



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:21 pm GMT

PDB ID : 2WG3  
Title : CRYSTAL STRUCTURE OF THE COMPLEX BETWEEN HUMAN HEDGEHOG-INTERACTING PROTEIN HIP AND DESERT HEDGEHOG WITHOUT CALCIUM  
Authors : Bishop, B.; Aricescu, A.R.; Harlos, K.; O'Callaghan, C.A.; Jones, E.Y.; Siebold, C.  
Deposited on : 2009-04-15  
Resolution : 2.60 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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

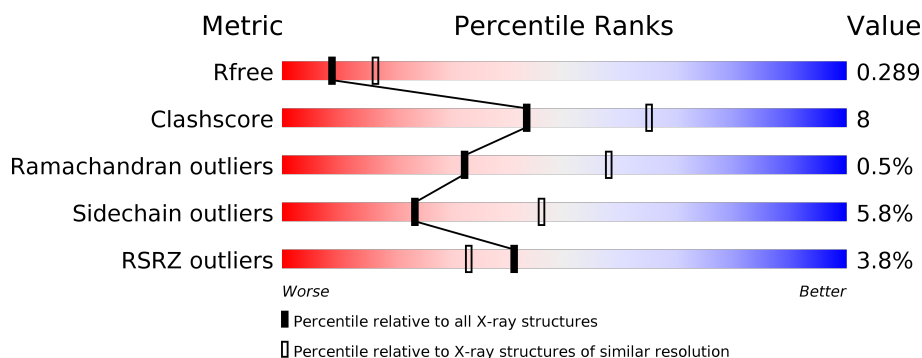
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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	164	
1	B	164	
2	C	463	
2	D	463	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	C	1641	-	-	-	X
6	NAG	D	1640	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8980 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 DESERT HEDGEHOG PROTEIN N-PRODUCT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	155	Total	C	N	O	S	0	0	0
			1235	774	231	226	4			
1	B	150	Total	C	N	O	S	0	0	0
			1192	746	222	220	4			

- Molecule 2 is a protein called HEDGEHOG-INTERACTING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	406	Total	C	N	O	S	0	0	0
			3186	2007	556	600	23			
2	D	409	Total	C	N	O	S	0	0	0
			3198	2014	556	606	22			

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

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

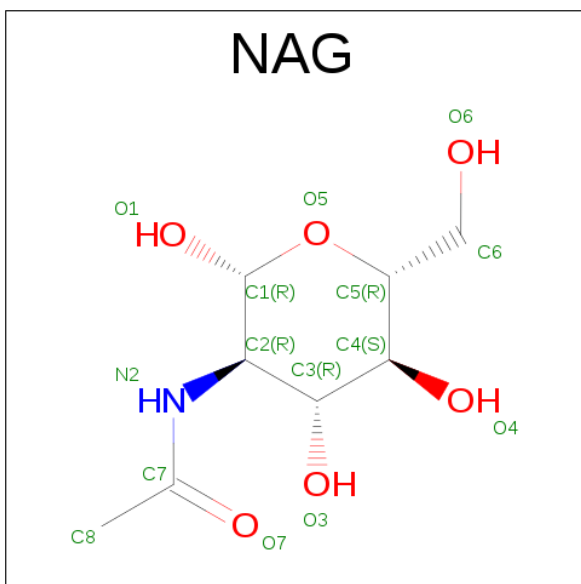
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	D	3	Total	Cl	0	0
			3	3		
4	C	2	Total	Cl	0	0
			2	2		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	N	O	0	0
			14	8	1	5		

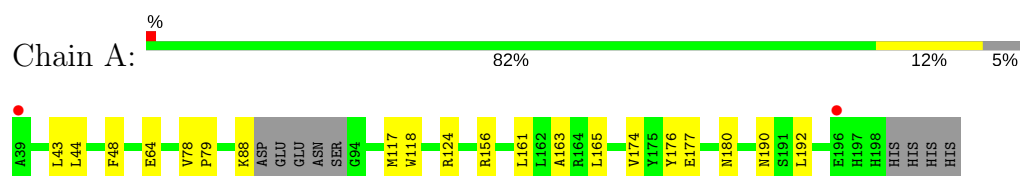
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	12	Total	O	0	0
			12	12		
7	B	18	Total	O	0	0
			18	18		
7	C	38	Total	O	0	0
			38	38		
7	D	55	Total	O	0	0
			55	55		

