



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:26 PM GMT

PDB ID : 1B3O  
Title : TERNARY COMPLEX OF HUMAN TYPE-II INOSINE MONOPHOSPHATE DEHYDROGENASE WITH 6-CL-IMP AND SELENAZOLE ADENINE DINUCLEOTIDE  
Authors : Colby, T.D.; Vanderveen, K.; Strickler, M.D.; Goldstein, B.M.  
Deposited on : 1998-12-14  
Resolution : 2.90 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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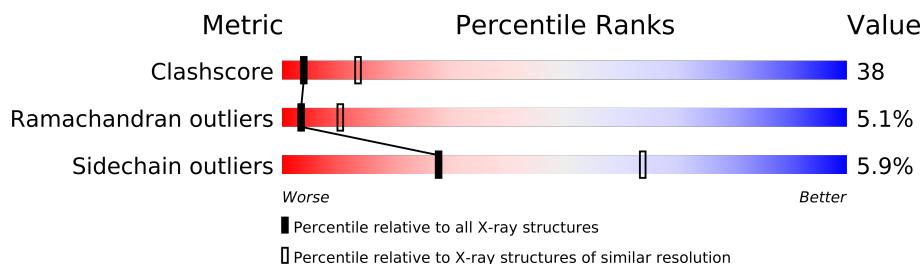
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : **FAILED**  
Percentile statistics : 21963  
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 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))
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (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  $\geq 3$ , 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.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	514	
1	B	514	

## 2 Entry composition i

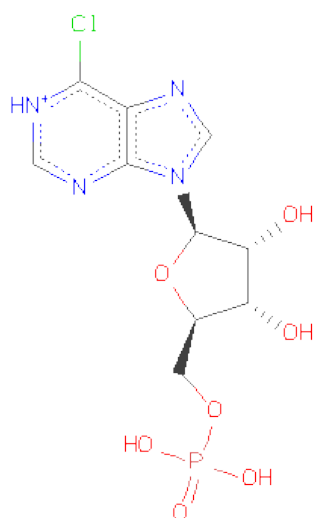
There are 5 unique types of molecules in this entry. The entry contains 5536 atoms, of which 0 are hydrogen and 0 are deuterium.

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 (INOSINE MONOPHOSPHATE DEHYDROGENASE 2).

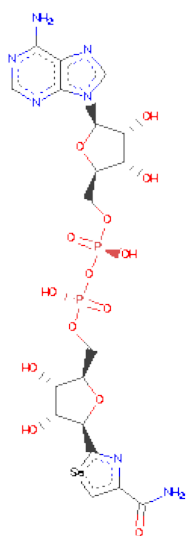
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	3
			2275	1434	389	439	13			
1	B	414	Total	C	N	O	S	0	0	4
			3085	1941	535	591	18			

- Molecule 2 is 6-CHLOROPURINE RIBOSIDE, 5'-MONOPHOSPHATE (three-letter code: CPR) (formula: C<sub>10</sub>H<sub>13</sub>ClN<sub>4</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	10	4	7	1		
2	B	1	Total	C	N	O	P	0	0
			22	10	4	7	1		

- Molecule 3 is SELENAZOLE-4-CARBOXYAMIDE-ADENINEDINUCLEOTIDE (three-letter code: SAE) (formula: C<sub>19</sub>H<sub>25</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>Se).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	Se	0	0
			43	19	7	14	2	1		
3	B	1	Total	C	N	O	P	Se	0	0
			43	19	7	14	2	1		

- Molecule 4 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	15	Total	X	15	0
			15	15		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total	O	0	0
			11	11		
5	B	20	Total	O	0	0
			20	20		



PHE	I1E	I373	I284	I211
	LYS	A374	N285	V212
	VAL	K375	M286	N213
	ALA	A376	I287	E214
	GLN	L377	K291	D215
	GLY	A378		D216
	VAL	L379	D292	E217
	SER	T383	K293	L218
	GLY		Y294	V219
	ALA	V384	P295	A220
	VAL	M385	Q298	I221
	GLN	M386		I222
	D449	G387	V299	A223
	K450	S388	I300	R224
	I453	L389	G301	T225
	H454	L390	N302	D226
	K455	A391	V303	L227
	F456	A392	V304	K228
	V457	E395	V305	K229
	P458		T306	V230
	Y459	G398	Q309	R231
	L460	E399		L235
	I461	PHE	L313	A236
	I464	PHE	V318	S237
	Q465	SER		D319
	I471	ASP	A320	D239
	G472	GLY	L321	A240
	A473	I1E	R322	K241
	L476	ARG	G328	K242
		LEU		Q243
	L476	LYS	S329	C246
	T477	LYS	I330	G247
	Q478	TYR	C331	A248
	M483	ARG	I332	A249
		GLY	T333	H253
	L488	MET	Q334	
		GLY	E335	D261
	R493	SER	V336	
	T494	LEU	L337	D263
	A497	ASP	A338	A264
ALA		Q343	Q265	
Q498	MET	ASP	K349	D269
V499	LYS	L346		
GLU	HIS	K349	V270	
GLY	LEU		S351	V271
VAL	SER	E352	V272	
HIS	GLN	R355	L273	
SER	ASN		D274	
LEU	ARG	TYR	Q277	S280
	HIS	R356		
	SER	PHE	F282	
	TYR	SER	Q283	
	GLU	GLU		
	LYS	ALA		
ARG	ASP			
LEU	LYS			

## 4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.26Å 142.26Å 174.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.90	Depositor
% Data completeness (in resolution range)	86.4 (100.00-2.90)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 2.85Å)	Xtriage
Refinement program	CNS 0.3	Depositor
R, $R_{free}$	0.244 , 0.270	Depositor
Wilson B-factor (Å <sup>2</sup> )	44.3	Xtriage
Anisotropy	0.068	Xtriage
Estimated twinning fraction	0.039 for -h,k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 33820 reflections (0.003%)	Xtriage
Total number of atoms	5536	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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: UNX, CPR, SAE

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	0.49	0/2308	0.77	0/3122
1	B	0.58	0/3125	0.85	2/4224 (0.0%)
All	All	0.54	0/5433	0.82	2/7346 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	181	LYS	N-CA-C	6.40	128.27	111.00
1	B	231	ARG	NE-CZ-NH1	-5.02	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	TYR	Sidechain

### 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	2275	0	2294	129	0
1	B	3085	0	3161	285	0
2	A	22	0	11	1	0
2	B	22	0	11	2	0
3	A	43	0	23	4	0
3	B	43	0	23	4	0
4	B	15	0	0	0	0
5	A	11	0	0	0	0
5	B	20	0	0	0	0
All	All	5536	0	5523	417	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 38.

