



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:58 PM GMT

PDB ID : 1W22  
Title : Crystal structure of inhibited human HDAC8  
Authors : Vannini, A.; Volpari, C.; Caroli Casavola, E.; Di Marco, S.  
Deposited on : 2004-06-25  
Resolution : 2.50 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

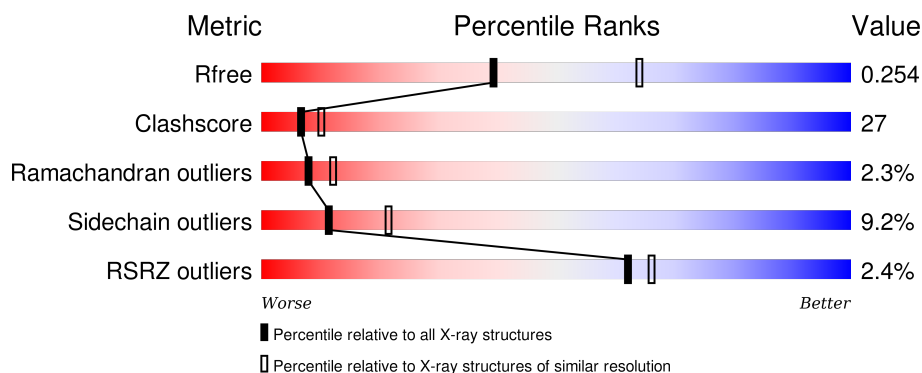
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	377	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, yellow 1%, yellow 55%, yellow 55%, yellow 83%, yellow 83%, orange 83%, orange 88%, red 88%, red 90%, grey 90%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>%</span> <span>55%</span> <span>33%</span> <span>5% • 6%</span> </div> </div>
1	B	377	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, yellow 3%, yellow 51%, yellow 51%, yellow 86%, yellow 86%, orange 86%, orange 91%, red 91%, red 93%, grey 93%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>3%</span> <span>51%</span> <span>36%</span> <span>6% • 7%</span> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5815 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 HISTONE DEACETYLASE 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	S	0	0	1
			2745	1763	456	507	19			
1	B	351	Total	C	N	O	S	0	0	1
			2732	1754	455	504	19			

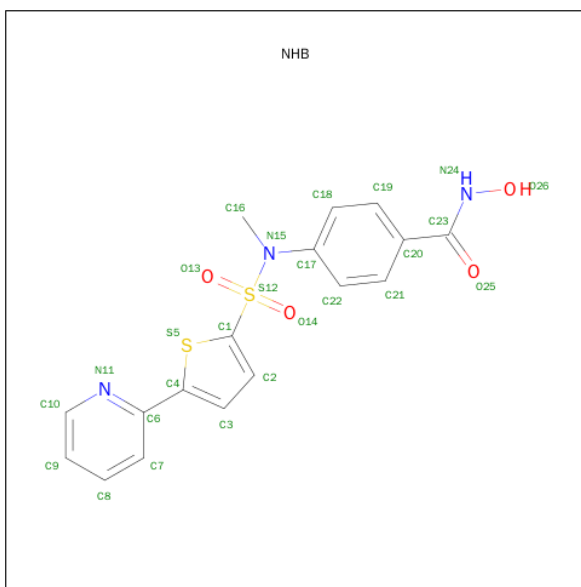
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	K	0	0
			2	2		
3	A	2	Total	K	0	0
			2	2		

- Molecule 4 is N-HYDROXY-4-(METHYL{[5-(2-PYRIDINYL)-2-THIENYL]SULFONYL} AMINO)BENZAMIDE (three-letter code: NHB) (formula: C<sub>17</sub>H<sub>15</sub>N<sub>3</sub>O<sub>4</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			26	17	3	4	2		
4	B	1	Total	C	N	O	S	0	0
			26	17	3	4	2		

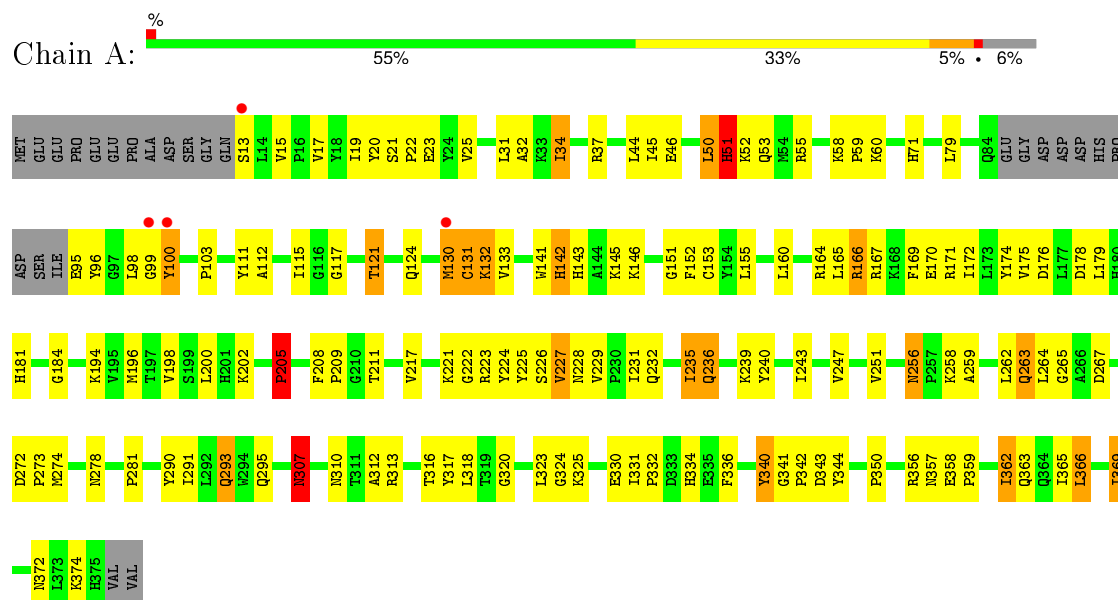
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	154	Total	O	0	0
			154	154		
5	B	126	Total	O	0	0
			126	126		