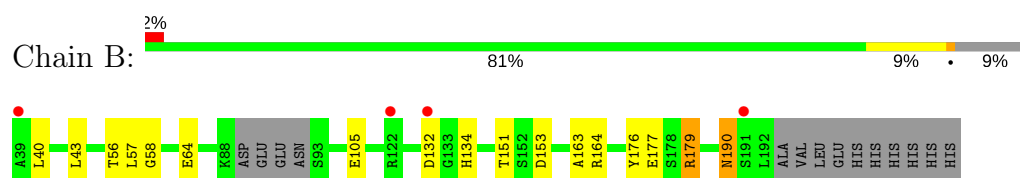
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

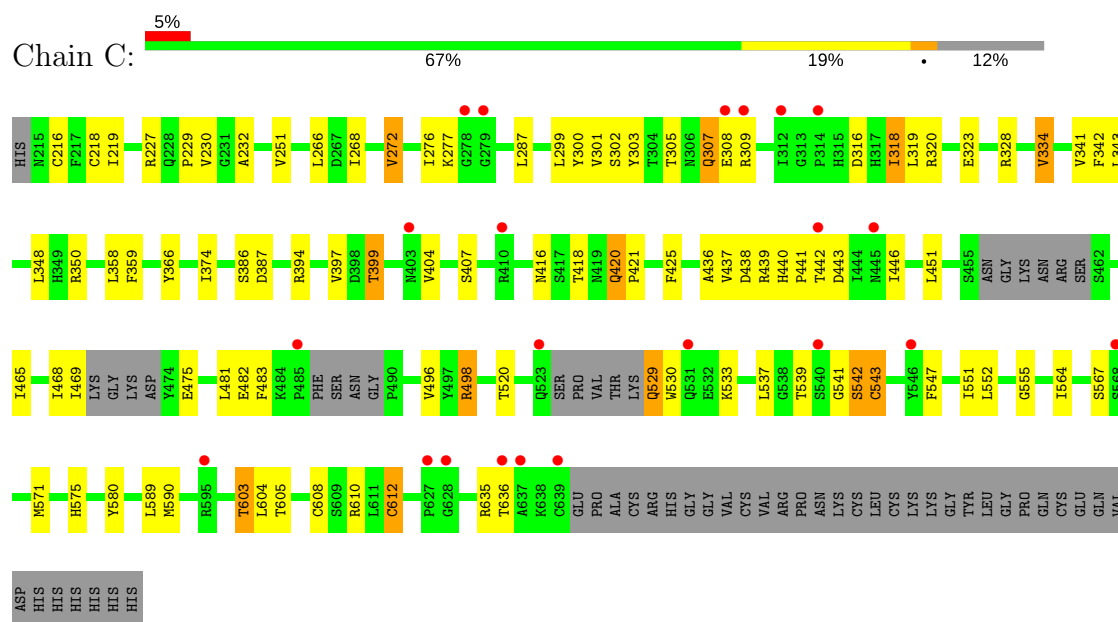
#### • Molecule 1: DESERT HEDGEHOG PROTEIN N-PRODUCT