All (417) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:105:ARG:HH12	1:B:109:LYS:HG2	1.18	1.06
1:B:181:LYS:HE2	1:B:181:LYS:H	1.20	1.01
1:B:224:ARG:HB3	1:B:227:LEU:HD11	1.46	0.97
1:B:227:LEU:HD13	1:B:228:LYS:N	1.80	0.96
1:B:198:ASN:HA	1:B:201:LEU:HD12	1.44	0.95
1:B:122:SER:N	1:B:148:GLY:HA2	1.81	0.94
1:B:270:VAL:HG12	1:B:298:GLN:HB2	1.49	0.94
1:B:201:LEU:HD22	1:B:206:LYS:HA	1.52	0.92
1:B:207:GLY:O	1:B:223:ALA:HA	1.70	0.90
1:A:270:VAL:HG12	1:A:298:GLN:HB2	1.54	0.90
1:A:277:GLN:C	1:A:277:GLN:HE21	1.75	0.89
1:B:203:ARG:HH21	1:B:205:LYS:HB2	1.39	0.88
1:B:212:VAL:HG11	1:B:216:ASP:HA	1.57	0.87
1:B:343:GLN:HE21	1:B:343:GLN:HA	1.40	0.87
1:B:239:ASP:OD2	1:B:243:GLN:HB2	1.75	0.86
1:B:198:ASN:O	1:B:201:LEU:HB2	1.76	0.85
1:B:203:ARG:NE	1:B:205:LYS:H	1.74	0.85
1:B:224:ARG:HB3	1:B:227:LEU:CD1	2.07	0.84
1:B:291:LYS:HA	1:B:291:LYS:HE2	1.60	0.83
1:B:277:GLN:C	1:B:277:GLN:HE21	1.82	0.82
1:B:204:SER:C	1:B:206:LYS:H	1.83	0.81
1:B:368:GLN:H	1:B:372:HIS:HD2	1.26	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:75:GLU:OE2	1:B:92:HIS:HE1	1.63	0.81
1:B:330:ILE:HG23	1:B:335:GLU:HB2	1.62	0.81
1:A:368:GLN:H	1:A:372:HIS:HD2	1.26	0.81
1:B:198:ASN:HB3	1:B:224:ARG:HH12	1.46	0.80
1:A:283:GLN:HE22	1:A:302:GLY:HA3	1.46	0.80
1:A:473:ALA:HA	1:A:478:GLN:NE2	1.97	0.79
1:B:92:HIS:HD2	1:B:94:ASN:HB3	1.45	0.79
1:A:239:ASP:OD2	1:A:243:GLN:HB2	1.83	0.79
1:B:203:ARG:HD2	1:B:204:SER:N	1.97	0.79
1:B:114:PHE:O	1:B:115:ILE:HD13	1.83	0.78
1:B:330:ILE:HG12	1:B:335:GLU:HG2	1.65	0.78
1:B:483:MET:HB3	1:B:488:LEU:HD23	1.63	0.78
1:B:153:ARG:HA	1:B:216:ASP:O	1.83	0.78
1:A:16:ASP:HB2	1:A:489:LYS:HG3	1.65	0.78
1:B:204:SER:O	1:B:206:LYS:N	2.16	0.78
1:A:493:ARG:HE	1:A:498:GLN:HG2	1.48	0.78
1:B:207:GLY:O	1:B:208:LYS:HD2	1.84	0.77
1:B:111:GLU:O	1:B:112:GLN:HG2	1.84	0.77
1:B:181:LYS:CE	1:B:181:LYS:H	1.98	0.77
1:A:31:THR:HG22	1:A:32:TYR:N	2.01	0.76
1:B:213:ASN:OD1	1:B:217:GLU:HB2	1.85	0.76
1:B:181:LYS:HE2	1:B:181:LYS:N	2.00	0.76
1:B:144:ILE:HG12	1:B:156:GLY:CA	2.16	0.76
1:B:12:TYR:CE2	1:B:14:PRO:HA	2.22	0.75
1:A:291:LYS:HE2	1:A:291:LYS:HA	1.69	0.74
1:B:144:ILE:HD11	1:B:179:MET:SD	2.28	0.74
1:B:203:ARG:NH1	1:B:204:SER:HB3	2.04	0.73
1:B:204:SER:O	1:B:206:LYS:HG3	1.88	0.73
1:B:261:ASP:O	1:B:265:GLN:HG3	1.87	0.73
1:B:105:ARG:HH12	1:B:109:LYS:CG	2.00	0.73
1:A:473:ALA:HA	1:A:478:GLN:HE21	1.54	0.73
1:B:115:ILE:HG22	1:B:118:PRO:HD3	1.70	0.72
1:B:31:THR:HG22	1:B:32:TYR:N	2.03	0.72
1:B:207:GLY:HA2	1:B:224:ARG:H	1.54	0.72
1:B:283:GLN:HE22	1:B:302:GLY:HA3	1.54	0.72
1:B:337:LEU:O	1:B:338:ALA:HB2	1.89	0.72
1:B:203:ARG:HD2	1:B:203:ARG:C	2.09	0.72
1:A:92:HIS:HD2	1:A:94:ASN:HB3	1.54	0.72
1:A:16:ASP:CB	1:A:489:LYS:HG3	2.20	0.72
1:B:471:ILE:HD12	1:B:488:LEU:HD13	1.71	0.71
1:A:26:CYS:HB3	1:A:28:ASP:OD2	1.89	0.71
1:B:150:MET:CE	1:B:220:ALA:HA	2.21	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:277:GLN:HE22	1:A:279:ASN:N	1.89	0.70
1:B:155:VAL:HG12	1:B:155:VAL:O	1.92	0.70
1:B:197:ALA:O	1:B:201:LEU:HG	1.92	0.69
1:A:277:GLN:HE22	1:A:279:ASN:H	1.39	0.69
1:B:157:ILE:O	1:B:158:ILE:HG23	1.91	0.69
1:B:227:LEU:C	1:B:227:LEU:HD13	2.12	0.69
1:B:105:ARG:NH1	1:B:109:LYS:HG2	2.02	0.69
1:B:120:VAL:HG11	1:B:150:MET:HB2	1.74	0.69
1:B:331:CYS:O	1:B:332:ILE:HB	1.92	0.69
1:B:198:ASN:CB	1:B:224:ARG:HH12	2.05	0.69
1:A:270:VAL:CG1	1:A:298:GLN:HB2	2.22	0.69
1:A:31:THR:HG22	1:A:33:ASN:H	1.56	0.69
1:A:283:GLN:O	1:A:287:ILE:HG12	1.93	0.69
1:A:386:MET:CE	1:A:389:LEU:HD23	2.23	0.69
1:B:193:THR:HG23	1:B:196:GLU:H	1.58	0.69
1:B:203:ARG:HG3	1:B:204:SER:H	1.57	0.68
1:B:157:ILE:HG22	1:B:158:ILE:N	2.08	0.68
1:B:305:VAL:H	1:B:309:GLN:NE2	1.92	0.68
