



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:03 PM UTC

PDB ID : 2WG3 / pdb_00002wg3
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

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

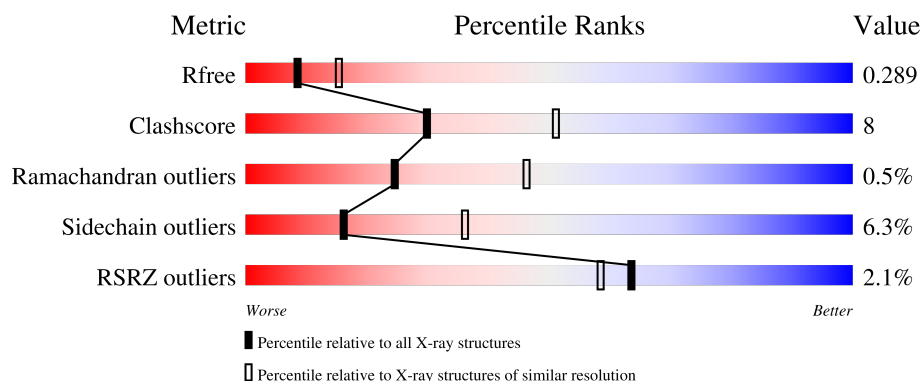
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 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	164	79% 14% • 5%
1	B	164	% 77% 13% • 9%
2	C	463	3% 67% 18% • 12%
2	D	463	% 73% 12% • 12%

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			

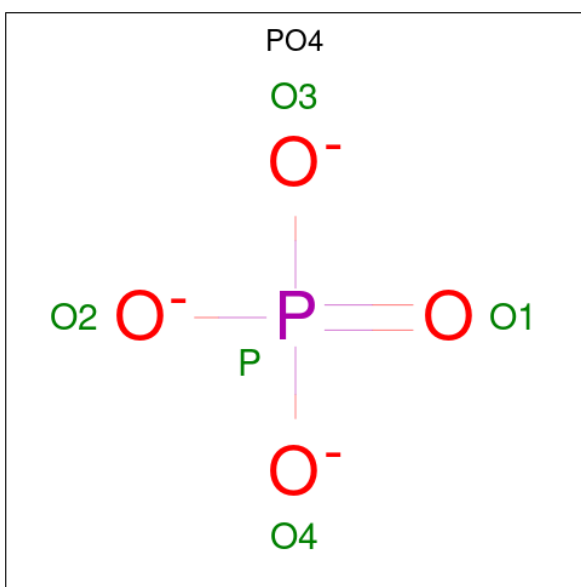
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

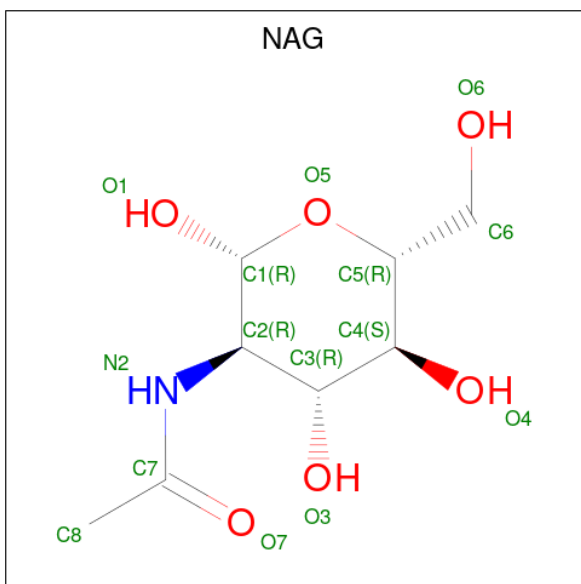
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	C	2	Total	Cl	0	0
			2	2		
4	D	3	Total	Cl	0	0
			3	3		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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, 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.