#### • Molecule 1: DESERT HEDGEHOG PROTEIN N-PRODUCT

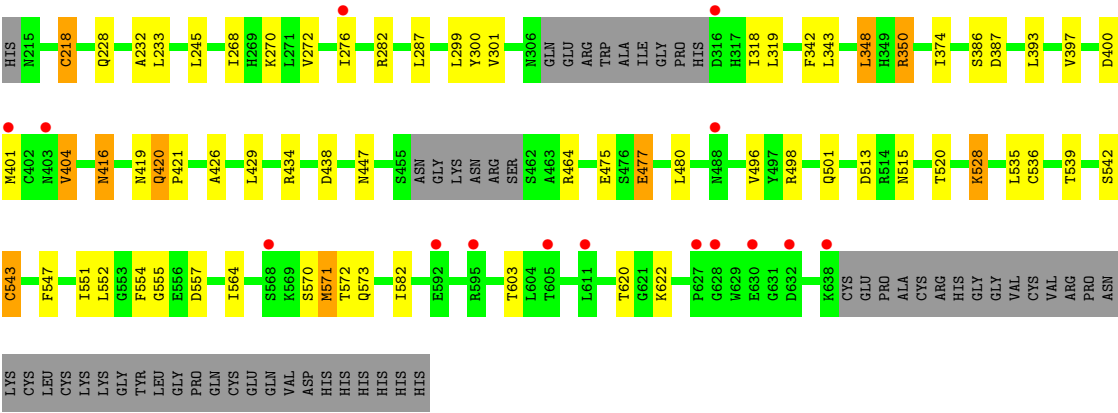


#### • Molecule 2: HEDGEHOG-INTERACTING PROTEIN



#### • Molecule 2: HEDGEHOG-INTERACTING PROTEIN







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.82Å 110.70Å 144.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 20.25 – 2.52	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.60) 99.3 (20.25-2.52)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 2.53Å)	Xtriage
Refinement program	REFMAC 5.5.0047	Depositor
R, $R_{free}$	0.224 , 0.281 0.234 , 0.289	Depositor DCC
$R_{free}$ test set	2592 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.3	Xtriage
Anisotropy	1.158	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 50.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8980	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.18 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.8059e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, CL, ZN, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.56	0/1263	0.73	0/1711
1	B	0.50	0/1218	0.66	0/1649
2	C	0.53	1/3258 (0.0%)	0.65	0/4403
2	D	0.56	1/3270 (0.0%)	0.68	0/4420
All	All	0.54	2/9009 (0.0%)	0.67	0/12183

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
2	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	536	CYS	CB-SG	-6.51	1.71	1.82
2	C	216	CYS	CB-SG	-5.28	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	528	LYS	Peptide

## 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	1235	0	1201	11	0
1	B	1192	0	1161	10	0
2	C	3186	0	3092	63	0
2	D	3198	0	3115	48	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	C	2	0	0	0	0
4	D	3	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	1	0
6	C	14	0	13	2	0
6	D	14	0	13	5	0
7	A	12	0	0	0	0
7	B	18	0	0	0	0
7	C	38	0	0	3	0
7	D	55	0	0	0	0
All	All	8980	0	8595	134	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 8.