1:B:283:GLN:O	1:B:287:ILE:HG12	1.94	0.68
1:B:494:THR:O	1:B:497:ALA:HB3	1.93	0.67
1:A:75:GLU:O	1:A:77:GLY:N	2.27	0.67
1:B:333:THR:O	1:B:334:GLN:HB3	1.95	0.67
1:A:456:PHE:O	1:A:459:TYR:HB3	1.95	0.67
1:B:206:LYS:C	1:B:206:LYS:HD2	2.16	0.67
1:A:483:MET:HB3	1:A:488:LEU:HD23	1.78	0.66
1:B:120:VAL:HG21	1:B:150:MET:N	2.11	0.66
1:B:211:ILE:O	1:B:218:LEU:HD12	1.95	0.66
1:B:203:ARG:NH2	1:B:205:LYS:HB2	2.09	0.66
1:B:473:ALA:HA	1:B:478:GLN:NE2	2.11	0.66
1:B:378:ALA:O	1:B:483:MET:HG2	1.95	0.66
1:B:227:LEU:O	1:B:227:LEU:HD22	1.97	0.65
1:A:31:THR:CG2	1:A:32:TYR:N	2.60	0.65
1:A:51:LEU:HD12	1:A:461:ILE:HG23	1.77	0.65
1:B:225:THR:HG22	1:B:225:THR:O	1.97	0.65
1:B:16:ASP:O	1:B:17:GLY:O	2.13	0.65
1:B:144:ILE:HG13	1:B:144:ILE:O	1.97	0.65
1:B:112:GLN:OE1	1:B:243:GLN:HG2	1.96	0.65
1:B:333:THR:O	1:B:333:THR:HG22	1.97	0.65
1:A:305:VAL:H	1:A:309:GLN:NE2	1.95	0.64
1:B:121:LEU:HA	1:B:148:GLY:O	1.97	0.64
1:A:104:VAL:O	1:A:108:LYS:HG2	1.98	0.64
1:A:494:THR:N	1:A:497:ALA:HB3	2.12	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:305:VAL:H	1:A:309:GLN:HE22	1.46	0.63
1:A:449:ASP:O	1:A:450:LYS:O	2.15	0.63
1:B:12:TYR:HE2	1:B:14:PRO:HA	1.62	0.63
1:B:303:ASN:OD1	1:B:322:ARG:HD3	1.99	0.63
1:B:203:ARG:CD	1:B:204:SER:N	2.62	0.63
1:B:75:GLU:O	1:B:77:GLY:N	2.32	0.62
1:B:69:PRO:HG3	1:B:90:PHE:HB2	1.82	0.62
1:B:471:ILE:HD12	1:B:488:LEU:CD1	2.29	0.62
1:B:204:SER:C	1:B:206:LYS:N	2.54	0.61
1:B:203:ARG:CG	1:B:204:SER:N	2.62	0.61
1:B:51:LEU:HD12	1:B:461:ILE:HG23	1.80	0.61
1:B:238:LYS:HA	1:B:243:GLN:O	2.00	0.61
1:B:64:PRO:HA	1:B:383:THR:HG22	1.82	0.61
1:B:457:VAL:O	1:B:461:ILE:HG13	2.00	0.61
1:B:142:ILE:HD12	1:B:142:ILE:N	2.16	0.60
1:B:201:LEU:CD2	1:B:206:LYS:HA	2.29	0.60
1:A:69:PRO:HG3	1:A:90:PHE:HB2	1.82	0.60
1:B:203:ARG:HD2	1:B:204:SER:HB3	1.83	0.60
1:B:121:LEU:C	1:B:148:GLY:HA2	2.21	0.60
1:B:212:VAL:CG1	1:B:216:ASP:HA	2.31	0.60
1:B:100:GLN:HG2	1:B:263:LEU:HD21	1.82	0.60
1:B:144:ILE:HG12	1:B:156:GLY:HA3	1.82	0.60
1:B:12:TYR:O	1:B:13:VAL:O	2.20	0.60
1:B:31:THR:HG22	1:B:32:TYR:H	1.66	0.60
1:B:337:LEU:O	1:B:338:ALA:CB	2.48	0.60
1:B:75:GLU:OE2	1:B:92:HIS:CE1	2.52	0.59
1:B:395:GLU:OE1	1:B:395:GLU:N	2.35	0.59
1:A:25:ASN:OD1	1:A:349:LYS:HE2	2.03	0.59
1:B:22:GLN:O	1:B:26:CYS:SG	2.60	0.59
1:B:55:LEU:HG	1:B:56:THR:HG23	1.83	0.58
1:B:150:MET:HE2	1:B:220:ALA:HA	1.84	0.58
1:B:270:VAL:CG1	1:B:298:GLN:HB2	2.29	0.58
1:A:74:THR:O	1:A:75:GLU:HG3	2.04	0.58
1:A:368:GLN:H	1:A:372:HIS:CD2	2.15	0.58
1:A:378:ALA:O	1:A:483:MET:HG2	2.04	0.58
1:A:303:ASN:CG	3:A:600:SAE:H62N	2.08	0.57
1:B:460:LEU:O	1:B:464:ILE:HG13	2.04	0.57
1:A:377:LEU:HD13	1:A:476:LEU:HD13	1.86	0.57
1:B:239:ASP:CG	1:B:243:GLN:HB2	2.25	0.57
1:B:292:ASP:O	1:B:295:PRO:HD3	2.03	0.57
1:B:118:PRO:HD2	1:B:150:MET:SD	2.44	0.57
1:B:368:GLN:H	1:B:372:HIS:CD2	2.15	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:12:TYR:C	1:B:13:VAL:HG13	2.25	0.57
1:A:31:THR:CG2	1:A:32:TYR:H	2.18	0.56
1:A:366:GLY:O	1:A:368:GLN:HG3	2.05	0.56
1:A:75:GLU:HA	1:A:91:ILE:HD12	1.87	0.56
1:B:386:MET:CE	1:B:389:LEU:HD23	2.34	0.56
1:B:31:THR:CG2	1:B:32:TYR:N	2.69	0.56
1:B:182:ARG:O	1:B:182:ARG:HD3	2.05	0.56
1:A:493:ARG:NE	1:A:498:GLN:HG2	2.19	0.56
1:B:198:ASN:CA	1:B:224:ARG:HH12	2.18	0.56
1:A:100:GLN:HG2	1:A:263:LEU:HD21	1.88	0.56
1:B:157:ILE:CG2	1:B:158:ILE:N	2.68	0.56
1:B:62:LYS:HB3	1:B:235:LEU:HD22	1.88	0.56
1:A:477:THR:HA	1:A:480:ARG:NH1	2.21	0.56
1:A:33:ASN:OD1	1:A:372:HIS:HE1	1.89	0.56
1:A:395:GLU:H	1:A:395:GLU:CD	2.08	0.56
1:A:277:GLN:NE2	1:A:279:ASN:H	2.02	0.55
1:B:103:GLU:OE1	1:B:106:LYS:HE3	2.07	0.55
1:B:144:ILE:CG1	1:B:144:ILE:O	2.54	0.55
1:A:303:ASN:ND2	3:A:600:SAE:H62N	2.03	0.55