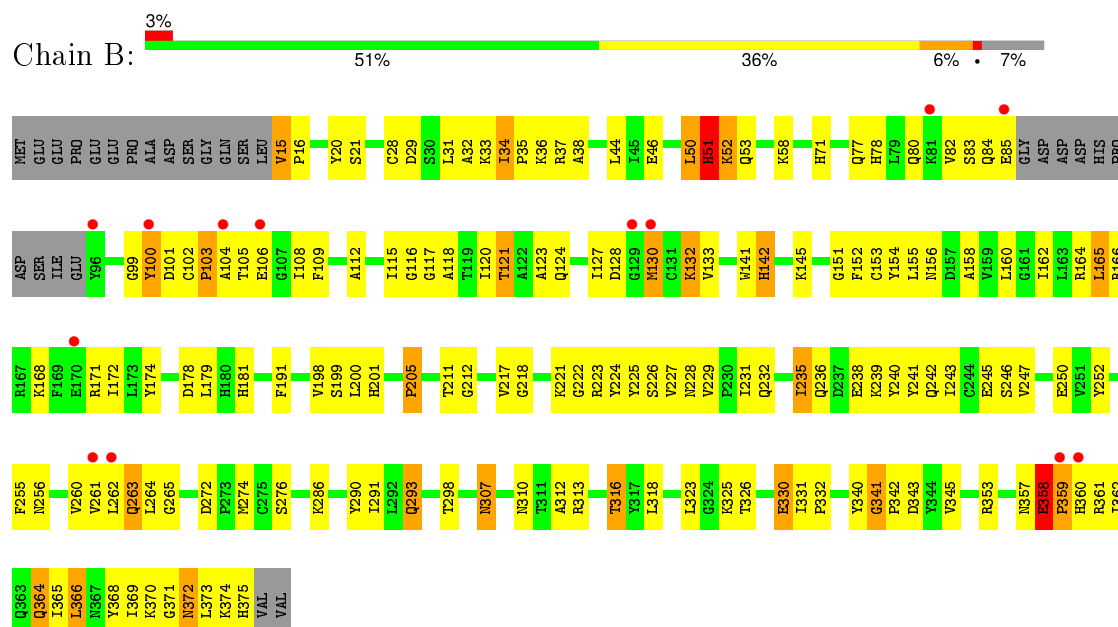
### 3 Residue-property plots

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: HISTONE DEACETYLASE 8



#### • Molecule 1: HISTONE DEACETYLASE 8



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.75Å 83.53Å 94.65Å 90.00° 97.48° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 32.58 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.50) 97.7 (32.58-2.50)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.90 (at 2.51Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, $R_{free}$	0.210 , 0.250 0.210 , 0.254	Depositor DCC
$R_{free}$ test set	1322 reflections (5.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.9	Xtriage
Anisotropy	0.769	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 44.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 27171 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5815	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.38	0/2812	0.65	1/3812 (0.0%)
1	B	0.36	0/2799	0.64	0/3795
All	All	0.37	0/5611	0.65	1/7607 (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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	307	ASN	N-CA-C	-5.04	97.38	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	340	TYR	Sidechain

### 5.2 Too-close contacts

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2745	0	2711	139	0
1	B	2732	0	2696	160	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	26	0	14	0	0
4	B	26	0	14	4	0
5	A	154	0	0	8	0
5	B	126	0	0	16	0
All	All	5815	0	5435	296	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 27.