All (134) 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)
2:D:447:ASN:HD22	6:D:1640:NAG:H83	1.09	1.16
2:D:447:ASN:ND2	6:D:1640:NAG:H83	1.63	1.10
2:C:348:LEU:HD12	2:C:374:ILE:HD12	1.47	0.94
2:D:348:LEU:HD22	2:D:374:ILE:HD12	1.49	0.93
2:D:434:ARG:NH2	5:D:1639:PO4:O1	2.07	0.88
2:D:348:LEU:CD2	2:D:374:ILE:HD12	2.04	0.87
2:C:287:LEU:HD13	2:C:301:VAL:HG12	1.61	0.81
2:C:266:LEU:CD1	2:C:334:VAL:HG21	2.11	0.81
2:C:443:ASP:HB3	2:C:446:ILE:HD12	1.65	0.77
2:C:266:LEU:HD13	2:C:334:VAL:HG21	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:305:THR:HG22	2:C:318:ILE:HG12	1.74	0.69
2:C:358:LEU:HD13	2:C:437:VAL:HG11	1.75	0.69
2:D:386:SER:O	2:D:387:ASP:HB2	1.92	0.68
2:D:287:LEU:HD13	2:D:301:VAL:HG12	1.74	0.67
2:C:308:GLU:N	2:C:309:ARG:HA	2.10	0.66
2:D:552:LEU:HD22	2:D:571:MET:HE3	1.76	0.66
2:D:539:THR:O	2:D:542:SER:O	2.15	0.65
2:C:608:CYS:O	2:C:612:CYS:HB3	1.97	0.64
2:C:551:ILE:HD12	2:C:564:ILE:HG21	1.80	0.64
1:A:78:VAL:HG12	1:A:79:PRO:HD2	1.80	0.64
2:D:438:ASP:HB2	2:D:496:VAL:HG21	1.80	0.64
2:C:551:ILE:HD12	2:C:564:ILE:CG2	2.27	0.64
2:C:359:PHE:O	2:C:439:ARG:NH2	2.31	0.64
2:C:425:PHE:CE2	2:C:468:ILE:HD12	2.33	0.64
1:B:43:LEU:HD22	1:B:163:ALA:HB1	1.79	0.63
2:C:319:LEU:C	2:C:319:LEU:HD23	2.20	0.62
2:D:464:ARG:NH1	2:D:480:LEU:O	2.32	0.62
2:C:465:ILE:HG22	2:C:481:LEU:HB2	1.82	0.62
2:D:276:ILE:O	2:D:572:THR:HG21	2.00	0.62
2:D:447:ASN:ND2	6:D:1640:NAG:C8	2.53	0.61
2:C:266:LEU:CD1	2:C:334:VAL:CG2	2.78	0.61
2:C:386:SER:O	2:C:387:ASP:HB2	2.02	0.60
1:A:64:GLU:CD	1:A:190:ASN:HD21	2.06	0.59
2:C:272:VAL:HG12	2:C:303:TYR:CD2	2.38	0.59
2:C:465:ILE:CG2	2:C:481:LEU:HB2	2.33	0.59
2:D:268:ILE:O	2:D:272:VAL:HG23	2.03	0.59
1:A:118:TRP:CZ2	1:A:161:LEU:HD12	2.38	0.58
2:C:610:ARG:NH2	7:C:2035:HOH:O	2.35	0.58
2:C:300:TYR:CE2	2:C:323:GLU:HG3	2.39	0.58
1:A:43:LEU:HD22	1:A:163:ALA:HB1	1.84	0.58
6:C:1641:NAG:H83	6:C:1641:NAG:H3	1.85	0.58
1:B:179:ARG:NH2	2:D:419:ASN:O	2.37	0.58
2:D:348:LEU:HD22	2:D:374:ILE:CD1	2.28	0.58
2:C:227:ARG:NH2	2:C:575:HIS:CE1	2.72	0.57
2:D:520:THR:HG23	2:D:535:LEU:HB2	1.86	0.57
2:C:268:ILE:O	2:C:272:VAL:HG13	2.05	0.56
2:D:287:LEU:CD1	2:D:301:VAL:HG12	2.35	0.56
2:D:552:LEU:HD13	2:D:571:MET:CE	2.36	0.56
2:C:348:LEU:CD1	2:C:374:ILE:HD12	2.29	0.55
2:D:282:ARG:NE	2:D:350:ARG:HD2	2.22	0.55
2:D:571:MET:CE	2:D:571:MET:HA	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:341:VAL:HG23	7:C:2013:HOH:O	2.05	0.55
2:C:469:ILE:O	2:C:469:ILE:HG22	2.07	0.55
2:C:219:ILE:CG2	2:C:537:LEU:HD11	2.36	0.55
2:C:307:GLN:HE21	2:C:307:GLN:HA	1.72	0.55
2:D:348:LEU:HD23	2:D:374:ILE:HD12	1.89	0.54
2:D:401:MET:HB2	2:D:404:VAL:HG12	1.89	0.54
1:A:64:GLU:OE1	1:A:190:ASN:ND2	2.38	0.53
1:B:40:LEU:HD22	1:B:164:ARG:CG	2.38	0.53
2:D:228:GLN:HA	2:D:571:MET:HE2	1.91	0.53
2:D:426:ALA:HA	2:D:477:GLU:HG2	1.90	0.53
2:C:266:LEU:HD12	2:C:334:VAL:CG2	2.39	0.53
2:D:570:SER:OG	2:D:573:GLN:OE1	2.27	0.53
1:B:40:LEU:HD22	1:B:164:ARG:HG3	1.91	0.53
1:A:44:LEU:HD22	2:C:418:THR:HB	1.91	0.53
2:C:425:PHE:CZ	2:C:468:ILE:HD12	2.44	0.52
2:C:229:PRO:O	2:C:571:MET:HE1	2.09	0.52
2:C:551:ILE:CD1	2:C:564:ILE:HG21	2.40	0.51
1:B:190:ASN:N	1:B:190:ASN:OD1	2.43	0.51
