0.42
1:A:241:LYS:HB2	1:A:241:LYS:HE3	1.93	0.42
1:A:237:LEU:O	1:A:238:ASP:HB3	2.20	0.42
2:B:329:GLY:HA3	2:B:345:VAL:HG11	2.02	0.42
1:A:287:ASP:HB2	2:B:245:LYS:NZ	2.34	0.41
2:B:102:LEU:HA	2:B:103:PRO:HD2	1.95	0.41
1:A:398:PRO:HB3	1:A:418:VAL:HA	2.01	0.41
2:B:69:TYR:CD2	4:B:401:BGC:H6C1	2.54	0.41
2:B:146:GLN:HA	2:B:274:LEU:HB3	2.01	0.41
1:A:230:THR:HG22	1:A:248:MET:HA	2.01	0.41
1:A:237:LEU:HD12	1:A:243:ILE:HD13	2.02	0.41
1:A:138:GLY:HA3	1:A:139:LEU:HA	1.69	0.41
1:A:257:THR:HG21	1:A:303:TRP:O	2.21	0.41
1:A:47:LEU:O	1:A:51:ARG:HG3	2.21	0.41
2:B:172:PHE:HB2	2:B:359:MET:CE	2.50	0.41
1:A:188:ILE:O	1:A:192:THR:HB	2.21	0.41
1:A:98:PRO:O	1:A:101:THR:HG22	2.21	0.41
1:A:101:THR:HG23	1:A:102:GLN:N	2.36	0.41
2:B:302:GLU:HB2	2:B:343:VAL:HG12	2.02	0.41
1:A:302:THR:O	1:A:305:ARG:HG2	2.20	0.41
2:B:129:ASP:H	2:B:130:GLN:CA	2.34	0.41
1:A:226:ASP:OD1	1:A:228:VAL:HG23	2.21	0.41
1:A:321:LEU:HA	1:A:423:LEU:HB3	2.03	0.41
1:A:414:LEU:HA	1:A:414:LEU:HD23	1.86	0.41
1:A:189:ASN:ND2	1:A:194:GLY:HA2	2.35	0.40
2:B:135:VAL:HG13	2:B:135:VAL:O	2.22	0.40
1:A:276:THR:CG2	1:A:277:MET:N	2.84	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	382/423 (90%)	326 (85%)	51 (13%)	5 (1%)	18	70
2	B	310/317 (98%)	253 (82%)	54 (17%)	3 (1%)	22	75
All	All	692/740 (94%)	579 (84%)	105 (15%)	8 (1%)	19	72

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	LYS
2	B	335	PRO
1	A	197	PRO
2	B	143	PRO
1	A	114	PRO
1	A	153	VAL
1	A	98	PRO
2	B	50	PRO

### 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	298/377 (79%)	274 (92%)	24 (8%)	17	58
2	B	239/275 (87%)	210 (88%)	29 (12%)	7	34
All	All	537/652 (82%)	484 (90%)	53 (10%)	11	44

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LEU

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Mol	Chain	Res	Type
1	A	96	THR
1	A	109	LEU
1	A	116	LYS
1	A	130	THR
1	A	140	THR
1	A	176	ASN
1	A	192	THR
1	A	211	LEU
1	A	222	LEU
1	A	237	LEU
1	A	253	LYS
1	A	299	LEU
1	A	303	TRP
1	A	311	ASN
1	A	341	SER
1	A	343	PHE
1	A	365	THR
1	A	367	ILE
1	A	369	VAL
1	A	411	LEU
1	A	412	LEU
1	A	414	LEU
1	A	422	LEU
2	B	66	ILE
2	B	83	GLU
2	B	94	THR
2	B	102	LEU
2	B	124	GLN
2	B	129	ASP
2	B	133	CYS
2	B	148	LEU
2	B	156	ASN
2	B	175	THR
2	B	182	LEU
2	B	184	ARG
2	B	187	THR
2	B	193	ASN
2	B	207	VAL
2	B	211	MET
2	B	251	LEU
2	B	260	LEU
2	B	263	TRP