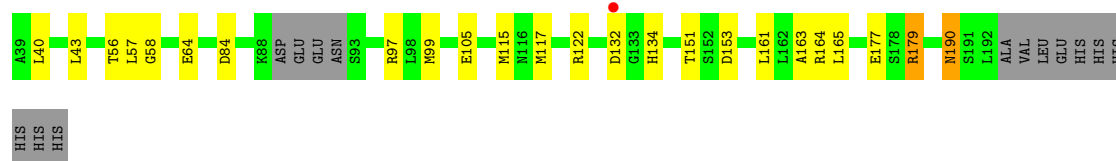
• Molecule 1: DESERT HEDGEHOG PROTEIN N-PRODUCT

Chain A: 



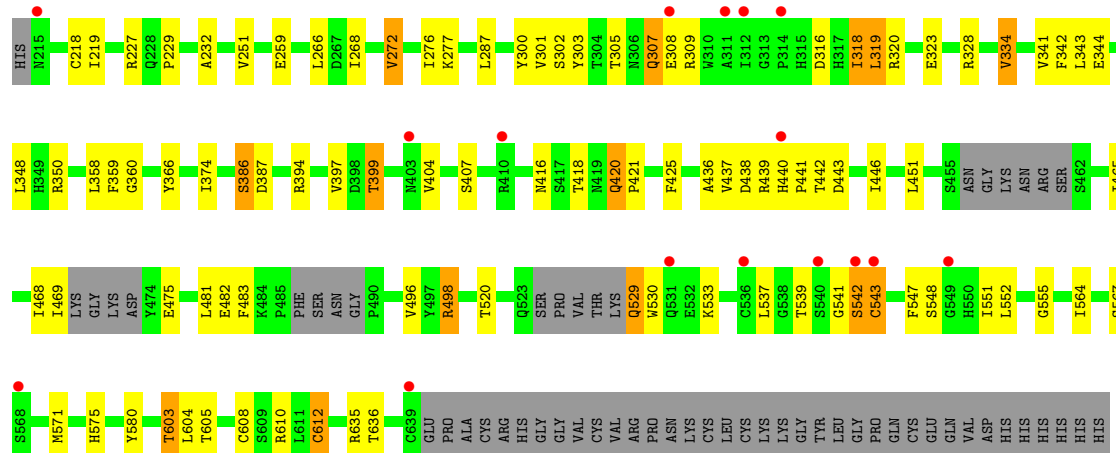
• Molecule 1: DESERT HEDGEHOG PROTEIN N-PRODUCT

Chain B: 



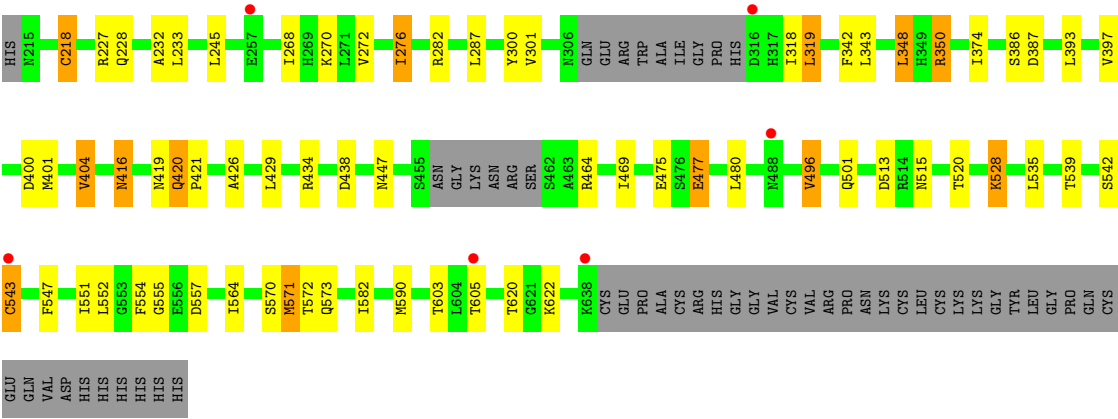
• Molecule 2: HEDGEHOG-INTERACTING PROTEIN