1:A:273:LEU:HD11	1:A:287:ILE:HD13	1.88	0.55
1:A:270:VAL:HG12	1:A:298:GLN:CB	2.32	0.55
1:B:291:LYS:CE	1:B:291:LYS:HA	2.34	0.55
1:B:333:THR:O	1:B:334:GLN:CB	2.55	0.55
1:B:291:LYS:CA	1:B:291:LYS:HE2	2.35	0.55
1:A:272:VAL:HG13	1:A:272:VAL:O	2.07	0.55
1:B:125:ASP:O	1:B:126:ARG:HD2	2.06	0.54
1:B:144:ILE:CD1	1:B:156:GLY:HA3	2.36	0.54
1:A:26:CYS:O	1:A:28:ASP:N	2.40	0.54
1:A:12:TYR:O	1:A:13:VAL:O	2.26	0.54
1:B:199:GLU:O	1:B:202:GLN:N	2.32	0.54
1:B:212:VAL:CG1	1:B:215:ASP:O	2.55	0.54
1:B:150:MET:HE1	1:B:220:ALA:HA	1.88	0.54
1:B:277:GLN:C	1:B:277:GLN:NE2	2.57	0.54
1:B:108:LYS:HB3	1:B:243:GLN:NE2	2.23	0.54
1:B:92:HIS:CD2	1:B:94:ASN:HB3	2.35	0.54
1:B:13:VAL:O	1:B:13:VAL:HG22	2.06	0.54
1:B:25:ASN:OD1	1:B:349:LYS:HE2	2.08	0.54
1:A:390:LEU:O	1:A:393:THR:HG23	2.08	0.54
1:B:334:GLN:O	1:B:335:GLU:HB2	2.08	0.54
1:B:456:PHE:O	1:B:459:TYR:HB3	2.08	0.53
1:A:257:LYS:O	1:A:260:LEU:HB3	2.07	0.53
1:B:154:LEU:HD12	1:B:218:LEU:HD13	1.91	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:190:ALA:HB2	1:B:219:VAL:HG11	1.90	0.53
1:B:26:CYS:O	1:B:28:ASP:N	2.41	0.53
1:A:313:LEU:O	1:A:318:VAL:HG13	2.09	0.53
1:B:203:ARG:HG3	1:B:204:SER:N	2.20	0.53
1:B:122:SER:OG	1:B:148:GLY:N	2.41	0.53
1:A:80:ILE:HG13	1:A:107:VAL:HG22	1.91	0.53
1:B:330:ILE:HG12	1:B:335:GLU:CG	2.36	0.53
1:A:74:THR:HG22	1:A:91:ILE:HD13	1.90	0.53
1:A:36:LEU:HG	1:A:493:ARG:HD3	1.91	0.52
1:A:277:GLN:C	1:A:277:GLN:NE2	2.56	0.52
1:A:493:ARG:HH21	1:A:498:GLN:HG2	1.74	0.52
1:B:203:ARG:HD2	1:B:204:SER:CB	2.40	0.52
1:B:207:GLY:H	1:B:224:ARG:HB2	1.75	0.52
1:B:343:GLN:NE2	1:B:343:GLN:HA	2.19	0.52
1:A:277:GLN:HE21	1:A:278:GLY:N	2.08	0.52
1:B:145:THR:OG1	1:B:146:ASP:N	2.43	0.52
1:B:328:GLY:HA2	2:B:631:CPR:O1P	2.09	0.52
1:B:26:CYS:O	1:B:27:GLY:C	2.47	0.52
1:A:93:HIS:HB3	1:A:100:GLN:HE22	1.75	0.52
1:A:343:GLN:HA	1:A:343:GLN:NE2	2.24	0.52
1:A:19:THR:O	1:A:20:ALA:C	2.47	0.52
1:B:56:THR:OG1	1:B:59:ILE:HG12	2.10	0.51
1:B:343:GLN:HE21	1:B:343:GLN:CA	2.10	0.51
1:B:212:VAL:HG13	1:B:217:GLU:O	2.10	0.51
1:B:196:GLU:O	1:B:199:GLU:HB2	2.10	0.51
1:B:270:VAL:HG12	1:B:298:GLN:CB	2.33	0.51
1:B:193:THR:HG22	1:B:196:GLU:CD	2.31	0.51
1:B:127:VAL:HG22	1:B:128:ARG:H	1.75	0.51
1:B:355:ARG:HG3	1:B:356:ARG:N	2.25	0.51
1:B:140:CYS:SG	1:B:141:GLY:N	2.83	0.50
1:B:198:ASN:HB3	1:B:224:ARG:NH1	2.20	0.50
1:A:494:THR:H	1:A:497:ALA:HB3	1.75	0.50
1:A:283:GLN:HE22	1:A:302:GLY:CA	2.22	0.50
1:B:346:ALA:O	1:B:350:VAL:HG23	2.11	0.50
1:B:181:LYS:HG2	1:B:183:GLU:HG2	1.93	0.50
1:B:493:ARG:NH2	1:B:498:GLN:HG2	2.25	0.50
1:B:12:TYR:O	1:B:13:VAL:HG13	2.11	0.50
1:A:395:GLU:N	1:A:395:GLU:CD	2.64	0.50
1:B:375:LYS:O	1:B:379:LEU:HG	2.11	0.50
1:B:218:LEU:HD11	1:B:220:ALA:O	2.12	0.50
1:B:76:ALA:O	1:B:80:ILE:HG13	2.11	0.50
1:B:120:VAL:O	1:B:121:LEU:HB3	2.12	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:71:ASP:HB3	1:B:92:HIS:CD2	2.46	0.50
1:B:190:ALA:HA	1:B:211:ILE:CG2	2.42	0.49
1:A:84:LEU:HD23	1:A:244:LEU:HD21	1.92	0.49
1:B:313:LEU:O	1:B:318:VAL:HG22	2.12	0.49
1:B:228:LYS:HB2	1:B:228:LYS:NZ	2.27	0.49
1:B:212:VAL:HG12	1:B:215:ASP:O	2.12	0.49
1:B:157:ILE:CG2	1:B:158:ILE:H	2.26	0.49
1:B:461:ILE:O	1:B:465:GLN:HG3	2.12	0.49
1:B:186:VAL:HG13	1:B:205:LYS:NZ	2.28	0.49
1:B:203:ARG:HH11	1:B:204:SER:HB3	1.77	0.49
1:B:227:LEU:HD22	1:B:227:LEU:C	2.33	0.49
1:B:206:LYS:HD2	1:B:207:GLY:N	2.28	0.49
1:A:277:GLN:NE2	1:A:278:GLY:N	2.60	0.49
1:B:31:THR:CG2	1:B:32:TYR:H	2.24	0.49
1:B:306:THR:OG1	1:B:309:GLN:HG3	2.13	0.49
1:B:336:VAL:HG23	1:B:336:VAL:O	2.13	0.49
1:B:377:LEU:HD13	1:B:476:LEU:HD13	1.95	0.48
1:B:203:ARG:O	1:B:204:SER:HB2	2.13	0.48
1:B:203:ARG:HE	1:B:205:LYS:CB	2.26	0.48
1:B:227:LEU:N	1:B:227:LEU:CD1	2.76	0.48