All (296) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:GLN:NE2	1:B:265:GLY:H	1.49	1.11
1:A:263:GLN:NE2	1:A:265:GLY:H	1.52	1.06
1:A:181:HIS:HD1	1:A:211:THR:HG23	1.25	1.00
1:B:117:GLY:O	1:B:121:THR:HG22	1.65	0.97
1:A:374:LYS:HB3	5:A:2151:HOH:O	1.63	0.97
1:B:124:GLN:HE21	1:B:164:ARG:HE	0.97	0.93
1:B:263:GLN:HE22	1:B:265:GLY:H	1.14	0.91
1:A:34:ILE:HD11	1:A:37:ARG:NE	1.89	0.88
1:B:232:GLN:H	1:B:357:ASN:HD21	1.22	0.88
1:A:205:PRO:HB2	1:B:353:ARG:HG3	1.58	0.86
1:B:124:GLN:NE2	1:B:164:ARG:HE	1.75	0.82
1:B:312:ALA:O	1:B:316:THR:HG23	1.78	0.81
1:B:364:GLN:C	1:B:364:GLN:HE21	1.86	0.79
1:B:123:ALA:HB1	1:B:165:LEU:HD13	1.65	0.78
1:B:357:ASN:O	1:B:358:GLU:HG3	1.83	0.78
1:A:181:HIS:ND1	1:A:211:THR:HG23	1.99	0.77
1:A:312:ALA:O	1:A:316:THR:HG23	1.83	0.77
1:B:51:HIS:O	1:B:52:LYS:HG2	1.83	0.77
1:A:169:PHE:HB2	1:A:172:ILE:HD11	1.67	0.77
1:A:166:ARG:HH11	1:A:166:ARG:HG2	1.51	0.76
1:A:34:ILE:HD11	1:A:37:ARG:CZ	2.16	0.76
1:A:263:GLN:HE21	1:A:265:GLY:H	1.34	0.75