Chain C: 



• Molecule 2: HEDGEHOG-INTERACTING PROTEIN

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	102.82Å 110.70Å 144.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.60) 99.7 (20.00-2.60)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	1.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

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: NAG, PO4, ZN, CL

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	0.72	0/1263	0.92	5/1711 (0.3%)
1	B	0.65	0/1218	0.82	0/1649
2	C	0.66	0/3258	0.83	3/4403 (0.1%)
2	D	0.71	0/3270	0.85	0/4420
All	All	0.69	0/9009	0.85	8/12183 (0.1%)

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

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	ALA	N-CA-C	8.60	119.25	107.73
1	A	194	VAL	N-CA-C	6.06	121.95	109.34
1	A	159	TYR	N-CA-C	5.34	118.02	111.82
2	C	360	GLY	CA-C-N	5.21	124.87	119.56
2	C	360	GLY	C-N-CA	5.21	124.87	119.56
2	C	386	SER	N-CA-C	5.18	119.65	112.45
1	A	188	ALA	N-CA-C	-5.08	103.69	110.55
1	A	192	LEU	N-CA-C	5.06	121.57	110.80

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	18	0
1	B	1192	0	1161	15	0
2	C	3186	0	3092	63	0
2	D	3198	0	3115	50	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	1	0
All	All	8980	0	8595	148	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 (148) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:571:MET:HE2	2:D:571:MET:HA	1.65	0.78
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
2:D:552:LEU:HD13	2:D:571:MET:HE3	1.68	0.74
1:B:117:MET:HE2	1:B:165:LEU:HD21	1.69	0.73
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:319:LEU:C	2:C:319:LEU:HD23	2.20	0.67
2:C:308:GLU:N	2:C:309:ARG:HA	2.10	0.66
1:A:117:MET:HE3	1:A:161:LEU:HD11	1.78	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
1:A:64:GLU:CD	1:A:190:ASN:HD21	2.06	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: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:D:228:GLN:HA	2:D:571:MET:HE1	1.83	0.61
2:D:552:LEU:HD22	2:D:571:MET:HE3	1.83	0.61
2:C:386:SER:O	2:C:387:ASP:HB2	2.02	0.60
1:B:84:ASP:CG	1:B:115:MET:HE1	2.26	0.60
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
1:B:179:ARG:NH2	2:D:419:ASN:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:1641:NAG:H3	6:C:1641:NAG:H83	1.85	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
1:A:115:MET:HE3	1:A:122:ARG:HD3	1.88	0.56
2:C:552:LEU:HD22	2:C:571:MET:HE2	1.88	0.55
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:HA	2:D:571:MET:CE	2.36	0.55
2:C:341:VAL:HG23	7:C:2013:HOH:O	2.05	0.55
1:B:115:MET:HE3	1:B:122:ARG:HD3	1.88	0.55
2:C:219:ILE:CG2	2:C:537:LEU:HD11	2.36	0.55
2:C:307:GLN:HA	2:C:307:GLN:HE21	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
2:C:469:ILE:HG22	2:C:469:ILE:O	2.07	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: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
1:B:97:ARG:O	1:B:99:MET:HE3	2.09	0.52
2:D:552:LEU:HD13	2:D:571:MET:CE	2.36	0.52
2:C:425:PHE:CZ	2:C:468:ILE:HD12	2.44	0.52
2:C:552:LEU:HB3	2:C:571:MET:HE2	1.92	0.51
2:D:401:MET:HE3	7:D:2022:HOH:O	2.08	0.51
2:C:551:ILE:CD1	2:C:564:ILE:HG21	2.40	0.51
1:B:190:ASN:OD1	1:B:190:ASN:N	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:D:552:LEU:HD22	2:D:571:MET:HG2	1.92	0.51
2:D:557:ASP:OD2	2:D:557:ASP:C	2.53	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
2:D:348:LEU:CD2	2:D:374:ILE:CD1	2.86	0.49
6:D:1640:NAG:H83	6:D:1640:NAG:C1	2.41	0.49
2:C:219:ILE:HD11	2:C:539:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:229:PRO:O	2:C:571:MET:HE1	2.13	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:319:LEU:C	2:C:319:LEU:CD2	2.86	0.49
2:D:513:ASP:C	2:D:513:ASP:OD1	2.57	0.48
2:C:539:THR:CG2	2:C:547:PHE:HA	2.44	0.48
1:A:115:MET:HE3	1:A:122:ARG:HG2	1.96	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
1:B:151:THR:OG1	1:B:153:ASP:OD1	2.29	0.46
1:A:117:MET:HE2	1:A:165:LEU:HD21	1.96	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
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
1:A:115:MET:HE3	1:A:122:ARG:CG	2.46	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:319:LEU:C	2:D:319:LEU:HD12	2.43	0.44
2:C:436:ALA:HB1	2:C:496:VAL:HG23	2.00	0.44
1:A:190:ASN:OD1	1:A:190:ASN:N	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:117:MET:HE3	1:B:161:LEU:HD21	2.00	0.43
1:A:115:MET:HE3	1:A:122:ARG:CD	2.48	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:318:ILE:HD12	2:C:344:GLU:CD	2.44	0.42
2:C:539:THR:HG21	2:C:547:PHE:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:232:ALA:O	2:C:555:GLY:HA2	2.19	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:D:590:MET:HE2	2:D:590:MET:HB2	1.88	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:D:552:LEU:CD1	2:D:571:MET:HE3	2.44	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:416:ASN:HD22	2:D:416:ASN:HA	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
2:C:541:GLY:O	2:C:542:SER:CB	2.69	0.40
1:A:84:ASP:OD1	1:A:115:MET:HE1	2.21	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%)	18	38
1	B	146/164 (89%)	142 (97%)	4 (3%)	0	100	100
2	C	396/463 (86%)	376 (95%)	16 (4%)	4 (1%)	12	28
2	D	403/463 (87%)	385 (96%)	18 (4%)	0	100	100
All	All	1096/1254 (87%)	1045 (95%)	46 (4%)	5 (0%)	24	46

