



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 07:13 PM UTC

PDB ID : 3PUR / pdb_00003pur
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

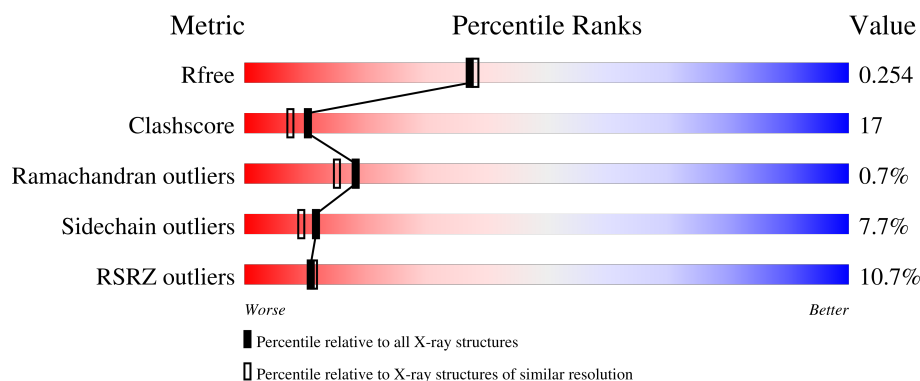
1 Overall quality at a glance

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 ≥ 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

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
1	A	483	Total	C	N	O	S	0	1	0
			3982	2548	673	733	28			
1	C	496	Total	C	N	O	S	0	1	0
			4094	2618	693	755	28			

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

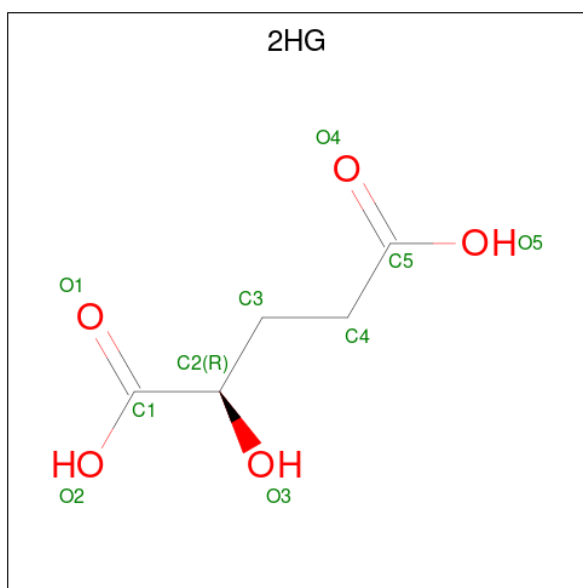
- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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 (CCD ID: 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		

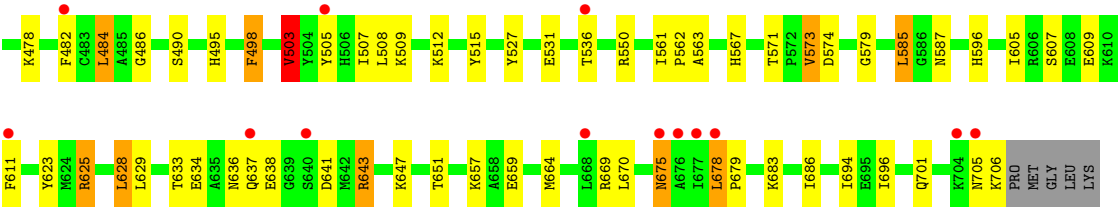
- Molecule 4 is (2R)-2-hydroxypentanedioic acid (CCD ID: 2HG) (formula: $C_5H_8O_5$).



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

- Molecule 5 is water.

