



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2024 – 05:15 PM EST

PDB ID : 3PUR  
Title : CEKDM7A from C.Elegans, complex with D-2-HG  
Authors : Yang, Y.; Wang, P.; Xu, W.; Xu, Y.  
Deposited on : 2010-12-06  
Resolution : 2.10 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

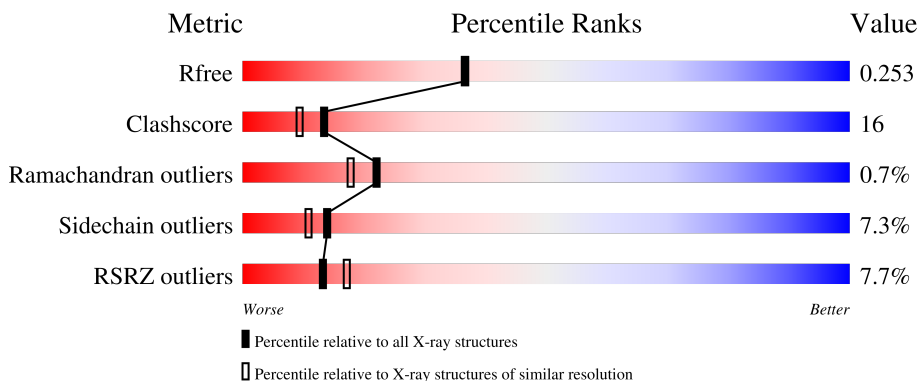
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	528	
1	C	528	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	2HG	A	1000	-	X	-	-
4	2HG	C	1000	-	X	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8399 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 Lysine-specific demethylase 7 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	483	3982	2548	673	733	28	0	1	0
1	C	496	4094	2618	693	755	28	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	184	GLU	-	expression tag	UNP Q9GYI0
A	185	PHE	-	expression tag	UNP Q9GYI0
A	186	HIS	-	expression tag	UNP Q9GYI0
A	187	MET	-	expression tag	UNP Q9GYI0
C	184	GLU	-	expression tag	UNP Q9GYI0
C	185	PHE	-	expression tag	UNP Q9GYI0
C	186	HIS	-	expression tag	UNP Q9GYI0
C	187	MET	-	expression tag	UNP Q9GYI0

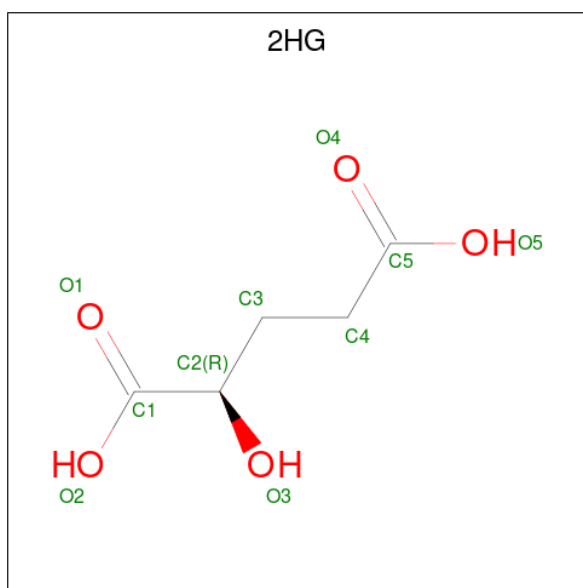
- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		
3	C	2	Total	Zn	0	0
			2	2		

- Molecule 4 is (2R)-2-hydroxypentanedioic acid (three-letter code: 2HG) (formula: C<sub>5</sub>H<sub>8</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 5 5	0	0
4	C	1	Total C O 10 5 5	0	0