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 ⓘ

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%)	125 (98%)	3 (2%)	44	71
1	B	124/137 (90%)	120 (97%)	4 (3%)	34	62
2	C	355/404 (88%)	324 (91%)	31 (9%)	9	21
2	D	358/404 (89%)	335 (94%)	23 (6%)	16	35
All	All	965/1082 (89%)	904 (94%)	61 (6%)	16	36

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	VAL
1	A	161	LEU
1	A	177	GLU
1	B	105	GLU
1	B	177	GLU
1	B	179	ARG
1	B	190	ASN
2	C	218	CYS
2	C	259	GLU
2	C	272	VAL
2	C	307	GLN
2	C	316	ASP
2	C	318	ILE
2	C	319	LEU
2	C	334	VAL

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Mol	Chain	Res	Type
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	548	SER
2	C	603	THR
2	C	604	LEU
2	C	605	THR
2	C	635	ARG
2	C	636	THR
2	D	218	CYS
2	D	227	ARG
2	D	270	LYS
2	D	276	ILE
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	469	ILE
2	D	475	GLU
2	D	477	GLU
2	D	496	VAL
2	D	501	GLN
2	D	515	ASN
2	D	528	LYS
2	D	543	CYS

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Mol	Chain	Res	Type
2	D	571	MET
2	D	603	THR
2	D	605	THR
2	D	622	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	134	HIS
2	C	220	GLN
2	C	307	GLN
2	C	416	ASN
2	C	529	GLN
2	C	575	HIS
2	D	416	ASN
2	D	517	ASN
2	D	531	GLN