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.01Å 144.09Å 78.09Å 90.00° 106.22° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 50.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	87.0 (50.00-2.10) 95.9 (50.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.68 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_353)	Depositor
R, R_{free}	0.214 , 0.251 0.218 , 0.254	Depositor DCC
R_{free} test set	3930 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	39.0	Xtriage
Anisotropy	0.768	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8399	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.52	0/4091	0.88	10/5518 (0.2%)
1	C	0.50	0/4205	0.83	6/5670 (0.1%)
All	All	0.51	0/8296	0.85	16/11188 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	464	LEU	N-CA-C	-6.33	104.44	111.71
1	A	197	ARG	N-CA-C	6.23	119.86	109.95
1	C	507	ILE	CB-CA-C	-6.21	105.21	111.80
1	A	609	GLU	N-CA-C	-5.89	105.59	112.89
1	A	507	ILE	CB-CA-C	-5.82	105.64	111.80
1	A	422	PHE	N-CA-C	5.80	119.71	109.96
1	A	471	LEU	CA-C-N	5.78	125.71	119.76
1	A	471	LEU	C-N-CA	5.78	125.71	119.76
1	C	422	PHE	N-CA-C	5.60	118.94	109.76
1	C	421	ASN	CA-C-N	-5.46	114.52	122.65
1	C	421	ASN	C-N-CA	-5.46	114.52	122.65
1	A	476	ARG	CA-C-N	-5.39	114.01	119.83
1	A	476	ARG	C-N-CA	-5.39	114.01	119.83
1	A	533	SER	CA-C-N	5.17	124.78	119.56
1	A	533	SER	C-N-CA	5.17	124.78	119.56
1	C	503	VAL	CB-CA-C	-5.10	102.65	110.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3982	0	3859	135	0
1	C	4094	0	3968	138	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	269	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 17.

All (269) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:361:MET:HE1	5:C:1294:HOH:O	1.88	0.73
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:643:ARG:HD2	1:C:701:GLN:CD	2.16	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
1:C:231:SER:HB2	1:C:260:GLN:HE22	1.59	0.68
1:A:643:ARG:HD2	1:A:701:GLN:CD	2.19	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: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
5:A:1295:HOH:O	1:C:361:MET:HE3	1.97	0.64
1:A:230:LYS:HZ3	1:A:610:LYS:HA	1.60	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:229:LYS:HZ3	1:A:232:HIS:HB3	1.65	0.61
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
1:A:687:MET:HE3	1:A:687:MET:O	2.04	0.57
1:A:669:ARG:C	1:A:670:LEU:HD23	2.29	0.57
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: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:C:461:TYR:CA	1:C:464:LEU:HB2	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:538:THR:OG1	5:A:1092:HOH:O	2.18	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
1:A:234:HIS:C	1:A:236:LYS:H	2.17	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:MET:HE3	1:A:687:MET:CA	2.43	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:703:ALA:C	1:A:705:ASN:H	2.22	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: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
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: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:A:470:TYR:O	1:A:471:LEU:HB2	2.16	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:A:193:LYS:NZ	1:A:205:THR:OG1	2.48	0.45
1:C:231:SER:HB2	1:C:260:GLN:NE2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:573:VAL:O	1:C:574:ASP:C	2.60	0.45
1:A:244:CYS:O	1:A:248:GLN:HA	2.17	0.45
1:A:452:LEU:C	1:A:454:PRO:HD3	2.42	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:C:194:GLU:C	1:C:196:ASP:H	2.24	0.44
1:C:425:LEU:HD12	1:C:425:LEU:C	2.43	0.44
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:A:661:GLU:OE1	1:A:687:MET:HE2	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:C:641:ASP:OD1	1:C:641:ASP:C	2.61	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: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
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:621:TRP:HA	1:A:660:MET:HE1	2.01	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
4:C:1000:2HG:H2	5:C:1041:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:471:LEU:O	1:C:472:PRO:C	2.63	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:669:ARG:C	1:C:670:LEU:HD23	2.45	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:C:607:SER:C	1:C:609:GLU:H	2.27	0.41
1:C:705:ASN:C	1:C:706:LYS:HG3	2.45	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:A:687:MET:HE3	1:A:687:MET:C	2.46	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:A:439:PRO:O	1:A:440:PRO:C	2.64	0.41
1:C:463:LYS:HE3	1:C:463:LYS:HB2	1.77	0.41
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:234:HIS:C	1:A:236:LYS:N	2.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:VAL:CG1	1:C:550:ARG:HB2	2.51	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