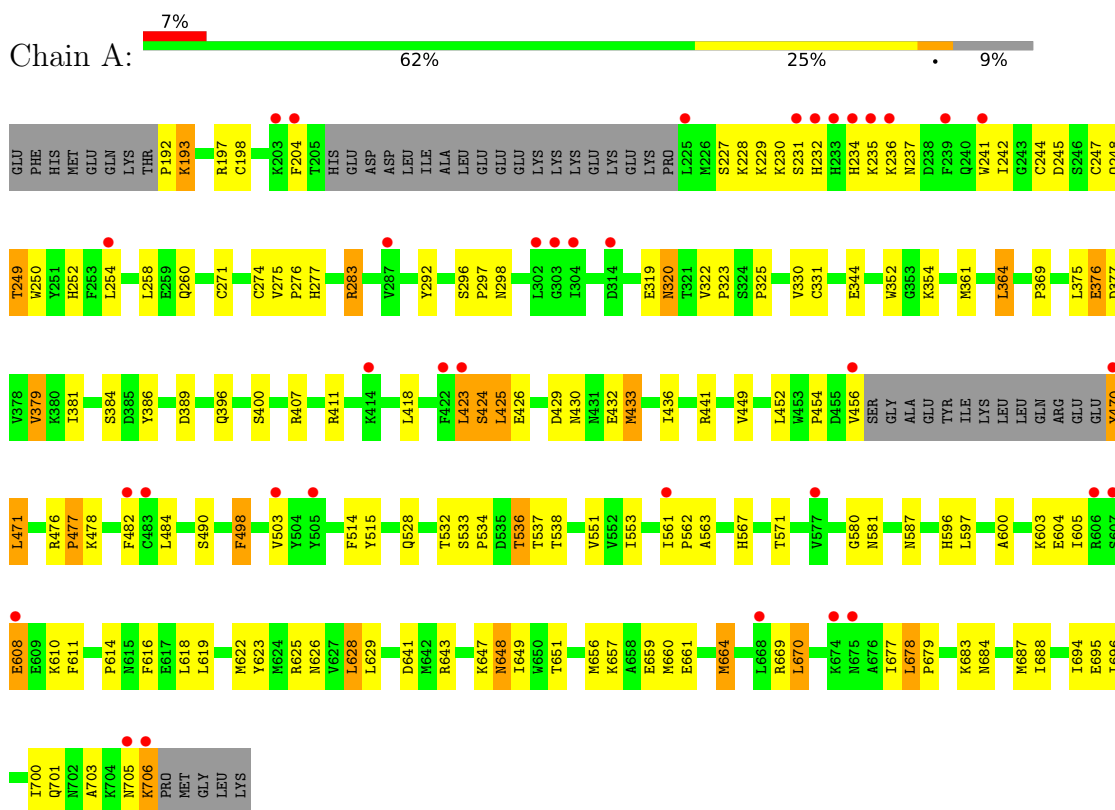
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	142	Total O 142 142	0	0
5	C	155	Total O 155 155	0	0

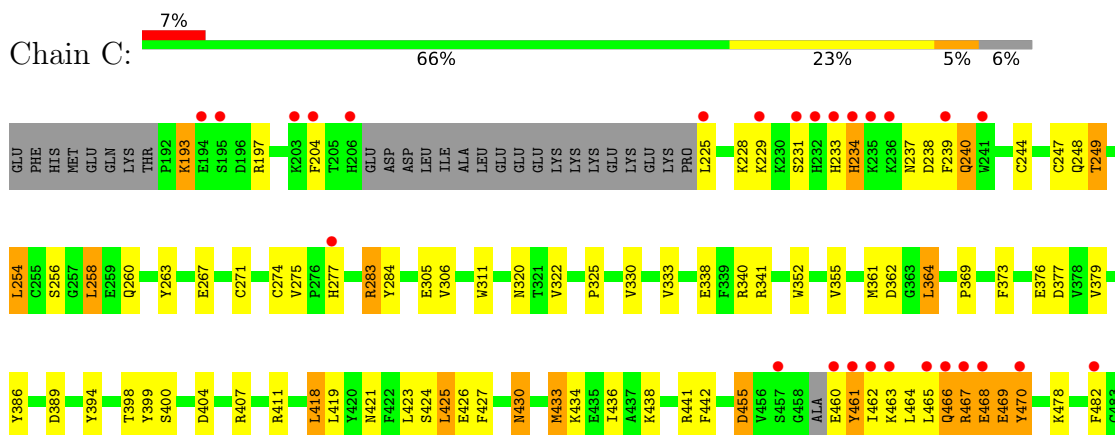
### 3 Residue-property plots [i](#)

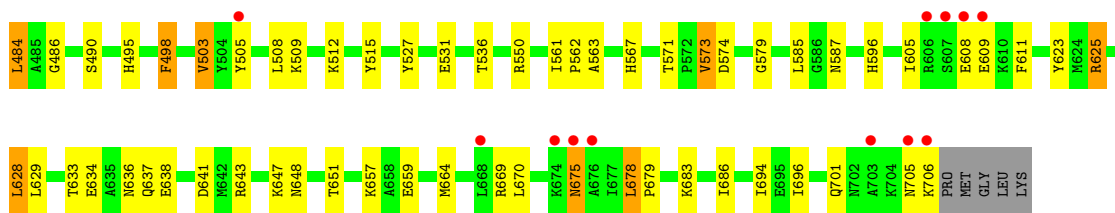
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Lysine-specific demethylase 7 homolog



- Molecule 1: Lysine-specific demethylase 7 homolog





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.01Å 144.09Å 78.09Å 90.00° 106.22° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 42.86 – 2.10	Depositor EDS
% Data completeness (in resolution range)	87.0 (50.00-2.10) 95.9 (42.86-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.68 (at 2.10Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.6.1_353)	Depositor
R, $R_{free}$	0.214 , 0.251 0.218 , 0.253	Depositor DCC
$R_{free}$ test set	3926 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.0	Xtrriage
Anisotropy	0.768	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8399	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, 2HG, ZN

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	0.43	0/4091	0.58	0/5518
1	C	0.42	0/4205	0.58	0/5670
All	All	0.43	0/8296	0.58	0/11188

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3982	0	3859	129	0
1	C	4094	0	3968	131	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	2	0	0	0	0
3	C	2	0	0	0	0
4	A	10	0	6	0	0
4	C	10	0	6	1	0
5	A	142	0	0	4	0
5	C	155	0	0	4	0
All	All	8399	0	7839	256	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 16.