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Mol	Chain	Res	Type
2	B	277	ARG
2	B	280	THR
2	B	281	LEU
2	B	283	GLU
2	B	310	HIS
2	B	320	GLU
2	B	331	LEU
2	B	343	VAL
2	B	345	VAL
2	B	353	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	GLN
1	A	185	ASN
1	A	189	ASN
1	A	272	GLN
1	A	323	GLN
2	B	124	GLN
2	B	128	HIS
2	B	156	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

7 ligands 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	$\# Z  > 2$
3	NAG	A	501	1	12,14,15	0.62	0	15,19,21	0.81	1 (6%)
3	NAG	A	502	1	12,14,15	0.66	1 (8%)	15,19,21	1.22	2 (13%)
4	BGC	B	401	-	10,11,12	0.80	0	11,15,17	0.86	1 (9%)
3	NAG	B	402	2	12,14,15	0.66	1 (8%)	15,19,21	1.03	1 (6%)
3	NAG	B	403	2	12,14,15	0.62	0	15,19,21	1.16	2 (13%)
3	NAG	B	404	2	12,14,15	0.58	0	15,19,21	1.13	2 (13%)
3	NAG	B	405	2	12,14,15	0.63	0	15,19,21	0.67	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
3	NAG	A	501	1	-	0/6/23/26	0/1/1/1
3	NAG	A	502	1	-	1/6/23/26	0/1/1/1
4	BGC	B	401	-	-	0/2/19/22	0/1/1/1
3	NAG	B	402	2	-	0/6/23/26	0/1/1/1
3	NAG	B	403	2	-	0/6/23/26	0/1/1/1
3	NAG	B	404	2	-	1/6/23/26	0/1/1/1
3	NAG	B	405	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	NAG	O5-C5	-2.02	1.41	1.45
3	B	402	NAG	O5-C5	-2.02	1.41	1.45

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	NAG	O5-C5-C6	3.04	110.17	106.98
3	A	502	NAG	C2-N2-C7	2.68	127.59	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	403	NAG	O5-C5-C6	2.61	109.72	106.98
3	B	404	NAG	C2-N2-C7	2.45	127.20	123.09
3	B	403	NAG	C2-N2-C7	2.27	126.91	123.09
4	B	401	BGC	O5-C5-C6	2.27	109.36	106.98
3	A	502	NAG	O5-C5-C6	2.23	109.32	106.98
3	B	404	NAG	O5-C5-C6	2.09	109.17	106.98
3	A	501	NAG	O5-C5-C6	2.08	109.16	106.98

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	404	NAG	C1-C2-N2-C7
3	A	502	NAG	C1-C2-N2-C7

There are no ring outliers.

## 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	384/423 (90%)	-0.17	2 (0%)	88 48	54, 76, 139, 164	0
2	B	312/317 (98%)	-0.03	3 (0%)	79 32	53, 89, 148, 200	0
All	All	696/740 (94%)	-0.10	5 (0%)	84 40	53, 82, 145, 200	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	269	ASP	3.2
2	B	270	LEU	2.8
1	A	385	THR	2.8
2	B	271	GLY	2.6
1	A	354	ARG	2.3

### 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	B	405	14/15	0.37	9.94	144,156,160,162	0
3	NAG	A	502	14/15	0.31	3.36	119,127,138,138	0
3	NAG	B	403	14/15	0.42	2.52	121,135,141,141	0
3	NAG	B	404	14/15	0.31	1.56	131,146,157,158	0
4	BGC	B	401	11/12	0.39	0.99	147,156,162,163	0
3	NAG	A	501	14/15	0.29	-0.81	149,159,163,163	0
3	NAG	B	402	14/15	0.47	-	155,180,189,192	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.