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%)	30	28
1	C	491/528 (93%)	466 (95%)	20 (4%)	5 (1%)	12	9
All	All	969/1056 (92%)	920 (95%)	42 (4%)	7 (1%)	18	15

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
1	C	469	GLU
1	C	470	TYR
1	A	471	LEU

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	435/475 (92%)	397 (91%)	38 (9%)	9	7
1	C	447/475 (94%)	417 (93%)	30 (7%)	15	12
All	All	882/950 (93%)	814 (92%)	68 (8%)	12	9

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	LYS
1	A	237	ASN
1	A	249	THR
1	A	258	LEU
1	A	283	ARG
1	A	298	ASN
1	A	320	ASN
1	A	340	ARG
1	A	344	GLU
1	A	364	LEU
1	A	376	GLU
1	A	379	VAL
1	A	381	ILE
1	A	384	SER
1	A	388	VAL
1	A	407	ARG
1	A	411	ARG
1	A	418	LEU
1	A	424	SER
1	A	425	LEU
1	A	433	MET
1	A	456	VAL
1	A	498	PHE
1	A	503	VAL
1	A	509	LYS
1	A	536	THR
1	A	573	VAL

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Mol	Chain	Res	Type
1	A	605	ILE
1	A	608	GLU
1	A	628	LEU
1	A	629	LEU
1	A	643	ARG
1	A	648	ASN
1	A	664	MET
1	A	668	LEU
1	A	670	LEU
1	A	678	LEU
1	A	695	GLU
1	C	193	LYS
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	455	ASP
1	C	461	TYR
1	C	466	GLN
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	585	LEU
1	C	625	ARG
1	C	628	LEU
1	C	629	LEU
1	C	643	ARG
1	C	664	MET
1	C	675	ASN
1	C	678	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	260	GLN
1	A	277	HIS
1	A	320	ASN
1	A	351	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	233	HIS
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	421	ASN
1	C	430	ASN
1	C	475	GLN
1	C	584	HIS
1	C	587	ASN
1	C	596	HIS
1	C	675	ASN
1	C	684	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 oligosaccharides 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	2HG	C	1000	2	9,9,9	2.22	3 (33%)	10,11,11	2.42	4 (40%)
4	2HG	A	1000	2	9,9,9	2.20	3 (33%)	10,11,11	2.66	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	4.86	1.38	1.22
4	C	1000	2HG	O4-C5	4.62	1.37	1.22
4	C	1000	2HG	O3-C2	-2.42	1.37	1.42
4	A	1000	2HG	O3-C2	-2.30	1.37	1.42
4	A	1000	2HG	O5-C5	2.27	1.38	1.30
4	C	1000	2HG	O5-C5	2.13	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	4.81	121.93	114.48
4	C	1000	2HG	O5-C5-O4	-4.58	111.56	123.33
4	A	1000	2HG	O5-C5-O4	-4.29	112.30	123.33
4	C	1000	2HG	O4-C5-C4	-3.43	112.23	123.09
4	A	1000	2HG	O2-C1-C2	3.19	119.49	112.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1000	2HG	O2-C1-C2	2.98	119.04	112.74
4	C	1000	2HG	C4-C3-C2	2.96	119.06	114.48
4	A	1000	2HG	O4-C5-C4	-2.50	115.17	123.09
4	A	1000	2HG	O1-C1-C2	-2.20	118.20	122.60