All (256) 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:C:247:CYS:SG	1:C:249:THR:HG23	1.99	1.01
1:A:247:CYS:SG	1:A:249:THR:HG23	2.01	1.00
1:C:193:LYS:H	1:C:193:LYS:HD3	1.29	0.98
1:A:482[B]:PHE:CD2	1:A:484:LEU:HD11	2.00	0.96
1:C:482[B]:PHE:CE1	1:C:484:LEU:HD11	2.00	0.96
1:C:463:LYS:HA	1:C:466:GLN:HB2	1.45	0.96
1:A:325:PRO:HG2	1:A:330:VAL:HG11	1.49	0.92
1:A:430:ASN:HD22	1:A:433:MET:H	1.18	0.91
1:C:461:TYR:HA	1:C:464:LEU:HB2	1.56	0.86
1:A:596:HIS:HE1	1:A:659:GLU:OE1	1.58	0.85
1:A:430:ASN:ND2	1:A:433:MET:H	1.75	0.84
1:A:283:ARG:HH22	1:A:418:LEU:CD2	1.91	0.83
1:C:361:MET:HE1	5:C:1294:HOH:O	1.78	0.82
1:C:482[B]:PHE:HE1	1:C:484:LEU:HD11	1.42	0.81
1:A:482[B]:PHE:CE2	1:A:484:LEU:HD11	2.14	0.81
1:C:333:VAL:HB	1:C:338:GLU:HG3	1.62	0.81
1:C:433:MET:HA	1:C:436:ILE:HD12	1.65	0.79
1:C:225:LEU:HD21	1:C:229:LYS:HB3	1.63	0.79
1:A:532:THR:HB	1:A:604:GLU:HG2	1.66	0.78
1:A:228:LYS:HE2	1:A:498:PHE:HE2	1.49	0.77
1:C:424:SER:HB2	1:C:482[A]:PHE:CD1	2.21	0.75
1:C:464:LEU:O	1:C:469:GLU:HB3	1.84	0.75
1:A:482[B]:PHE:HD2	1:A:484:LEU:HD11	1.50	0.74
1:C:482[B]:PHE:CD1	1:C:484:LEU:HD11	2.22	0.74
1:A:231:SER:HB2	1:A:260:GLN:HE22	1.54	0.73
1:C:430:ASN:ND2	1:C:433:MET:H	1.87	0.72
1:C:260:GLN:NE2	1:C:400:SER:H	1.87	0.72
1:C:283:ARG:HH22	1:C:418:LEU:HD22	1.54	0.70
1:C:466:GLN:O	1:C:467:ARG:HG3	1.91	0.70
1:A:648:ASN:HD22	1:A:648:ASN:H	1.37	0.70
1:A:537:THR:OG1	5:A:1092:HOH:O	2.09	0.70
1:C:678:LEU:HD22	1:C:679:PRO:HD2	1.72	0.70
1:A:424:SER:HB3	1:A:482[A]:PHE:CE1	2.26	0.69
1:C:462:ILE:O	1:C:466:GLN:N	2.24	0.69
1:A:596:HIS:CE1	1:A:659:GLU:OE1	2.43	0.69
1:A:369:PRO:HG3	1:A:436:ILE:HG22	1.75	0.69
1:A:563:ALA:H	1:A:587:ASN:ND2	1.91	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:SER:HB2	1:C:260:GLN:HE22	1.59	0.68
1:A:232:HIS:HA	1:A:235:LYS:HE3	1.75	0.68
1:C:234:HIS:HE1	1:C:398:THR:O	1.76	0.67
1:A:231:SER:HB2	1:A:260:GLN:NE2	2.09	0.67
1:C:193:LYS:HD3	1:C:193:LYS:N	2.05	0.67
1:A:376:GLU:OE2	1:A:411:ARG:NH1	2.25	0.67
1:A:553:ILE:N	1:A:553:ILE:HD12	2.10	0.66
1:C:503:VAL:HG23	1:C:561:ILE:HB	1.78	0.66
1:A:227:SER:HB3	1:A:478:LYS:HB3	1.78	0.65
1:A:596:HIS:CD2	1:C:362:ASP:OD2	2.49	0.65
1:C:643:ARG:HD2	1:C:701:GLN:CD	2.16	0.65
1:A:596:HIS:HD2	1:C:362:ASP:OD2	1.80	0.65
1:C:237:ASN:HA	1:C:240:GLN:OE1	1.97	0.65
1:A:228:LYS:HE2	1:A:498:PHE:CE2	2.32	0.64
1:C:563:ALA:H	1:C:587:ASN:ND2	1.94	0.64
1:C:325:PRO:HG2	1:C:330:VAL:HG11	1.80	0.64
1:A:643:ARG:HD2	1:A:701:GLN:CD	2.19	0.63
1:A:705:ASN:O	1:A:706:LYS:HD3	1.98	0.63
1:A:641:ASP:OD1	1:A:643:ARG:HD3	1.99	0.63
1:C:461:TYR:HE1	1:C:470:TYR:CG	2.16	0.63
1:C:260:GLN:HE21	1:C:400:SER:H	1.45	0.63
1:C:369:PRO:HG3	1:C:436:ILE:HG22	1.80	0.63
1:C:647:LYS:O	1:C:651:THR:HG23	1.99	0.62
1:A:386:TYR:CE2	1:A:425:LEU:HD13	2.34	0.62
1:C:234:HIS:CE1	1:C:398:THR:O	2.53	0.61
1:A:230:LYS:NZ	1:A:610:LYS:HA	2.16	0.61
1:C:376:GLU:OE2	1:C:411:ARG:NH1	2.34	0.61