2:C:219:ILE:HG23	2:C:537:LEU:HD11	1.92	0.51
2:C:529:GLN:HE21	2:C:529:GLN:N	2.07	0.51
2:C:230:VAL:HG12	2:C:571:MET:HE3	1.93	0.51
2:D:552:LEU:HD22	2:D:571:MET:HG2	1.92	0.51
2:D:233:LEU:CD2	2:D:245:LEU:HD11	2.41	0.50
2:C:420:GLN:HG3	2:C:421:PRO:HD2	1.94	0.50
6:D:1640:NAG:H83	6:D:1640:NAG:C1	2.41	0.49
2:D:348:LEU:CD2	2:D:374:ILE:CD1	2.86	0.49
2:C:219:ILE:HD11	2:C:539:THR:HG22	1.94	0.49
2:D:552:LEU:HD13	2:D:571:MET:HE3	1.93	0.49
2:D:343:LEU:HD21	2:D:393:LEU:CD1	2.42	0.49
2:D:400:ASP:OD1	2:D:620:THR:OG1	2.27	0.49
2:D:564:ILE:HG12	2:D:582:ILE:HD11	1.94	0.49
1:B:56:THR:HG22	1:B:58:GLY:H	1.77	0.49
2:C:539:THR:CG2	2:C:547:PHE:HA	2.44	0.48
1:B:64:GLU:OE1	1:B:190:ASN:ND2	2.43	0.47
2:C:266:LEU:HD12	2:C:334:VAL:HG22	1.96	0.47
2:C:342:PHE:HE1	2:C:397:VAL:HG12	1.78	0.47
2:C:307:GLN:NE2	2:C:308:GLU:O	2.48	0.47
2:D:557:ASP:OD2	2:D:557:ASP:C	2.53	0.46
2:C:358:LEU:HD22	2:C:437:VAL:CG2	2.45	0.46
2:C:439:ARG:HB2	2:C:440:HIS:CE1	2.51	0.46
2:D:287:LEU:HD12	2:D:300:TYR:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LYS:HD2	1:A:124:ARG:NH2	2.31	0.46
2:C:443:ASP:CB	2:C:446:ILE:HD12	2.42	0.46
2:D:547:PHE:CE2	2:D:551:ILE:HD11	2.50	0.45
1:A:117:MET:CE	1:A:165:LEU:HD21	2.46	0.45
2:C:366:TYR:CE1	2:C:394:ARG:HD2	2.51	0.45
2:C:276:ILE:HD12	2:C:277:LYS:N	2.32	0.45
2:C:425:PHE:CE2	2:C:468:ILE:CD1	2.99	0.45
1:B:56:THR:HG22	1:B:57:LEU:N	2.32	0.45
2:C:438:ASP:OD1	2:C:498:ARG:NH1	2.51	0.44
2:D:232:ALA:O	2:D:555:GLY:HA2	2.17	0.44
2:D:342:PHE:HE1	2:D:397:VAL:HG12	1.82	0.44
2:D:571:MET:HA	2:D:571:MET:HE3	2.00	0.44
2:D:552:LEU:CD2	2:D:571:MET:HE3	2.47	0.44
2:C:436:ALA:HB1	2:C:496:VAL:HG23	2.00	0.44
2:C:319:LEU:CD2	2:C:319:LEU:C	2.86	0.44
2:D:513:ASP:OD1	2:D:513:ASP:C	2.57	0.43
1:A:190:ASN:N	1:A:190:ASN:OD1	2.50	0.43
2:C:469:ILE:HG22	7:C:2028:HOH:O	2.18	0.43
2:C:552:LEU:HD11	2:C:567:SER:HB2	2.00	0.43
1:B:132:ASP:HB2	1:B:134:HIS:CD2	2.53	0.43
2:C:328:ARG:O	2:C:603:THR:OG1	2.37	0.43
2:C:539:THR:HG21	2:C:547:PHE:HA	2.01	0.42
2:C:232:ALA:O	2:C:555:GLY:HA2	2.19	0.42
1:B:151:THR:OG1	1:B:153:ASP:OD1	2.29	0.42
2:D:420:GLN:HG3	2:D:421:PRO:HD2	2.01	0.42
2:D:429:LEU:HG	2:D:480:LEU:HD11	2.02	0.42
2:D:554:PHE:CD1	2:D:564:ILE:HD13	2.55	0.42
2:C:219:ILE:HB	2:C:580:TYR:HB3	2.02	0.42
1:A:156:ARG:HD3	1:A:180:ASN:OD1	2.20	0.42
2:D:218:CYS:HB3	2:D:543:CYS:HB3	1.88	0.41
2:C:552:LEU:HD22	2:C:571:MET:HE2	2.03	0.41
1:A:48:PHE:HA	1:A:174:VAL:O	2.20	0.41
2:C:251:VAL:HG21	2:C:287:LEU:HD22	2.02	0.41
2:C:302:SER:HA	2:C:320:ARG:O	2.20	0.41
2:D:233:LEU:HD21	2:D:245:LEU:HD11	2.03	0.41
2:C:399:THR:HG23	2:C:407:SER:HB3	2.01	0.41
2:D:228:GLN:HA	2:D:571:MET:CE	2.50	0.41
2:C:589:LEU:HD22	2:C:590:MET:HE2	2.03	0.41
2:D:416:ASN:HA	2:D:416:ASN:HD22	1.68	0.41
6:C:1641:NAG:H82	6:C:1641:NAG:C1	2.51	0.41
6:D:1640:NAG:C8	6:D:1640:NAG:C1	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:541:GLY:O	2:C:542:SER:CB	2.69	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	151/164 (92%)	142 (94%)	8 (5%)	1 (1%)	25	49
1	B	146/164 (89%)	142 (97%)	4 (3%)	0	100	100
2	C	396/463 (86%)	376 (95%)	16 (4%)	4 (1%)	18	37
2	D	403/463 (87%)	385 (96%)	18 (4%)	0	100	100
All	All	1096/1254 (87%)	1045 (95%)	46 (4%)	5 (0%)	32	58