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	483/528 (91%)	0.84	53 (10%)	10 11	25, 54, 82, 103	1 (0%)
1	C	496/528 (93%)	0.79	52 (10%)	11 12	24, 53, 86, 107	1 (0%)
All	All	979/1056 (92%)	0.82	105 (10%)	11 11	24, 54, 84, 107	2 (0%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	465	LEU	8.2
1	A	225	LEU	7.2
1	C	470	TYR	7.0
1	C	464	LEU	6.4
1	A	470	TYR	5.6
1	C	458	GLY	5.4
1	A	192	PRO	5.4
1	C	462	ILE	5.3
1	A	456	VAL	5.0
1	A	705	ASN	4.6
1	C	466	GLN	4.6
1	C	277	HIS	4.6
1	C	192	PRO	4.5
1	C	468	GLU	4.5
1	C	463	LYS	4.3
1	A	423	LEU	4.2
1	C	461	TYR	4.2
1	C	225	LEU	4.2
1	C	307	GLY	4.0
1	A	505	TYR	4.0
1	C	231	SER	3.9
1	C	195	SER	3.9
1	C	239	PHE	3.7
1	A	234	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	505	TYR	3.5
1	A	231	SER	3.5
1	C	460	GLU	3.4
1	A	235	LYS	3.4
1	C	234	HIS	3.4
1	A	314	ASP	3.1
1	C	678	LEU	3.1
1	C	423	LEU	3.1
1	A	608	GLU	3.1
1	C	206	HIS	3.1
1	C	233	HIS	3.1
1	A	681	ASP	3.0
1	A	239	PHE	3.0
1	A	204	PHE	3.0
1	A	704	LYS	2.9
1	C	230	LYS	2.9
1	A	685	LYS	2.9
1	A	303	GLY	2.9
1	C	204	PHE	2.9
1	C	611	PHE	2.9
1	A	482[A]	PHE	2.8
1	A	675	ASN	2.8
1	A	703	ALA	2.8
1	C	203	LYS	2.8
1	A	676	ALA	2.8
1	A	236	LYS	2.7
1	A	226	MET	2.7
1	A	706	LYS	2.7
1	C	229	LYS	2.7
1	C	236	LYS	2.7
1	A	611	PHE	2.6
1	C	249	THR	2.6
1	A	304	ILE	2.6
1	A	637	GLN	2.6
1	A	233	HIS	2.6
1	A	330	VAL	2.5
1	C	456	VAL	2.5
1	A	536	THR	2.5
1	C	371	PRO	2.5
1	C	471	LEU	2.5
1	A	603	LYS	2.5
1	A	664	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	668	LEU	2.4
1	C	374	ASP	2.4
1	A	674	LYS	2.4
1	C	675	ASN	2.4
1	A	277	HIS	2.4
1	C	705	ASN	2.3
1	A	316	ILE	2.3
1	C	250	TRP	2.3
1	C	482[A]	PHE	2.3
1	C	536	THR	2.3
1	A	230	LYS	2.3
1	A	232	HIS	2.3
1	C	640	SER	2.2
1	A	196	ASP	2.2
1	A	203	LYS	2.2
1	A	651	THR	2.2
1	C	196	ASP	2.2
1	A	471	LEU	2.2
1	A	607	SER	2.2
1	A	692	LYS	2.2
1	A	680	THR	2.2
1	A	229	LYS	2.1
1	C	704	LYS	2.1
1	C	226	MET	2.1
1	C	311	TRP	2.1
1	C	637	GLN	2.1
1	C	251	TYR	2.1
1	A	639	GLY	2.1
1	A	193	LYS	2.1
1	A	686	ILE	2.1
1	C	677	ILE	2.1
1	C	379	VAL	2.1
1	A	371	PRO	2.0
1	A	546	GLY	2.0
1	C	422	PHE	2.0
1	C	469	GLU	2.0
1	C	676	ALA	2.0
1	A	528	GLN	2.0
1	A	202	GLY	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	2HG	C	1000	10/10	0.92	0.14	43,48,55,60	3
4	2HG	A	1000	10/10	0.94	0.12	38,47,53,59	3
3	ZN	A	2	1/1	0.99	0.03	65,65,65,65	0
3	ZN	A	3	1/1	0.99	0.03	55,55,55,55	0
3	ZN	C	2	1/1	1.00	0.02	72,72,72,72	0
3	ZN	C	3	1/1	1.00	0.02	58,58,58,58	0
2	FE2	A	1	1/1	1.00	0.05	39,39,39,39	0
2	FE2	C	1	1/1	1.00	0.05	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.