1:A:678:LEU:HD22	1:A:679:PRO:HD2	1.83	0.61
1:C:430:ASN:HD22	1:C:433:MET:H	1.49	0.60
1:A:618:LEU:HD22	1:A:677:ILE:HB	1.84	0.60
1:C:465:LEU:O	1:C:467:ARG:N	2.35	0.59
1:A:605:ILE:HD12	1:A:605:ILE:O	2.02	0.59
1:C:465:LEU:HD23	1:C:470:TYR:HB3	1.85	0.59
1:A:386:TYR:HE2	1:A:425:LEU:HD13	1.67	0.59
1:C:229:LYS:HB2	5:C:1291:HOH:O	2.02	0.58
1:C:461:TYR:HA	1:C:464:LEU:HD12	1.83	0.58
1:C:325:PRO:HG2	1:C:330:VAL:CG1	2.34	0.58
1:A:193:LYS:HE2	1:A:241:TRP:CD2	2.39	0.58
1:C:705:ASN:O	1:C:706:LYS:HG3	2.03	0.58
1:C:256:SER:OG	1:C:258:LEU:HB2	2.03	0.58
1:C:434:LYS:O	1:C:438:LYS:HD3	2.02	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:LYS:O	1:C:467:ARG:HD2	2.05	0.57
1:C:596:HIS:HE1	1:C:659:GLU:OE1	1.87	0.57
1:A:534:PRO:O	1:A:536:THR:HG22	2.05	0.56
1:C:469:GLU:O	1:C:470:TYR:O	2.23	0.56
1:A:260:GLN:HE21	1:A:400:SER:H	1.52	0.56
1:A:430:ASN:HD22	1:A:433:MET:N	1.97	0.55
1:C:636:ASN:ND2	1:C:696:ILE:HB	2.21	0.55
1:C:455:ASP:OD2	1:C:455:ASP:N	2.38	0.55
1:A:538:THR:OG1	5:A:1092:HOH:O	2.18	0.55
1:A:193:LYS:HE2	1:A:241:TRP:CE2	2.42	0.55
1:C:333:VAL:HB	1:C:338:GLU:CG	2.34	0.55
1:A:283:ARG:NH2	1:A:418:LEU:CD2	2.68	0.55
1:C:283:ARG:NH2	1:C:418:LEU:HD22	2.22	0.55
1:C:641:ASP:OD1	1:C:643:ARG:HD3	2.07	0.55
1:A:320:ASN:H	1:A:320:ASN:HD22	1.56	0.54
1:C:505:TYR:OH	1:C:512:LYS:HE3	2.06	0.54
1:A:229:LYS:HZ3	1:A:232:HIS:HB3	1.73	0.54
1:C:461:TYR:CA	1:C:464:LEU:HB2	2.32	0.54
1:A:482[B]:PHE:HD2	1:A:484:LEU:CD1	2.21	0.53
1:C:469:GLU:HG2	1:C:470:TYR:N	2.22	0.53
1:C:460:GLU:HG2	1:C:462:ILE:HG22	1.90	0.53
1:A:687:MET:HE3	1:A:687:MET:O	2.08	0.53
1:A:603:LYS:HD2	1:C:341:ARG:CZ	2.38	0.53
1:C:263:TYR:HB2	5:C:1292:HOH:O	2.08	0.53
1:C:623:TYR:CD1	1:C:628:LEU:HD22	2.43	0.53
1:A:669:ARG:C	1:A:670:LEU:HD23	2.29	0.53
1:A:254:LEU:HD23	1:A:254:LEU:O	2.09	0.52
1:A:283:ARG:HH22	1:A:418:LEU:HD22	1.70	0.52
1:C:271:CYS:O	1:C:275:VAL:HG23	2.10	0.52
1:C:421:ASN:ND2	1:C:486:GLY:HA3	2.25	0.52
1:C:623:TYR:HD1	1:C:628:LEU:HD22	1.73	0.52
1:A:471:LEU:HD21	1:A:622:MET:SD	2.50	0.52
1:A:600:ALA:HA	1:C:341:ARG:HH21	1.75	0.52
1:A:648:ASN:H	1:A:648:ASN:ND2	2.04	0.51
1:C:461:TYR:O	1:C:465:LEU:N	2.43	0.51
1:C:197:ARG:HB3	1:C:204:PHE:CD2	2.45	0.51
1:C:305:GLU:HG2	1:C:536:THR:HG23	1.93	0.51
1:C:482[B]:PHE:CE1	1:C:579:GLY:HA3	2.45	0.51
1:C:426:GLU:HG2	1:C:482[A]:PHE:CD1	2.45	0.51
1:C:490:SER:HB2	1:C:571:THR:HB	1.92	0.51
1:C:306:VAL:O	1:C:311:TRP:CE3	2.64	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:LYS:H	1:C:193:LYS:CD	2.04	0.50
1:C:338:GLU:HB3	1:C:341:ARG:NH1	2.27	0.50
1:A:608:GLU:HA	1:A:608:GLU:OE1	2.11	0.50
1:C:563:ALA:H	1:C:587:ASN:HD22	1.58	0.49
1:C:426:GLU:HG2	1:C:482[A]:PHE:CE1	2.48	0.49
1:A:647:LYS:O	1:A:651:THR:HG23	2.12	0.49
1:C:498:PHE:CD2	1:C:611:PHE:HD2	2.31	0.49
1:A:625:ARG:HD2	1:A:626:ASN:OD1	2.13	0.49
1:C:633:THR:O	1:C:637:GLN:HG3	2.13	0.49
1:A:319:GLU:O	1:A:322:VAL:HG23	2.13	0.48