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 [i](#)

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	$\# Z > 2$
6	NAG	D	1640	2	14,14,15	0.65	0	17,19,21	1.42	2 (11%)
5	PO4	D	1639	-	4,4,4	1.00	0	6,6,6	1.28	1 (16%)
6	NAG	C	1641	2	14,14,15	0.69	0	17,19,21	1.56	4 (23%)
5	PO4	C	1640	-	4,4,4	1.00	0	6,6,6	0.46	0

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
6	NAG	D	1640	2	-	3/6/23/26	0/1/1/1
6	NAG	C	1641	2	-	6/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1641	NAG	C1-C2-N2	3.62	116.13	110.43
6	D	1640	NAG	C3-C4-C5	3.60	116.75	110.23
6	D	1640	NAG	C4-C3-C2	3.03	115.46	111.02
6	C	1641	NAG	C8-C7-N2	2.56	120.36	116.12
6	C	1641	NAG	O5-C1-C2	-2.55	107.34	111.29
6	C	1641	NAG	C3-C4-C5	2.07	113.98	110.23
5	D	1639	PO4	O3-P-O2	2.04	114.26	107.91

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1641	NAG	C8-C7-N2-C2
6	C	1641	NAG	O7-C7-N2-C2
6	D	1640	NAG	C8-C7-N2-C2
6	D	1640	NAG	O7-C7-N2-C2
6	C	1641	NAG	C4-C5-C6-O6
6	C	1641	NAG	O5-C5-C6-O6
6	C	1641	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
6	D	1640	NAG	C1-C2-N2-C7
6	C	1641	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1640	NAG	5	0
5	D	1639	PO4	1	0
6	C	1641	NAG	2	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	155/164 (94%)	-0.14	0 100 100	15, 20, 25, 29	0
1	B	150/164 (91%)	-0.17	1 (0%) 84 82	15, 20, 25, 28	0
2	C	406/463 (87%)	0.20	16 (3%) 43 38	11, 19, 31, 38	0
2	D	409/463 (88%)	-0.05	6 (1%) 72 68	10, 19, 26, 31	0
All	All	1120/1254 (89%)	0.01	23 (2%) 63 58	10, 19, 28, 38	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	540	SER	5.6
2	C	308	GLU	5.1
2	C	312	ILE	5.0
2	C	215	ASN	4.2
2	D	257	GLU	3.7
2	C	314	PRO	3.6
2	D	638	LYS	3.5
2	D	488	ASN	3.4
2	C	639	CYS	3.4
2	C	542	SER	3.3
2	D	605	THR	3.2
2	C	531	GLN	2.9
2	D	543	CYS	2.8
2	C	403	ASN	2.7
2	C	543	CYS	2.7
2	C	568	SER	2.7
2	D	316	ASP	2.4
2	C	549	GLY	2.4
1	B	132	ASP	2.3
2	C	440	HIS	2.3
2	C	536	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	410	ARG	2.1
2	C	311	ALA	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
6	NAG	C	1641	14/15	0.64	0.17	54,59,62,62	0
6	NAG	D	1640	14/15	0.79	0.11	41,45,47,50	0
4	CL	D	1642	1/1	0.83	0.19	60,60,60,60	0
4	CL	A	1200	1/1	0.86	0.16	59,59,59,59	0
4	CL	D	1643	1/1	0.89	0.16	71,71,71,71	0
5	PO4	C	1640	5/5	0.92	0.13	67,67,67,68	0
4	CL	C	1642	1/1	0.94	0.09	50,50,50,50	0
4	CL	D	1641	1/1	0.95	0.16	60,60,60,60	0
4	CL	C	1643	1/1	0.95	0.12	54,54,54,54	0
5	PO4	D	1639	5/5	0.96	0.09	34,36,37,38	0
3	ZN	B	1193	1/1	0.99	0.04	30,30,30,30	0
3	ZN	A	1199	1/1	1.00	0.04	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.