1:B:115:ILE:O	1:B:117:ASP:N	2.47	0.48
1:B:368:GLN:N	1:B:372:HIS:HD2	2.05	0.48
1:B:386:MET:HE2	1:B:389:LEU:HD23	1.96	0.48
1:A:477:THR:HA	1:A:480:ARG:HH11	1.78	0.48
1:B:19:THR:HG22	1:B:21:GLN:H	1.79	0.48
1:B:105:ARG:HH11	1:B:105:ARG:HG2	1.78	0.48
1:B:224:ARG:NE	1:B:225:THR:H	2.11	0.48
1:B:212:VAL:HG12	1:B:213:ASN:N	2.29	0.48
1:B:115:ILE:HG22	1:B:118:PRO:CD	2.42	0.48
1:B:283:GLN:HE22	1:B:302:GLY:CA	2.24	0.48
1:B:127:VAL:HG22	1:B:128:ARG:N	2.28	0.48
1:A:455:LYS:C	1:A:458:PRO:HD2	2.33	0.48
1:B:193:THR:HG22	1:B:196:GLU:OE2	2.13	0.47
1:B:150:MET:HG2	1:B:150:MET:O	2.14	0.47
3:B:601:SAE:H51A	3:B:601:SAE:PN	2.54	0.47
1:B:93:HIS:CD2	1:B:93:HIS:H	2.31	0.47
1:A:103:GLU:OE1	1:A:103:GLU:HA	2.14	0.47
1:B:28:ASP:HB3	1:B:30:LEU:HG	1.95	0.47
1:A:343:GLN:HE21	1:A:343:GLN:HA	1.79	0.47
1:B:80:ILE:HG13	1:B:107:VAL:HG22	1.97	0.47
1:A:265:GLN:C	1:A:267:GLY:H	2.16	0.47
1:B:198:ASN:CB	1:B:224:ARG:NH1	2.75	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:31:THR:HG22	1:A:32:TYR:H	1.74	0.47
1:B:144:ILE:CG1	1:B:156:GLY:HA3	2.44	0.47
1:A:100:GLN:OE1	1:A:259:ARG:HD3	2.15	0.47
1:B:105:ARG:NH1	1:B:105:ARG:HG2	2.30	0.47
1:A:291:LYS:HA	1:A:291:LYS:CE	2.41	0.47
1:B:494:THR:H	1:B:497:ALA:CB	2.27	0.47
1:A:56:THR:OG1	1:A:59:ILE:HG12	2.14	0.47
1:A:26:CYS:O	1:A:27:GLY:C	2.54	0.47
1:A:18:LEU:N	1:A:18:LEU:HD22	2.29	0.47
1:A:66:VAL:O	1:A:385:MET:HA	2.15	0.47
1:B:363:ALA:HB3	1:B:384:VAL:HG22	1.96	0.47
1:B:121:LEU:HD22	1:B:121:LEU:C	2.35	0.46
1:B:125:ASP:O	1:B:126:ARG:CD	2.63	0.46
1:B:205:LYS:O	1:B:206:LYS:O	2.33	0.46
1:B:213:ASN:ND2	1:B:215:ASP:OD2	2.48	0.46
1:B:494:THR:H	1:B:497:ALA:HB2	1.81	0.46
1:A:19:THR:O	1:A:21:GLN:N	2.47	0.46
1:B:51:LEU:CD1	1:B:461:ILE:HG23	2.45	0.46
1:B:124:LYS:H	1:B:124:LYS:HD2	1.80	0.46
1:B:303:ASN:HA	1:B:322:ARG:O	2.16	0.46
1:B:471:ILE:HG13	1:B:471:ILE:O	2.15	0.46
1:A:80:ILE:HG23	1:A:244:LEU:CD1	2.46	0.46
1:B:455:LYS:C	1:B:458:PRO:HD2	2.36	0.46
1:B:203:ARG:CZ	1:B:204:SER:HB3	2.45	0.46
3:A:600:SAE:H51A	3:A:600:SAE:PN	2.55	0.46
1:B:13:VAL:O	1:B:13:VAL:CG2	2.63	0.46
1:B:453:ILE:HG23	1:B:457:VAL:HG23	1.97	0.46
1:B:388:SER:N	2:B:631:CPR:O3P	2.38	0.46
1:B:96:THR:OG1	1:B:99:PHE:HB2	2.15	0.46
1:B:390:LEU:O	1:B:392:ALA:N	2.49	0.46
1:A:23:LEU:HD11	1:A:492:LYS:CG	2.46	0.46
1:A:483:MET:CB	1:A:488:LEU:HD23	2.45	0.46
1:A:303:ASN:OD1	1:A:322:ARG:HD3	2.16	0.46
1:A:460:LEU:O	1:A:464:ILE:HG13	2.16	0.46
1:A:303:ASN:HA	1:A:322:ARG:O	2.16	0.45
1:B:188:ALA:HB1	1:B:192:ILE:HD13	1.98	0.45
1:B:303:ASN:CG	3:B:601:SAE:H62N	2.20	0.45
1:A:75:GLU:OE2	1:A:92:HIS:HE1	1.98	0.45
1:B:300:ILE:HG12	1:B:320:ALA:HB3	1.97	0.45
1:B:227:LEU:CD1	1:B:227:LEU:C	2.82	0.45
1:A:26:CYS:C	1:A:28:ASP:N	2.70	0.45
1:B:90:PHE:HA	1:B:247:GLY:O	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:398:GLY:O	1:B:399:GLU:C	2.54	0.45
1:B:154:LEU:N	1:B:216:ASP:O	2.48	0.45
1:A:483:MET:HB3	1:A:488:LEU:CD2	2.44	0.45
1:A:343:GLN:HE21	1:A:343:GLN:CA	2.29	0.45
1:B:181:LYS:O	1:B:182:ARG:CB	2.62	0.45
1:B:115:ILE:C	1:B:117:ASP:H	2.20	0.45
1:A:12:TYR:HE2	1:A:14:PRO:HA	1.82	0.45
1:B:20:ALA:O	1:B:24:PHE:HD2	1.99	0.45
1:B:157:ILE:HG22	1:B:158:ILE:H	1.80	0.45
1:A:293:LYS:O	1:A:294:TYR:CG	2.70	0.45
1:B:386:MET:HE3	1:B:389:LEU:HD23	1.98	0.44
1:A:395:GLU:OE1	1:A:453:ILE:HG12	2.17	0.44
1:A:23:LEU:O	1:A:28:ASP:OD2	2.35	0.44
1:A:13:VAL:HA	1:A:14:PRO:HD3	1.85	0.44
1:B:246:CYS:N	1:B:269:ASP:OD2	2.37	0.44
1:A:28:ASP:HB3	1:A:30:LEU:HD21	1.98	0.44
1:A:49:VAL:HA	1:A:474:LYS:O	2.17	0.44
1:B:198:ASN:CA	1:B:224:ARG:NH1	2.80	0.44
1:A:273:LEU:HD12	1:A:287:ILE:HD11	1.99	0.44
1:B:125:ASP:HB3	1:B:126:ARG:H	1.40	0.44
1:B:281:ILE:HG13	1:B:285:ASN:ND2	2.33	0.44