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	542	SER
2	C	612	CYS
1	A	192	LEU
2	C	543	CYS
2	C	441	PRO

### 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	128/137 (93%)	126 (98%)	2 (2%)	68	87
1	B	124/137 (90%)	119 (96%)	5 (4%)	36	64
2	C	355/404 (88%)	326 (92%)	29 (8%)	13	26
2	D	358/404 (89%)	338 (94%)	20 (6%)	25	48
All	All	965/1082 (89%)	909 (94%)	56 (6%)	23	46

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	TYR
1	A	177	GLU
1	B	105	GLU
1	B	176	TYR
1	B	177	GLU
1	B	179	ARG
1	B	190	ASN
2	C	218	CYS
2	C	272	VAL
2	C	299	LEU
2	C	307	GLN
2	C	316	ASP
2	C	318	ILE
2	C	334	VAL
2	C	343	LEU
2	C	350	ARG
2	C	399	THR
2	C	404	VAL
2	C	416	ASN
2	C	420	GLN
2	C	442	THR
2	C	451	LEU
2	C	475	GLU
2	C	482	GLU
2	C	483	PHE
2	C	498	ARG
2	C	520	THR
2	C	529	GLN
2	C	530	TRP
2	C	533	LYS
2	C	543	CYS
2	C	603	THR
2	C	604	LEU

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Mol	Chain	Res	Type
2	C	605	THR
2	C	635	ARG
2	C	636	THR
2	D	218	CYS
2	D	270	LYS
2	D	299	LEU
2	D	318	ILE
2	D	319	LEU
2	D	348	LEU
2	D	350	ARG
2	D	404	VAL
2	D	416	ASN
2	D	420	GLN
2	D	475	GLU
2	D	477	GLU
2	D	498	ARG
2	D	501	GLN
2	D	515	ASN
2	D	528	LYS
2	D	543	CYS
2	D	571	MET
2	D	603	THR
2	D	622	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	307	GLN
2	C	575	HIS
2	D	228	GLN
2	D	416	ASN
2	D	531	GLN