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ASN:HD22	1:A:310:ASN:H	1.35	0.74
1:A:141:TRP:HB3	1:A:153:CYS:SG	2.28	0.74
1:B:358:GLU:CD	1:B:358:GLU:O	2.27	0.73
1:A:290:TYR:O	1:A:293:GLN:HG3	1.89	0.73
1:B:174:TYR:HD2	1:B:261:VAL:HG13	1.54	0.73
1:A:51:HIS:O	1:A:52:LYS:HG2	1.89	0.73
1:B:171:ARG:HH21	1:B:256:ASN:HB3	1.55	0.72
1:A:235:ILE:HD12	1:A:240:TYR:HB2	1.72	0.72
1:A:209:PRO:HG2	1:A:211:THR:HG22	1.71	0.72
1:B:124:GLN:HE21	1:B:164:ARG:NE	1.81	0.70
1:A:95:GLU:HG3	5:B:2102:HOH:O	1.91	0.70
1:A:60:LYS:H	1:A:121:THR:HG21	1.54	0.70
1:A:205:PRO:CB	1:B:353:ARG:HG3	2.22	0.70
1:B:263:GLN:HE22	1:B:265:GLY:N	1.90	0.69
1:A:179:LEU:HD23	1:A:274:MET:HG2	1.73	0.69
1:A:263:GLN:NE2	1:A:265:GLY:N	2.36	0.69
1:B:179:LEU:HD23	1:B:274:MET:HG2	1.74	0.69
1:B:264:LEU:HD13	1:B:318:LEU:HD13	1.73	0.69
1:B:361:ARG:O	1:B:365:ILE:HG12	1.93	0.69
1:B:53:GLN:HE22	1:B:325:LYS:NZ	1.91	0.68
1:B:34:ILE:HD11	1:B:37:ARG:NE	2.09	0.68
1:B:132:LYS:HD3	1:B:133:VAL:HG23	1.75	0.68
1:B:99:GLY:O	1:B:103:PRO:HA	1.92	0.68
1:A:178:ASP:HB2	1:A:263:GLN:NE2	2.08	0.68
1:B:16:PRO:HG3	1:B:132:LYS:HE3	1.76	0.67
1:B:307:ASN:ND2	1:B:310:ASN:H	1.92	0.67
1:A:217:VAL:HA	1:A:226:SER:O	1.93	0.67
1:A:164:ARG:HD2	1:A:167:ARG:HD2	1.77	0.67
1:B:307:ASN:C	1:B:307:ASN:HD22	1.97	0.66
1:A:132:LYS:HD2	1:A:133:VAL:HG23	1.77	0.66
1:B:238:GLU:O	1:B:242:GLN:HG3	1.97	0.65
1:A:46:GLU:HG3	1:A:51:HIS:CE1	2.32	0.65
1:B:28:CYS:SG	1:B:115:ILE:HD11	2.37	0.64
1:B:44:LEU:HB3	1:B:316:THR:HG21	1.78	0.64
1:A:31:LEU:HD23	1:A:34:ILE:CG2	2.27	0.63
1:A:31:LEU:HD23	1:A:34:ILE:HG21	1.81	0.63
1:B:100:TYR:O	1:B:103:PRO:HD3	1.98	0.63
1:A:307:ASN:ND2	1:A:310:ASN:H	1.97	0.63
1:A:100:TYR:O	1:A:103:PRO:HD3	1.97	0.63
1:B:34:ILE:O	1:B:34:ILE:HG12	1.99	0.62
1:A:53:GLN:HE22	1:A:325:LYS:NZ	1.98	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LYS:HE2	1:A:258:LYS:HA	1.82	0.61
1:A:363:GLN:HG3	5:A:2143:HOH:O	2.00	0.61
1:B:155:LEU:HD13	1:B:156:ASN:N	2.15	0.61
1:A:117:GLY:O	1:A:121:THR:HG23	2.01	0.60
1:A:365:ILE:O	1:A:369:ILE:HG22	2.00	0.60
1:A:325:LYS:HB3	1:A:325:LYS:HZ3	1.66	0.60
1:B:174:TYR:CD2	1:B:261:VAL:HG13	2.37	0.60
1:A:205:PRO:HB2	1:B:353:ARG:CG	2.30	0.60
1:A:263:GLN:HE22	1:A:265:GLY:H	1.42	0.60
1:A:235:ILE:HD13	1:A:236:GLN:N	2.16	0.60
1:A:235:ILE:HD13	1:A:236:GLN:H	1.67	0.59
1:A:71:HIS:HA	1:A:146:LYS:O	2.03	0.59
1:B:51:HIS:C	1:B:53:GLN:H	2.04	0.59
1:B:343:ASP:HB2	1:B:345:VAL:HG22	1.85	0.59
1:B:101:ASP:HB3	4:B:1378:NHB:C16	2.33	0.58
1:B:191:PHE:O	1:B:221:LYS:HB2	2.04	0.58
1:B:179:LEU:CD2	1:B:274:MET:HG2	2.33	0.58
1:A:31:LEU:HD22	1:A:111:TYR:OH	2.03	0.58
1:B:366:LEU:O	1:B:369:ILE:HG22	2.04	0.58
1:B:53:GLN:HG2	5:B:2017:HOH:O	2.03	0.57
1:B:145:LYS:HE3	5:B:2044:HOH:O	2.05	0.57
1:A:295:GLN:HB2	5:A:2118:HOH:O	2.03	0.57
1:A:19:ILE:HG22	1:A:59:PRO:HG3	1.86	0.57
1:B:263:GLN:NE2	1:B:265:GLY:N	2.35	0.57
1:B:51:HIS:O	1:B:53:GLN:N	2.38	0.57
1:A:179:LEU:CD2	1:A:274:MET:HG2	2.33	0.57
1:B:217:VAL:HA	1:B:226:SER:O	2.04	0.57
1:B:231:ILE:HG22	1:B:232:GLN:N	2.20	0.57