1:B:225:THR:O	1:B:225:THR:CG2	2.64	0.44
1:B:334:GLN:CD	3:B:601:SAE:SE1N	3.06	0.44
1:A:71:ASP:HB3	1:A:92:HIS:CD2	2.53	0.44
1:A:355:ARG:HG3	1:A:356:ARG:N	2.32	0.44
1:B:249:ALA:HB1	1:B:274:ASP:HB2	2.00	0.44
1:B:280:SER:O	1:B:284:ILE:HG13	2.18	0.44
1:B:147:THR:C	1:B:149:ARG:H	2.22	0.43
1:B:199:GLU:O	1:B:200:ILE:C	2.56	0.43
1:A:277:GLN:NE2	1:A:279:ASN:N	2.61	0.43
1:B:112:GLN:OE1	1:B:243:GLN:CG	2.64	0.43
1:B:494:THR:N	1:B:497:ALA:HB3	2.34	0.43
1:A:375:LYS:O	1:A:379:LEU:HG	2.18	0.43
1:A:93:HIS:H	1:A:93:HIS:CD2	2.36	0.43
1:A:343:GLN:CA	1:A:343:GLN:NE2	2.82	0.43
1:B:213:ASN:C	1:B:215:ASP:H	2.22	0.43
1:B:144:ILE:CD1	1:B:179:MET:SD	3.04	0.43
1:A:69:PRO:HG3	1:A:90:PHE:CB	2.48	0.43
1:B:203:ARG:CD	1:B:203:ARG:C	2.79	0.43
1:B:272:VAL:HG13	1:B:272:VAL:O	2.19	0.43
1:B:122:SER:CB	1:B:123:PRO:HD2	2.49	0.43
1:B:153:ARG:HH11	1:B:153:ARG:HB2	1.84	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:219:VAL:O	1:B:220:ALA:HB2	2.19	0.43
1:A:108:LYS:HG3	1:A:266:ALA:O	2.19	0.43
1:A:362:ILE:HG12	1:A:383:THR:OG1	2.19	0.43
1:B:62:LYS:CB	1:B:235:LEU:HD22	2.49	0.42
1:A:395:GLU:OE1	1:A:453:ILE:N	2.49	0.42
1:A:13:VAL:HG23	1:A:13:VAL:O	2.18	0.42
1:B:30:LEU:HD22	1:B:34:ASP:HB3	1.99	0.42
1:B:303:ASN:ND2	3:B:601:SAE:H62N	2.16	0.42
1:B:144:ILE:HG12	1:B:156:GLY:C	2.40	0.42
1:B:53:SER:OG	1:B:64:PRO:HB3	2.20	0.42
1:B:102:ASN:O	1:B:106:LYS:HG3	2.19	0.42
1:B:202:GLN:CG	1:B:203:ARG:N	2.82	0.42
1:B:111:GLU:HG3	1:B:242:LYS:O	2.20	0.42
1:A:28:ASP:HB3	1:A:30:LEU:CD2	2.49	0.42
1:A:461:ILE:O	1:A:465:GLN:HG3	2.19	0.42
1:B:373:ILE:HG21	1:B:464:ILE:HD11	2.02	0.42
1:B:120:VAL:HG23	1:B:121:LEU:N	2.34	0.42
1:A:90:PHE:CD1	1:A:90:PHE:N	2.87	0.42
1:A:108:LYS:O	1:A:243:GLN:NE2	2.53	0.42
1:B:203:ARG:HE	1:B:205:LYS:HB3	1.83	0.42
1:B:203:ARG:CZ	1:B:205:LYS:H	2.31	0.41
1:B:343:GLN:NE2	1:B:343:GLN:CA	2.81	0.41
1:B:68:SER:HA	1:B:69:PRO:HD3	1.81	0.41
1:A:312:ASN:HD22	1:A:312:ASN:N	2.18	0.41
1:B:193:THR:CG2	1:B:196:GLU:HG3	2.50	0.41
1:B:155:VAL:O	1:B:155:VAL:CG1	2.63	0.41
1:A:80:ILE:HG12	1:A:107:VAL:HG13	2.01	0.41
1:B:293:LYS:O	1:B:293:LYS:HG2	2.20	0.41
1:A:463:GLY:O	1:A:466:HIS:HB3	2.21	0.41
1:A:19:THR:HG22	1:A:21:GLN:H	1.85	0.41
1:B:198:ASN:HA	1:B:224:ARG:NH1	2.36	0.41
1:B:194:LEU:HD23	1:B:222:ILE:HD13	2.02	0.41
1:B:181:LYS:H	1:B:181:LYS:CD	2.34	0.41
1:B:110:TYR:HE2	1:B:117:ASP:OD1	2.03	0.41
1:B:115:ILE:CG2	1:B:118:PRO:HD3	2.45	0.41
1:B:142:ILE:N	1:B:142:ILE:CD1	2.82	0.41
1:B:199:GLU:O	1:B:202:GLN:CB	2.68	0.41
1:B:199:GLU:O	1:B:202:GLN:HB3	2.21	0.41
1:B:218:LEU:CD1	1:B:220:ALA:O	2.69	0.41
1:B:188:ALA:HA	1:B:189:PRO:HD3	1.87	0.41
1:A:293:LYS:O	1:A:293:LYS:HG2	2.21	0.41
1:B:253:HIS:O	1:B:256:ASP:HB2	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:31:THR:N	1:A:34:ASP:OD2	2.46	0.41
1:A:273:LEU:HD11	1:A:287:ILE:CD1	2.50	0.41
1:A:16:ASP:HB3	1:A:489:LYS:HG3	2.02	0.41
1:A:457:VAL:O	1:A:461:ILE:HG13	2.21	0.41
1:A:455:LYS:HA	1:A:455:LYS:HD3	1.91	0.41
1:B:225:THR:O	1:B:228:LYS:HD3	2.22	0.40
1:A:492:LYS:HB3	1:A:492:LYS:HE2	1.84	0.40
1:B:141:GLY:O	1:B:208:LYS:HG2	2.21	0.40
1:B:494:THR:N	1:B:497:ALA:CB	2.84	0.40
1:B:146:ASP:HB3	1:B:152:SER:OG	2.21	0.40
1:B:352:GLU:O	1:B:355:ARG:HG2	2.21	0.40
1:A:272:VAL:O	1:A:274:ASP:N	2.55	0.40
1:B:231:ARG:H	1:B:231:ARG:HG3	1.36	0.40
1:A:82:MET:HG3	1:A:88:ILE:H	1.87	0.40
1:B:83:ALA:O	1:B:236:ALA:HA	2.21	0.40
2:A:631:CPR:O2'	3:A:600:SAE:N6N	2.55	0.40
1:A:265:GLN:C	1:A:267:GLY:N	2.74	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	299/514 (58%)	249 (83%)	39 (13%)	11 (4%)	5	20
1	B	406/514 (79%)	304 (75%)	77 (19%)	25 (6%)	2	6
All	All	705/1028 (69%)	553 (78%)	116 (16%)	36 (5%)	3	10