### 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 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
5	PO4	C	1640	-	4,4,4	0.83	0	6,6,6	0.39	0
6	NAG	C	1641	2	14,14,15	0.68	0	15,19,21	1.60	4 (26%)
5	PO4	D	1639	-	4,4,4	0.88	0	6,6,6	1.08	0
6	NAG	D	1640	2	14,14,15	0.63	0	15,19,21	1.55	2 (13%)

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
5	PO4	C	1640	-	-	0/0/0/0	0/0/0/0
6	NAG	C	1641	2	-	0/6/23/26	0/1/1/1
5	PO4	D	1639	-	-	0/0/0/0	0/0/0/0
6	NAG	D	1640	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1641	NAG	O5-C1-C2	-2.97	107.34	111.47
6	C	1641	NAG	C3-C4-C5	2.13	113.98	110.22
6	C	1641	NAG	C8-C7-N2	2.35	120.36	116.11
6	D	1640	NAG	C4-C3-C2	3.03	115.46	111.02
6	C	1641	NAG	C1-C2-N2	3.30	116.13	110.49
6	D	1640	NAG	C3-C4-C5	3.71	116.75	110.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1641	NAG	2	0
5	D	1639	PO4	1	0
6	D	1640	NAG	5	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, 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	155/164 (94%)	-0.10	2 (1%) 77 73	15, 20, 25, 29	0
1	B	150/164 (91%)	-0.09	4 (2%) 55 48	15, 20, 25, 28	0
2	C	406/463 (87%)	0.18	22 (5%) 26 20	11, 19, 31, 38	0
2	D	409/463 (88%)	-0.03	15 (3%) 42 34	10, 19, 26, 31	0
All	All	1120/1254 (89%)	0.03	43 (3%) 41 33	10, 19, 28, 38	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	308	GLU	5.3
2	C	568	SER	5.0
2	D	605	THR	4.5
2	C	627	PRO	4.5
2	C	314	PRO	4.3
2	C	403	ASN	4.2
1	A	39	ALA	4.1
2	C	279	GLY	3.8
2	C	595	ARG	3.7
1	B	39	ALA	3.5
2	C	540	SER	3.5
2	C	531	GLN	3.4
2	C	639	CYS	3.3
2	D	595	ARG	3.3
2	D	568	SER	3.2
2	D	632	ASP	3.2
1	B	132	ASP	3.2
2	D	403	ASN	3.1
2	C	278	GLY	3.0
2	D	401	MET	3.0
2	C	312	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
2	C	546	TYR	3.0
1	A	196	GLU	2.7
2	C	410	ARG	2.7
2	D	276	ILE	2.6
2	C	637	ALA	2.5
2	C	309	ARG	2.5
2	D	630	GLU	2.4
2	C	442	THR	2.4
2	C	628	GLY	2.4
2	C	445	ASN	2.3
2	C	485	PRO	2.3
2	D	638	LYS	2.3
2	D	611	LEU	2.2
2	D	316	ASP	2.2
2	D	628	GLY	2.2
2	D	488	ASN	2.2
2	D	592	GLU	2.1
1	B	191	SER	2.1
2	C	636	THR	2.0
2	D	627	PRO	2.0
2	C	523	GLN	2.0
1	B	122	ARG	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 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
6	NAG	D	1640	14/15	0.90	0.36	7.16	41,45,47,50	0
6	NAG	C	1641	14/15	0.78	0.43	3.38	54,59,62,62	0
5	PO4	C	1640	5/5	0.97	0.20	0.17	67,67,67,68	0
4	CL	D	1641	1/1	0.97	0.17	-0.31	60,60,60,60	0
4	CL	D	1642	1/1	0.88	0.11	-1.03	60,60,60,60	0
3	ZN	A	1199	1/1	1.00	0.11	-1.30	27,27,27,27	0
3	ZN	B	1193	1/1	0.99	0.10	-1.73	30,30,30,30	0
4	CL	D	1643	1/1	0.80	0.12	-2.15	71,71,71,71	0
4	CL	C	1642	1/1	0.94	0.08	-2.63	50,50,50,50	0
5	PO4	D	1639	5/5	0.99	0.09	-2.88	34,36,37,38	0
4	CL	A	1200	1/1	0.93	0.10	-	59,59,59,59	0
4	CL	C	1643	1/1	0.97	0.04	-	54,54,54,54	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.