1:A:172:ILE:HD12	1:A:259:ALA:HB3	1.87	0.57
1:B:371:GLY:O	1:B:373:LEU:N	2.38	0.57
1:B:178:ASP:HB2	1:B:263:GLN:NE2	2.19	0.56
1:B:330:GLU:HB3	5:B:2100:HOH:O	2.06	0.56
1:A:32:ALA:HB1	5:A:2010:HOH:O	2.06	0.56
1:A:372:ASN:O	1:A:374:LYS:HG2	2.06	0.56
1:A:239:LYS:O	1:A:243:ILE:HG13	2.06	0.56
1:A:175:VAL:HA	1:A:198:VAL:HG13	1.86	0.56
1:B:15:VAL:HG12	1:B:130:MET:HE2	1.88	0.56
1:B:232:GLN:H	1:B:357:ASN:ND2	1.98	0.56
1:A:272:ASP:OD2	1:A:274:MET:HB2	2.07	0.55
1:B:118:ALA:O	1:B:121:THR:HG23	2.06	0.55
1:A:247:VAL:HG22	1:A:369:ILE:HD13	1.87	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:VAL:HG12	1:B:130:MET:CE	2.37	0.55
1:B:112:ALA:HB1	1:B:155:LEU:HB2	1.88	0.55
1:A:44:LEU:HB3	1:A:316:THR:HG21	1.89	0.54
1:B:241:TYR:CD2	1:B:286:LYS:HE2	2.42	0.54
1:B:358:GLU:O	1:B:360:HIS:N	2.40	0.54
1:A:34:ILE:HD11	1:A:37:ARG:CD	2.37	0.54
1:B:276:SER:O	1:B:353:ARG:NH2	2.39	0.54
1:A:53:GLN:CD	1:A:325:LYS:HZ1	2.10	0.54
1:A:132:LYS:CD	1:A:133:VAL:HG23	2.37	0.54
1:A:325:LYS:CB	1:A:325:LYS:NZ	2.71	0.54
1:B:199:SER:OG	1:B:201:HIS:HD2	1.90	0.54
1:A:53:GLN:NE2	1:A:325:LYS:HZ1	2.06	0.53
1:A:13:SER:OG	1:A:15:VAL:HG22	2.08	0.53
1:A:34:ILE:CD1	1:A:37:ARG:CZ	2.86	0.53
1:B:250:GLU:HG3	1:B:373:LEU:HD21	1.91	0.53
1:B:313:ARG:NH2	5:B:2103:HOH:O	2.42	0.53
1:A:71:HIS:CD2	1:A:155:LEU:HD22	2.43	0.53
1:B:372:ASN:O	1:B:373:LEU:HD12	2.09	0.52
1:B:46:GLU:HG3	1:B:51:HIS:CE1	2.45	0.52
1:A:208:PHE:CE1	1:A:209:PRO:HB3	2.45	0.52
1:A:171:ARG:HH21	1:A:256:ASN:HB3	1.75	0.52
1:B:174:TYR:HD2	1:B:261:VAL:CG1	2.21	0.52
1:A:45:ILE:HG13	1:A:316:THR:HG22	1.91	0.51
1:B:341:GLY:N	5:B:2103:HOH:O	2.27	0.51
1:B:171:ARG:HD2	1:B:255:PHE:CE1	2.45	0.51
1:B:252:TYR:O	1:B:255:PHE:O	2.29	0.51
1:A:142:HIS:CD2	1:A:142:HIS:H	2.26	0.51
1:A:130:MET:O	1:A:131:CYS:HB2	2.10	0.51
1:B:366:LEU:O	1:B:366:LEU:HD23	2.11	0.51
1:B:32:ALA:O	1:B:35:PRO:HD3	2.11	0.51
1:B:373:LEU:C	1:B:374:LYS:HG3	2.30	0.51
1:A:334:HIS:CD2	1:A:336:PHE:H	2.29	0.51
1:A:366:LEU:O	1:A:369:ILE:HG23	2.11	0.50
1:B:20:TYR:CG	1:B:21:SER:N	2.78	0.50
1:A:174:TYR:O	1:A:198:VAL:HG12	2.11	0.50
1:A:117:GLY:O	1:A:121:THR:CG2	2.59	0.50
1:B:243:ILE:O	1:B:247:VAL:HG23	2.11	0.49
1:B:357:ASN:O	1:B:358:GLU:CG	2.58	0.49
1:B:218:GLY:HA3	5:B:2063:HOH:O	2.12	0.49
1:B:34:ILE:HD11	1:B:37:ARG:CZ	2.42	0.49
1:B:342:PRO:HA	5:B:2049:HOH:O	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ILE:O	1:A:34:ILE:HG12	2.10	0.49
1:B:116:GLY:O	1:B:120:ILE:HG13	2.13	0.49
1:A:55:ARG:NH2	5:A:2022:HOH:O	2.46	0.49
1:B:235:ILE:HD12	1:B:240:TYR:HB2	1.93	0.49
1:A:374:LYS:O	1:A:374:LYS:HG3	2.12	0.49
1:A:247:VAL:HG13	1:A:369:ILE:HD11	1.95	0.49
1:A:170:GLU:HG3	1:A:194:LYS:HE3	1.95	0.49
1:B:104:ALA:HB3	5:B:2035:HOH:O	2.12	0.49
1:B:340:TYR:O	1:B:341:GLY:O	2.31	0.48
1:A:236:GLN:HG3	5:A:2101:HOH:O	2.13	0.48
1:A:60:LYS:O	1:A:117:GLY:HA3	2.13	0.48
1:B:84:GLN:O	1:B:85:GLU:HB2	2.13	0.48
1:A:196:MET:SD	1:A:251:VAL:HG13	2.53	0.48
1:A:166:ARG:CZ	1:A:194:LYS:HG2	2.43	0.48
1:A:273:PRO:HB3	4:B:1378:NHB:C1	2.43	0.48
1:A:124:GLN:OE1	1:A:164:ARG:NE	2.46	0.48