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	14	PRO
1	A	17	GLY

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Mol	Chain	Res	Type
1	A	76	ALA
1	A	450	LYS
1	B	14	PRO
1	B	17	GLY
1	B	76	ALA
1	B	114	PHE
1	B	205	LYS
1	B	206	LYS
1	B	228	LYS
1	B	229	LYS
1	B	332	ILE
1	B	334	GLN
1	B	335	GLU
1	B	450	LYS
1	A	16	ASP
1	A	27	GLY
1	B	13	VAL
1	B	27	GLY
1	B	123	PRO
1	B	126	ARG
1	B	150	MET
1	B	204	SER
1	B	302	GLY
1	B	338	ALA
1	B	391	ALA
1	A	20	ALA
1	A	273	LEU
1	A	391	ALA
1	B	125	ASP
1	B	236	ALA
1	B	293	LYS
1	B	181	LYS
1	A	289	TYR

### 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	242/420 (58%)	237 (98%)	5 (2%)	66	92
1	B	333/420 (79%)	304 (91%)	29 (9%)	15	41
All	All	575/840 (68%)	541 (94%)	34 (6%)	28	64

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	93	HIS
1	A	277	GLN
1	A	291	LYS
1	A	483	MET
1	B	16	ASP
1	B	93	HIS
1	B	112	GLN
1	B	114	PHE
1	B	120	VAL
1	B	121	LEU
1	B	124	LYS
1	B	126	ARG
1	B	149	ARG
1	B	153	ARG
1	B	158	ILE
1	B	179	MET
1	B	181	LYS
1	B	182	ARG
1	B	183	GLU
1	B	203	ARG
1	B	206	LYS
1	B	209	LEU
1	B	227	LEU
1	B	228	LYS
1	B	229	LYS
1	B	231	ARG
1	B	241	LYS
1	B	277	GLN
1	B	291	LYS
1	B	343	GLN
1	B	449	ASP
1	B	471	ILE
1	B	483	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	A	94	ASN
1	A	243	GLN
1	A	265	GLN
1	A	277	GLN
1	A	283	GLN
1	A	285	ASN
1	A	309	GLN
1	A	312	ASN
1	A	343	GLN
1	A	372	HIS
1	A	478	GLN
1	B	92	HIS
1	B	93	HIS
1	B	94	ASN
1	B	243	GLN
1	B	265	GLN
1	B	277	GLN
1	B	283	GLN
1	B	285	ASN
1	B	309	GLN
1	B	312	ASN
1	B	343	GLN
1	B	372	HIS
1	B	478	GLN