1:A:498:PHE:HD1	1:A:498:PHE:O	1.95	0.48
1:A:377:ASP:O	1:A:381:ILE:HG12	2.13	0.48
1:A:484:LEU:N	1:A:484:LEU:HD12	2.28	0.48
1:A:331:CYS:HB2	1:A:354:LYS:HD2	1.94	0.48
1:A:482[B]:PHE:CE1	1:A:580:GLY:HA2	2.48	0.48
1:A:260:GLN:NE2	1:A:400:SER:H	2.10	0.48
1:A:426:GLU:HG2	1:A:482[A]:PHE:CD1	2.49	0.48
1:C:466:GLN:O	1:C:467:ARG:CG	2.60	0.48
1:A:230:LYS:HZ1	1:A:610:LYS:HA	1.77	0.48
1:C:228:LYS:HB3	1:C:424:SER:OG	2.14	0.48
1:C:325:PRO:CG	1:C:330:VAL:HG11	2.43	0.47
1:C:675:ASN:H	1:C:675:ASN:ND2	2.10	0.47
1:A:661:GLU:OE1	1:A:687:MET:HE1	2.14	0.47
1:C:404:ASP:OD1	1:C:407:ARG:NH1	2.47	0.47
1:A:242:ILE:HD12	5:A:1190:HOH:O	2.13	0.47
1:C:386:TYR:CE2	1:C:425:LEU:HD13	2.49	0.47
1:C:197:ARG:HB3	1:C:204:PHE:CE2	2.50	0.47
1:C:468:GLU:OE1	1:C:469:GLU:N	2.47	0.47
1:A:296:SER:HA	1:A:297:PRO:HD3	1.77	0.47
1:A:325:PRO:HG2	1:A:330:VAL:CG1	2.33	0.47
1:A:449:VAL:HG22	1:A:477:PRO:HG2	1.96	0.47
1:A:503:VAL:HG23	1:A:561:ILE:HB	1.97	0.47
1:A:563:ALA:H	1:A:587:ASN:HD22	1.62	0.47
1:C:424:SER:HB2	1:C:482[A]:PHE:CG	2.50	0.47
1:C:634:GLU:O	1:C:638:GLU:HG2	2.15	0.47
1:C:678:LEU:HD13	1:C:683:LYS:HG3	1.97	0.47
1:A:234:HIS:C	1:A:236:LYS:H	2.17	0.47
1:A:274:CYS:HA	1:A:277:HIS:CE1	2.50	0.47
1:C:238:ASP:O	1:C:254:LEU:HB2	2.14	0.47
1:C:369:PRO:HG3	1:C:436:ILE:CG2	2.45	0.47
1:A:271:CYS:O	1:A:275:VAL:HG23	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:GLN:HE21	1:C:399:TYR:HA	1.79	0.46
1:A:325:PRO:HB2	1:A:330:VAL:HG12	1.96	0.46
1:A:470:TYR:O	1:A:471:LEU:HB2	2.16	0.46
1:A:532:THR:CB	1:A:604:GLU:HG2	2.42	0.46
1:A:664:MET:HG3	1:A:687:MET:HG3	1.98	0.46
1:A:376:GLU:H	1:A:376:GLU:HG2	1.51	0.46
1:C:657:LYS:HD2	1:C:694:ILE:HD12	1.96	0.46
1:A:198:CYS:HB2	1:A:241:TRP:CH2	2.51	0.46
1:C:482[B]:PHE:CD1	1:C:484:LEU:CD1	2.98	0.46
1:A:430:ASN:ND2	1:A:433:MET:HB2	2.31	0.46
1:A:628:LEU:HD12	1:A:649:ILE:HG23	1.97	0.45
1:C:386:TYR:HE2	1:C:425:LEU:HD13	1.81	0.45
1:A:657:LYS:HD2	1:A:694:ILE:HD12	1.98	0.45
1:C:509:LYS:HB2	1:C:509:LYS:HE3	1.67	0.45
1:C:267:GLU:HG3	1:C:284:TYR:CE1	2.51	0.45
1:C:352:TRP:CE2	1:C:562:PRO:HB3	2.52	0.45
1:C:427:PHE:CD1	1:C:433:MET:HB3	2.52	0.45
1:C:231:SER:HB2	1:C:260:GLN:NE2	2.30	0.45
1:A:244:CYS:O	1:A:248:GLN:HA	2.17	0.45
1:A:616:PHE:O	1:A:619:LEU:HB3	2.16	0.45
1:C:231:SER:HB3	1:C:389:ASP:OD2	2.17	0.45
1:A:352:TRP:CE2	1:A:562:PRO:HB3	2.51	0.45
1:A:503:VAL:CG2	1:A:561:ILE:HB	2.47	0.45
1:A:192:PRO:HD2	1:A:250:TRP:HH2	1.83	0.44
1:A:241:TRP:CZ2	1:A:252:HIS:NE2	2.86	0.44
1:A:684:ASN:O	1:A:688:ILE:HD13	2.18	0.44
1:C:625:ARG:HG3	1:C:686:ILE:HG12	2.00	0.44
1:A:515:TYR:O	1:A:567:HIS:HA	2.18	0.44
1:C:361:MET:O	1:C:364:LEU:HB2	2.18	0.43
1:A:498:PHE:CD2	1:A:611:PHE:HD2	2.36	0.43
1:A:623:TYR:CD1	1:A:628:LEU:HD22	2.53	0.43
1:A:490:SER:HB2	1:A:571:THR:HB	2.01	0.43
1:A:678:LEU:HB3	1:A:683:LYS:HE3	2.00	0.43
1:A:389:ASP:HB3	1:A:423:LEU:HD12	2.01	0.43
1:A:275:VAL:N	1:A:276:PRO:CD	2.81	0.43