1:B:99:GLY:O	1:B:103:PRO:CA	2.59	0.48
1:A:178:ASP:OD1	1:A:265:GLY:HA3	2.14	0.48
1:B:155:LEU:HD11	1:B:160:LEU:CD1	2.44	0.48
1:A:53:GLN:HE22	1:A:325:LYS:HZ1	1.60	0.47
1:A:51:HIS:C	1:A:53:GLN:N	2.68	0.47
1:B:31:LEU:HD23	1:B:34:ILE:CG2	2.44	0.47
1:B:369:ILE:HG23	1:B:370:LYS:N	2.30	0.47
1:A:263:GLN:HE22	1:A:265:GLY:N	2.07	0.47
1:B:108:ILE:HD11	1:B:154:TYR:CD1	2.49	0.47
1:B:246:SER:OG	1:B:366:LEU:HD11	2.15	0.47
1:A:166:ARG:NH1	1:A:166:ARG:HG2	2.26	0.47
1:A:235:ILE:HD11	1:A:240:TYR:N	2.29	0.47
1:A:278:ASN:ND2	1:A:350:PRO:HB2	2.29	0.47
1:A:175:VAL:HG22	1:A:198:VAL:CG1	2.45	0.47
1:B:53:GLN:NE2	1:B:325:LYS:NZ	2.62	0.46
1:B:71:HIS:CD2	1:B:155:LEU:HD22	2.49	0.46
1:B:201:HIS:HE1	1:B:212:GLY:O	1.98	0.46
1:B:44:LEU:HD12	1:B:44:LEU:HA	1.75	0.46
1:B:239:LYS:O	1:B:243:ILE:HG13	2.14	0.46
1:A:273:PRO:HB3	4:B:1378:NHB:C2	2.45	0.46
1:B:375:HIS:N	5:B:2124:HOH:O	2.48	0.46
1:A:22:PRO:HG2	1:A:23:GLU:OE1	2.15	0.46
1:B:325:LYS:CB	1:B:325:LYS:NZ	2.79	0.46
1:B:166:ARG:HG2	1:B:166:ARG:HH11	1.80	0.46
1:A:34:ILE:O	1:A:34:ILE:HG23	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ASP:HB2	1:B:263:GLN:CD	2.36	0.46
1:B:21:SER:HB3	1:B:58:LYS:HG3	1.98	0.46
1:B:358:GLU:OE2	1:B:358:GLU:O	2.34	0.46
1:A:320:GLY:O	1:A:324:GLY:N	2.49	0.46
1:B:343:ASP:HB3	5:B:2105:HOH:O	2.16	0.46
1:B:83:SER:HB2	1:B:109:PHE:HB2	1.97	0.46
1:A:223:ARG:O	1:A:224:TYR:HB2	2.17	0.45
1:B:142:HIS:CD2	1:B:142:HIS:H	2.34	0.45
1:B:132:LYS:HD2	1:B:133:VAL:N	2.30	0.45
1:A:142:HIS:O	1:A:184:GLY:HA3	2.16	0.45
1:B:50:LEU:HD11	1:B:325:LYS:HE2	1.98	0.45
1:B:102:CYS:HB3	1:B:154:TYR:CE1	2.52	0.45
1:B:80:GLN:O	1:B:83:SER:HB3	2.16	0.45
1:A:151:GLY:O	1:A:152:PHE:HB2	2.16	0.45
1:B:141:TRP:HB3	1:B:153:CYS:SG	2.56	0.45
1:B:325:LYS:CB	1:B:325:LYS:HZ2	2.30	0.45
1:B:325:LYS:NZ	1:B:325:LYS:HB3	2.31	0.45
1:B:181:HIS:CD2	1:B:228:ASN:ND2	2.85	0.45
1:B:200:LEU:HD13	1:B:229:VAL:HB	1.99	0.45
1:A:221:LYS:HE3	1:A:221:LYS:HB3	1.78	0.45
1:B:223:ARG:HG3	1:B:223:ARG:HH11	1.81	0.45
1:A:313:ARG:NH2	5:A:2125:HOH:O	2.49	0.45
1:A:143:HIS:O	1:A:145:LYS:HD2	2.17	0.45
1:B:222:GLY:O	1:B:225:TYR:HB2	2.17	0.45
1:B:29:ASP:OD2	1:B:38:ALA:HB3	2.17	0.45
1:A:205:PRO:CG	1:B:353:ARG:HG3	2.48	0.45
1:B:127:ILE:HG23	1:B:168:LYS:CD	2.47	0.45
1:B:217:VAL:C	1:B:226:SER:HB2	2.37	0.44
1:A:281:PRO:HB2	1:A:317:TYR:CD2	2.52	0.44
1:B:290:TYR:O	1:B:293:GLN:HG3	2.17	0.44
1:B:35:PRO:O	1:B:36:LYS:HB2	2.18	0.44
1:A:343:ASP:O	1:A:344:TYR:HB2	2.17	0.44
1:A:20:TYR:CG	1:A:21:SER:N	2.85	0.44
1:B:198:VAL:O	1:B:198:VAL:HG23	2.16	0.44
1:A:99:GLY:O	1:A:103:PRO:CA	2.66	0.44
1:A:247:VAL:HG13	1:A:369:ILE:CD1	2.47	0.44
1:B:375:HIS:N	5:B:2125:HOH:O	2.51	0.44
1:B:171:ARG:HB3	1:B:255:PHE:CZ	2.53	0.44
1:B:307:ASN:ND2	1:B:307:ASN:C	2.68	0.43
1:B:247:VAL:HG13	1:B:369:ILE:HD13	1.99	0.43
1:B:224:TYR:CD2	1:B:374:LYS:HD2	2.52	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ALA:CB	1:B:165:LEU:HD13	2.40	0.43
1:B:272:ASP:OD2	1:B:274:MET:HB2	2.18	0.43
1:A:227:VAL:HG21	1:A:369:ILE:HD12	1.99	0.43