### 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 ⓘ

Of 19 ligands modelled in this entry, 15 are unknown - leaving 4 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$
3	SAE	A	600	-	45,47,47	1.17	3 (6%)	66,72,72	2.57	17 (25%)
2	CPR	A	631	-	22,24,25	1.27	3 (13%)	32,36,38	2.35	12 (37%)
3	SAE	B	601	-	45,47,47	1.18	3 (6%)	66,72,72	2.58	17 (25%)
2	CPR	B	631	1	22,24,25	1.46	5 (22%)	32,36,38	2.67	13 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAE	A	600	-	-	0/24/62/62	0/2/5/5
2	CPR	A	631	-	-	0/10/26/26	0/1/3/3
3	SAE	B	601	-	-	0/24/62/62	0/2/5/5
2	CPR	B	631	1	-	0/10/26/26	0/1/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	SAE	O4B-C1B	3.88	1.47	1.41
3	A	600	SAE	O4B-C1B	3.85	1.47	1.41
2	B	631	CPR	C4-N9	-3.41	1.32	1.37
3	B	601	SAE	C5N-C4N	-3.21	1.35	1.38
3	A	600	SAE	C5N-C4N	-3.17	1.35	1.38
2	A	631	CPR	C2-N3	3.10	1.37	1.31
2	B	631	CPR	C2-N3	2.80	1.36	1.31
3	B	601	SAE	C4N-N3N	-2.38	1.33	1.38
3	A	600	SAE	C4N-N3N	-2.37	1.33	1.38
2	B	631	CPR	C5-N7	-2.35	1.31	1.40
2	B	631	CPR	P-O3P	-2.31	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	631	CPR	O4'-C1'	2.22	1.44	1.41
2	A	631	CPR	C5-N7	-2.08	1.32	1.40
2	A	631	CPR	O4'-C1'	2.05	1.44	1.41

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	SAE	N3A-C2A-N1A	-10.95	119.56	128.71
3	A	600	SAE	N3A-C2A-N1A	-10.90	119.59	128.71
2	B	631	CPR	O4'-C1'-N9	8.32	116.18	108.44
2	A	631	CPR	N3-C4-N9	7.53	139.04	125.43
3	A	600	SAE	O4B-C1B-N9A	7.28	115.21	108.44
3	B	601	SAE	O4B-C1B-N9A	7.27	115.20	108.44
3	B	601	SAE	N3A-C4A-N9A	6.71	137.56	125.43
3	A	600	SAE	N3A-C4A-N9A	6.71	137.55	125.43
2	B	631	CPR	N3-C4-N9	6.31	136.83	125.43
3	B	601	SAE	C4B-O4B-C1B	-5.22	104.08	109.75
3	A	600	SAE	C4B-O4B-C1B	-5.21	104.09	109.75
3	A	600	SAE	O4D-C1D-C2N	-4.87	102.98	110.62
3	B	601	SAE	O4D-C1D-C2N	-4.86	102.99	110.62
2	A	631	CPR	C5-C4-N3	-4.49	115.92	125.70
3	A	600	SAE	C5N-C4N-N3N	4.48	116.53	109.74
3	B	601	SAE	C5N-C4N-N3N	4.47	116.51	109.74
3	A	600	SAE	O4B-C4B-C5B	-4.33	93.91	109.36
3	B	601	SAE	O4B-C4B-C5B	-4.32	93.92	109.36
3	B	601	SAE	O3B-C3B-C2B	3.90	124.52	111.83
3	A	600	SAE	O3B-C3B-C2B	3.89	124.50	111.83
2	B	631	CPR	C5-C4-N3	-3.88	117.26	125.70
2	B	631	CPR	N1-C2-N3	-3.78	116.87	125.75
2	B	631	CPR	C2-N3-C4	3.66	122.09	113.48
2	A	631	CPR	N1-C2-N3	-3.65	117.18	125.75
2	A	631	CPR	C2-N3-C4	3.54	121.81	113.48
3	B	601	SAE	C5A-C4A-N3A	-3.54	118.00	125.70
3	A	600	SAE	C5A-C4A-N3A	-3.53	118.01	125.70
2	B	631	CPR	C8-N9-C4	-3.52	104.21	106.90
2	A	631	CPR	O2P-P-O5'	-3.51	96.96	106.65
2	B	631	CPR	C3'-C2'-C1'	3.21	105.93	100.91
3	B	601	SAE	O4B-C4B-C3B	3.13	111.52	105.17
3	A	600	SAE	O4B-C4B-C3B	3.13	111.52	105.17
2	A	631	CPR	O3'-C3'-C4'	3.10	120.22	111.08
2	B	631	CPR	O4'-C1'-C2'	-3.04	102.12	106.77
2	B	631	CPR	O3'-C3'-C4'	3.02	119.98	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	631	CPR	O4'-C1'-N9	2.87	111.11	108.44
3	B	601	SAE	C4A-C5A-N7A	2.80	111.92	109.52
3	A	600	SAE	C4A-C5A-N7A	2.79	111.91	109.52
3	A	600	SAE	C2A-N3A-C4A	2.75	121.83	114.01
3	B	601	SAE	C2A-N3A-C4A	2.75	121.83	114.01
3	A	600	SAE	O5D-C5D-C4D	2.69	118.81	108.94
3	B	601	SAE	O5D-C5D-C4D	2.69	118.80	108.94
2	A	631	CPR	C2'-C3'-C4'	-2.59	97.49	102.65
3	B	601	SAE	C2A-N1A-C6A	2.55	123.37	118.77
2	B	631	CPR	C5'-C4'-C3'	-2.53	105.06	115.21
3	A	600	SAE	C2A-N1A-C6A	2.51	123.31	118.77
3	A	600	SAE	C5B-C4B-C3B	-2.49	105.24	115.21
3	B	601	SAE	C5B-C4B-C3B	-2.48	105.28	115.21
3	A	600	SAE	O5D-PN-O1N	2.47	119.06	109.37
3	B	601	SAE	O5D-PN-O1N	2.46	119.00	109.37
2	B	631	CPR	C8-N9-C1'	2.31	130.93	126.38
2	A	631	CPR	C2'-C1'-N9	2.30	119.16	113.27
2	A	631	CPR	C3'-C2'-C1'	2.27	104.46	100.91
3	B	601	SAE	O4B-C1B-C2B	-2.22	103.37	106.77
3	A	600	SAE	O4B-C1B-C2B	-2.21	103.38	106.77
2	A	631	CPR	O4'-C1'-C2'	-2.16	103.47	106.77
2	A	631	CPR	O2P-P-O1P	2.09	117.28	110.44
2	B	631	CPR	O2P-P-O1P	2.07	117.22	110.44
2	B	631	CPR	C2'-C3'-C4'	-2.02	98.63	102.65

There are no chirality outliers.

There are no torsion outliers.

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 ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.