1:A:669:ARG:O	1:A:670:LEU:HD23	2.19	0.43
1:A:551:VAL:O	1:A:551:VAL:HG13	2.19	0.43
1:A:703:ALA:C	1:A:705:ASN:H	2.22	0.43
1:C:260:GLN:HE21	1:C:400:SER:N	2.16	0.43
1:A:193:LYS:HE2	1:A:241:TRP:CG	2.54	0.43
1:A:611:PHE:CZ	1:A:614:PRO:HG3	2.54	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:426:GLU:HG3	1:C:478:LYS:O	2.19	0.43
1:A:656:MET:O	1:A:660:MET:HG3	2.19	0.42
1:C:233:HIS:CD2	1:C:609:GLU:HG2	2.54	0.42
1:A:375:LEU:O	1:A:379:VAL:HG13	2.19	0.42
1:C:274:CYS:HA	1:C:277:HIS:CE1	2.54	0.42
1:A:476:ARG:NH2	1:A:478:LYS:HG3	2.34	0.42
1:A:432:GLU:O	1:A:436:ILE:HG12	2.19	0.42
1:A:533:SER:HA	1:A:534:PRO:HD3	1.83	0.42
1:C:233:HIS:NE2	1:C:609:GLU:HA	2.34	0.42
1:C:585:LEU:HD12	1:C:585:LEU:HA	1.81	0.42
1:C:193:LYS:N	1:C:193:LYS:CD	2.74	0.42
5:A:1295:HOH:O	1:C:361:MET:HE3	2.18	0.42
4:C:1000:2HG:H2	5:C:1041:HOH:O	2.20	0.42
1:A:424:SER:HB3	1:A:482[A]:PHE:CD1	2.55	0.42
1:A:603:LYS:NZ	1:C:341:ARG:NH2	2.68	0.42
1:A:426:GLU:HG2	1:A:482[A]:PHE:CE1	2.55	0.42
1:A:503:VAL:CG1	1:A:581:ASN:ND2	2.83	0.42
1:A:193:LYS:HB2	1:A:250:TRP:CE2	2.54	0.41
1:A:449:VAL:CG2	1:A:477:PRO:HG2	2.50	0.41
1:A:623:TYR:HD1	1:A:628:LEU:HD22	1.85	0.41
1:C:394:TYR:CZ	1:C:419:LEU:HG	2.55	0.41
1:C:498:PHE:HD2	1:C:611:PHE:HD2	1.67	0.41
1:A:361:MET:O	1:A:364:LEU:HB2	2.20	0.41
1:A:678:LEU:HD22	1:A:679:PRO:CD	2.50	0.41
1:C:244:CYS:O	1:C:248:GLN:HA	2.20	0.41
1:C:462:ILE:O	1:C:465:LEU:HB3	2.20	0.41
1:C:467:ARG:HB3	1:C:468:GLU:H	1.68	0.41
1:C:320:ASN:ND2	1:C:320:ASN:H	2.17	0.41
1:A:528:GLN:HB2	1:A:597:LEU:HD11	2.02	0.41
1:A:426:GLU:CG	1:A:482[A]:PHE:CE1	3.03	0.41
1:C:484:LEU:N	1:C:484:LEU:HD12	2.35	0.41
1:A:514:PHE:HB2	1:A:551:VAL:CG1	2.51	0.41
1:A:678:LEU:HA	1:A:679:PRO:HD3	1.86	0.41
1:C:461:TYR:HA	1:C:464:LEU:CB	2.39	0.41
1:A:648:ASN:ND2	1:A:648:ASN:N	2.68	0.41
1:C:527:TYR:CZ	1:C:531:GLU:HG3	2.56	0.41
1:A:197:ARG:HB3	1:A:204:PHE:CD2	2.56	0.41
1:A:376:GLU:OE2	1:A:411:ARG:HD2	2.21	0.41
1:C:495:HIS:HA	1:C:527:TYR:OH	2.21	0.41
1:A:429:ASP:OD1	1:A:429:ASP:N	2.51	0.41
1:C:463:LYS:HE3	1:C:463:LYS:HB2	1.77	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:515:TYR:O	1:C:567:HIS:HA	2.20	0.41
1:C:669:ARG:O	1:C:670:LEU:HD23	2.20	0.41
1:A:322:VAL:HA	1:A:323:PRO:HD3	1.91	0.41
1:C:239:PHE:CZ	1:C:254:LEU:HD12	2.56	0.41
1:C:376:GLU:HA	1:C:379:VAL:HG12	2.03	0.41
1:C:678:LEU:HD22	1:C:679:PRO:CD	2.46	0.41
1:C:322:VAL:CG1	1:C:550:ARG:HB2	2.51	0.40
1:C:573:VAL:O	1:C:574:ASP:C	2.60	0.40
1:C:605:ILE:HD12	1:C:605:ILE:O	2.21	0.40
1:C:373:PHE:HA	1:C:377:ASP:OD1	2.20	0.40
1:A:696:ILE:O	1:A:700:ILE:HG13	2.21	0.40
1:C:233:HIS:CD2	1:C:609:GLU:HA	2.56	0.40
1:A:292:TYR:CE2	1:A:396:GLN:HG3	2.56	0.40
1:A:452:LEU:C	1:A:454:PRO:HD3	2.42	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	478/528 (90%)	454 (95%)	22 (5%)	2 (0%)	34	32
1	C	491/528 (93%)	466 (95%)	20 (4%)	5 (1%)	15	11
All	All	969/1056 (92%)	920 (95%)	42 (4%)	7 (1%)	22	18