1:A:176:ASP:CG	1:A:263:GLN:HG2	2.39	0.43
1:B:50:LEU:HA	1:B:50:LEU:HD12	1.79	0.43
1:A:112:ALA:HB1	1:A:155:LEU:HB2	2.00	0.43
1:A:178:ASP:HB2	1:A:263:GLN:CD	2.38	0.43
1:B:50:LEU:C	1:B:51:HIS:O	2.54	0.43
1:A:231:ILE:HG22	1:A:232:GLN:N	2.34	0.43
1:A:171:ARG:HA	1:A:194:LYS:O	2.19	0.43
1:B:78:HIS:O	1:B:82:VAL:HG13	2.18	0.43
1:B:231:ILE:CG2	1:B:232:GLN:N	2.81	0.43
1:A:50:LEU:C	1:A:51:HIS:O	2.56	0.43
1:B:132:LYS:HD2	1:B:132:LYS:H	1.84	0.43
1:B:223:ARG:HG3	1:B:223:ARG:NH1	2.32	0.43
1:B:198:VAL:HA	1:B:227:VAL:HG22	2.01	0.43
1:B:77:GLN:NE2	5:B:2026:HOH:O	2.52	0.43
1:B:174:TYR:HA	1:B:261:VAL:HG13	2.00	0.43
1:A:217:VAL:C	1:A:226:SER:HB2	2.40	0.43
1:A:20:TYR:HE1	1:A:25:VAL:HG21	1.83	0.43
1:A:331:ILE:HA	1:A:332:PRO:HD3	1.76	0.43
1:A:172:ILE:CD1	1:A:259:ALA:HB3	2.49	0.43
1:B:127:ILE:HG23	1:B:168:LYS:HD2	2.01	0.43
1:B:21:SER:CB	1:B:58:LYS:HG3	2.49	0.43
1:A:202:LYS:HA	1:A:231:ILE:O	2.19	0.43
1:B:171:ARG:HH11	1:B:171:ARG:HG3	1.84	0.42
1:B:83:SER:HA	1:B:108:ILE:HG22	2.00	0.42
1:B:293:GLN:HB2	1:B:293:GLN:HE21	1.51	0.42
1:A:111:TYR:O	1:A:115:ILE:HG12	2.19	0.42
1:A:51:HIS:O	1:A:53:GLN:N	2.52	0.42
1:A:155:LEU:HD11	1:A:160:LEU:CD1	2.49	0.42
1:B:245:GLU:O	1:B:246:SER:C	2.56	0.42
1:B:373:LEU:O	1:B:374:LYS:HG3	2.18	0.42
1:B:151:GLY:O	1:B:152:PHE:HB2	2.19	0.42
1:B:358:GLU:HB3	5:B:2116:HOH:O	2.18	0.42
1:A:340:TYR:N	1:A:340:TYR:CD1	2.87	0.42
1:B:235:ILE:HD13	1:B:236:GLN:N	2.35	0.42
1:A:51:HIS:C	1:A:53:GLN:H	2.23	0.42
1:A:274:MET:HE3	5:B:2087:HOH:O	2.20	0.42
1:A:243:ILE:HG12	1:A:362:ILE:HD11	2.02	0.42
1:B:158:ALA:O	1:B:162:ILE:HG13	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:HIS:CD2	1:A:142:HIS:N	2.83	0.42
1:B:199:SER:OG	1:B:201:HIS:CD2	2.72	0.41
1:B:262:LEU:HD22	1:B:291:ILE:HD12	2.03	0.41
1:A:262:LEU:HD22	1:A:291:ILE:HD12	2.01	0.41
1:A:181:HIS:NE2	1:A:228:ASN:ND2	2.67	0.41
1:A:200:LEU:HD22	1:A:229:VAL:HG21	2.02	0.41
1:A:358:GLU:HA	1:A:359:PRO:HD3	1.93	0.41
1:B:34:ILE:CD1	1:B:37:ARG:CZ	2.98	0.41
1:A:17:VAL:HG23	1:A:131:CYS:SG	2.61	0.41
1:B:162:ILE:HG23	1:B:172:ILE:HG21	2.03	0.41
1:A:222:GLY:O	1:A:225:TYR:HB2	2.21	0.41
1:A:325:LYS:CB	1:A:325:LYS:HZ3	2.32	0.41
1:A:50:LEU:HA	1:A:50:LEU:HD12	1.59	0.41
1:A:155:LEU:HD11	1:A:160:LEU:HD11	2.03	0.41
1:B:223:ARG:O	1:B:224:TYR:HB2	2.21	0.41
1:B:331:ILE:HA	1:B:332:PRO:HD3	1.94	0.41
1:A:264:LEU:HD13	1:A:318:LEU:HD13	2.02	0.41
1:B:263:GLN:O	1:B:263:GLN:HG3	2.21	0.41
4:B:1378:NHB:H3	5:B:2126:HOH:O	2.20	0.41
1:B:235:ILE:HD11	1:B:239:LYS:HG2	2.02	0.41
1:B:85:GLU:HA	1:B:85:GLU:OE1	2.21	0.41
1:A:211:THR:HG21	5:A:2072:HOH:O	2.19	0.40
1:B:198:VAL:O	1:B:198:VAL:CG2	2.69	0.40
1:A:96:TYR:HB2	1:A:98:LEU:HD23	2.02	0.40
1:B:260:VAL:O	1:B:298:THR:HA	2.21	0.40
1:B:263:GLN:HE21	1:B:265:GLY:H	1.51	0.40
1:B:340:TYR:C	1:B:341:GLY:O	2.59	0.40
1:A:232:GLN:HB2	1:A:357:ASN:OD1	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	349/377 (93%)	316 (90%)	27 (8%)	6 (2%)	11	19
1	B	347/377 (92%)	309 (89%)	28 (8%)	10 (3%)	6	8
All	All	696/754 (92%)	625 (90%)	55 (8%)	16 (2%)	8	12

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	128	ASP
1	B	130	MET
1	B	359	PRO
1	B	372	ASN
1	A	51	HIS
1	A	205	PRO
1	A	341	GLY
1	B	103	PRO
1	B	341	GLY
1	A	131	CYS
1	B	51	HIS
1	B	52	LYS
1	A	356	ARG
1	B	205	PRO
1	A	342	PRO
1	B	358	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	A	293/316 (93%)	267 (91%)	26 (9%)	12	23
1	B	292/316 (92%)	264 (90%)	28 (10%)	10	19
All	All	585/632 (93%)	531 (91%)	54 (9%)	11	21

All (54) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	34	ILE
1	A	50	LEU
1	A	51	HIS
1	A	58	LYS
1	A	79	LEU
1	A	100	TYR
1	A	121	THR
1	A	130	MET
1	A	132	LYS
1	A	142	HIS
1	A	165	LEU
1	A	166	ARG
1	A	205	PRO
1	A	227	VAL
1	A	235	ILE
1	A	236	GLN
1	A	256	ASN
1	A	263	GLN
1	A	267	ASP
1	A	293	GLN
1	A	307	ASN
1	A	323	LEU
1	A	330	GLU
1	A	362	ILE
1	A	366	LEU
1	A	369	ILE
1	B	15	VAL
1	B	33	LYS
1	B	34	ILE
1	B	50	LEU
1	B	51	HIS
1	B	100	TYR
1	B	105	THR
1	B	106	GLU
1	B	121	THR
1	B	132	LYS
1	B	142	HIS
1	B	165	LEU
1	B	205	PRO
1	B	211	THR
1	B	235	ILE
1	B	263	GLN
1	B	293	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	307	ASN
1	B	316	THR
1	B	323	LEU
1	B	326	THR
1	B	330	GLU
1	B	358	GLU
1	B	359	PRO
1	B	362	ILE
1	B	364	GLN
1	B	366	LEU
1	B	368	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	77	GLN
1	A	80	GLN
1	A	136	ASN
1	A	228	ASN
1	A	263	GLN
1	A	293	GLN
1	A	307	ASN
1	A	372	ASN
1	B	51	HIS
1	B	77	GLN
1	B	80	GLN
1	B	124	GLN
1	B	201	HIS
1	B	228	ASN
1	B	236	GLN
1	B	253	GLN
1	B	263	GLN
1	B	293	GLN
1	B	307	ASN
1	B	357	ASN
1	B	363	GLN
1	B	364	GLN
1	B	372	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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$
4	NHB	A	1378	2	26,28,28	2.31	7 (26%)	26,40,40	2.20	6 (23%)
4	NHB	B	1378	2	26,28,28	2.53	7 (26%)	26,40,40	2.02	5 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NHB	A	1378	2	-	0/18/26/26	0/3/3/3
4	NHB	B	1378	2	-	0/18/26/26	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1378	NHB	C17-N15	-6.37	1.33	1.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1378	NHB	C17-N15	-6.18	1.34	1.44
4	B	1378	NHB	C1-S5	-4.79	1.63	1.72
4	B	1378	NHB	C6-C4	-4.41	1.39	1.49
4	A	1378	NHB	C6-C4	-3.95	1.40	1.49
4	A	1378	NHB	C1-S5	-2.53	1.67	1.72
4	A	1378	NHB	O26-N24	-2.09	1.36	1.39
4	B	1378	NHB	O26-N24	-2.02	1.36	1.39
4	B	1378	NHB	C20-C23	2.47	1.55	1.50
4	A	1378	NHB	C20-C23	2.58	1.55	1.50
4	A	1378	NHB	O13-S12	4.66	1.49	1.43
4	B	1378	NHB	O13-S12	5.21	1.50	1.43
4	B	1378	NHB	O14-S12	6.25	1.51	1.43
4	A	1378	NHB	O14-S12	6.32	1.51	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1378	NHB	O14-S12-O13	-5.98	109.15	119.47
4	B	1378	NHB	O14-S12-O13	-3.50	113.42	119.47
4	A	1378	NHB	C17-N15-S12	2.06	121.25	116.63
4	B	1378	NHB	C4-C6-N11	2.16	120.35	116.72
4	A	1378	NHB	C10-N11-C6	2.19	120.22	117.20
4	A	1378	NHB	C4-C6-N11	2.21	120.43	116.72
4	B	1378	NHB	C10-N11-C6	2.66	120.87	117.20
4	B	1378	NHB	C17-N15-S12	2.68	122.65	116.63
4	A	1378	NHB	O13-S12-N15	4.80	112.55	106.84
4	A	1378	NHB	O14-S12-N15	5.84	113.78	106.84
4	B	1378	NHB	O14-S12-N15	7.07	115.24	106.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1378	NHB	4	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	353/377 (93%)	-0.06	4 (1%) 82 84	19, 37, 61, 82	0
1	B	351/377 (93%)	0.08	13 (3%) 45 50	20, 41, 77, 96	0
All	All	704/754 (93%)	0.01	17 (2%) 62 66	19, 39, 68, 96	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	130	MET	4.4
1	B	100	TYR	3.8
1	B	130	MET	3.8
1	B	106	GLU	3.4
1	B	261	VAL	2.9
1	B	85	GLU	2.8
1	A	100	TYR	2.8
1	B	104	ALA	2.8
1	B	360	HIS	2.8
1	A	99	GLY	2.6
1	B	170	GLU	2.5
1	B	129	GLY	2.5
1	A	13	SER	2.5
1	B	81	LYS	2.4
1	B	359	PRO	2.3
1	B	96	TYR	2.3
1	B	262	LEU	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 [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NHB	B	1378	26/26	0.93	0.17	0.75	40,49,55,56	0
3	K	A	1376	1/1	0.99	0.22	0.71	21,21,21,21	0
3	K	A	1377	1/1	0.97	0.14	0.68	42,42,42,42	0
4	NHB	A	1378	26/26	0.93	0.17	0.52	40,48,53,54	0
3	K	B	1376	1/1	0.98	0.16	-0.51	31,31,31,31	0
2	ZN	A	1375	1/1	0.96	0.11	-1.38	25,25,25,25	0
3	K	B	1377	1/1	0.97	0.11	-2.19	40,40,40,40	0
2	ZN	B	1375	1/1	0.95	0.10	-2.30	27,27,27,27	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.