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	423	LEU
1	C	423	LEU
1	C	466	GLN
1	C	467	ARG

Continued on next page...



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	469	GLU
1	C	470	TYR
1	A	471	LEU

### 5.3.2 Protein sidechains [i](#)

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	435/475 (92%)	403 (93%)	32 (7%)	13	10
1	C	447/475 (94%)	415 (93%)	32 (7%)	14	11
All	All	882/950 (93%)	818 (93%)	64 (7%)	14	11

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	LYS
1	A	237	ASN
1	A	245	ASP
1	A	249	THR
1	A	258	LEU
1	A	283	ARG
1	A	298	ASN
1	A	320	ASN
1	A	344	GLU
1	A	364	LEU
1	A	376	GLU
1	A	379	VAL
1	A	384	SER
1	A	407	ARG
1	A	424	SER
1	A	425	LEU
1	A	433	MET
1	A	441	ARG
1	A	456	VAL
1	A	470	TYR

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	477	PRO
1	A	498	PHE
1	A	536	THR
1	A	608	GLU
1	A	628	LEU
1	A	629	LEU
1	A	648	ASN
1	A	664	MET
1	A	670	LEU
1	A	678	LEU
1	A	695	GLU
1	A	706	LYS
1	C	193	LYS
1	C	234	HIS
1	C	240	GLN
1	C	249	THR
1	C	254	LEU
1	C	258	LEU
1	C	283	ARG
1	C	340	ARG
1	C	355	VAL
1	C	364	LEU
1	C	418	LEU
1	C	425	LEU
1	C	430	ASN
1	C	433	MET
1	C	441	ARG
1	C	442	PHE
1	C	455	ASP
1	C	461	TYR
1	C	468	GLU
1	C	484	LEU
1	C	498	PHE
1	C	503	VAL
1	C	508	LEU
1	C	573	VAL
1	C	608	GLU
1	C	625	ARG
1	C	628	LEU
1	C	629	LEU
1	C	648	ASN
1	C	664	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	675	ASN
1	C	678	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	260	GLN
1	A	277	HIS
1	A	320	ASN
1	A	395	ASN
1	A	421	ASN
1	A	430	ASN
1	A	587	ASN
1	A	596	HIS
1	A	648	ASN
1	A	705	ASN
1	C	234	HIS
1	C	260	GLN
1	C	277	HIS
1	C	298	ASN
1	C	320	ASN
1	C	395	ASN
1	C	396	GLN
1	C	421	ASN
1	C	430	ASN
1	C	587	ASN
1	C	596	HIS
1	C	675	ASN
1	C	705	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	2HG	C	1000	2	9,9,9	2.16	3 (33%)	10,11,11	2.47	4 (40%)
4	2HG	A	1000	2	9,9,9	2.15	3 (33%)	10,11,11	2.78	5 (50%)

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	2HG	C	1000	2	-	6/9/9/9	-
4	2HG	A	1000	2	-	4/9/9/9	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1000	2HG	O4-C5	4.78	1.38	1.22
4	C	1000	2HG	O4-C5	4.55	1.37	1.22
4	C	1000	2HG	O3-C2	-2.43	1.37	1.42
4	A	1000	2HG	O3-C2	-2.31	1.37	1.42
4	A	1000	2HG	O5-C5	2.25	1.38	1.30
4	C	1000	2HG	O5-C5	2.12	1.37	1.30

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1000	2HG	C4-C3-C2	5.47	121.93	114.46
4	C	1000	2HG	O5-C5-O4	-4.71	111.56	123.30
4	A	1000	2HG	O5-C5-O4	-4.41	112.30	123.30
4	C	1000	2HG	O4-C5-C4	-3.38	112.23	123.08
4	C	1000	2HG	C4-C3-C2	3.37	119.06	114.46
4	A	1000	2HG	O2-C1-C2	3.08	119.49	112.72
4	C	1000	2HG	O2-C1-C2	2.88	119.04	112.72
4	A	1000	2HG	O4-C5-C4	-2.46	115.17	123.08
4	A	1000	2HG	O1-C1-C2	-2.22	118.20	122.54

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1000	2HG	C2-C3-C4-C5
4	C	1000	2HG	O1-C1-C2-O3
4	C	1000	2HG	O2-C1-C2-C3
4	C	1000	2HG	O3-C2-C3-C4
4	A	1000	2HG	C2-C3-C4-C5
4	A	1000	2HG	O2-C1-C2-O3
4	A	1000	2HG	O1-C1-C2-C3
4	A	1000	2HG	O2-C1-C2-C3
4	C	1000	2HG	O1-C1-C2-C3
4	C	1000	2HG	O2-C1-C2-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1000	2HG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	483/528 (91%)	0.57	36 (7%)	14 18	32, 54, 82, 103	0
1	C	496/528 (93%)	0.47	39 (7%)	12 16	32, 53, 86, 107	0
All	All	979/1056 (92%)	0.52	75 (7%)	13 17	32, 54, 84, 107	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	462	ILE	10.2
1	C	233	HIS	6.4
1	C	236	LYS	6.1
1	A	236	LYS	5.6
1	C	461	TYR	5.6
1	C	460	GLU	5.6
1	C	470	TYR	5.6
1	A	456	VAL	5.4
1	C	225	LEU	5.3
1	A	674	LYS	5.1
1	A	235	LYS	5.1
1	C	206	HIS	5.1
1	C	606	ARG	5.0
1	C	234	HIS	5.0
1	A	234	HIS	4.8
1	A	233	HIS	4.7
1	A	470	TYR	4.4
1	C	465	LEU	4.3
1	C	239	PHE	4.3
1	A	482[A]	PHE	4.3
1	A	232	HIS	4.3
1	C	231	SER	4.2
1	A	705	ASN	4.1
1	C	674	LYS	4.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	675	ASN	4.0
1	A	231	SER	4.0
1	C	468	GLU	4.0
1	A	505	TYR	3.9
1	C	608	GLU	3.8
1	A	225	LEU	3.8
1	C	609	GLU	3.7
1	A	239	PHE	3.7
1	C	466	GLN	3.7
1	C	607	SER	3.7
1	C	277	HIS	3.6
1	A	414	LYS	3.4
1	A	606	ARG	3.3
1	A	204	PHE	3.3
1	A	607	SER	3.1
1	C	235	LYS	3.1
1	C	706	LYS	3.1
1	C	232	HIS	2.9
1	C	505	TYR	2.9
1	A	241	TRP	2.9
1	C	204	PHE	2.8
1	C	675	ASN	2.8
1	A	314	ASP	2.8
1	A	422	PHE	2.7
1	C	463	LYS	2.6
1	C	195	SER	2.6
1	C	482[A]	PHE	2.6
1	A	503	VAL	2.6
1	C	194	GLU	2.6
1	C	241	TRP	2.5
1	A	706	LYS	2.5
1	C	668	LEU	2.5
1	C	676	ALA	2.4
1	C	467	ARG	2.4
1	A	254	LEU	2.4
1	C	229	LYS	2.4
1	A	668	LEU	2.3
1	C	705	ASN	2.3
1	A	423	LEU	2.3
1	C	203	LYS	2.2
1	A	303	GLY	2.2
1	A	561	ILE	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	287	VAL	2.1
1	A	608	GLU	2.1
1	A	203	LYS	2.1
1	C	457	SER	2.1
1	A	302	LEU	2.0
1	A	304	ILE	2.0
1	A	483	CYS	2.0
1	C	703	ALA	2.0
1	A	577	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å <sup>2</sup> )	Q<0.9
4	2HG	A	1000	10/10	0.94	0.26	38,47,53,59	3
4	2HG	C	1000	10/10	0.94	0.25	43,48,55,60	3
3	ZN	A	3	1/1	0.97	0.12	55,55,55,55	0
3	ZN	A	2	1/1	0.98	0.07	65,65,65,65	0
3	ZN	C	2	1/1	0.99	0.06	72,72,72,72	0
3	ZN	C	3	1/1	0.99	0.11	58,58,58,58	0
2	FE2	A	1	1/1	1.00	0.20	39,39,39,39	0
2	FE2	C	1	1/1	1.00	0.20	39,39,39,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.