



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:05 PM UTC

PDB ID : 1FPN / pdb_00001fpn
Title : HUMAN RHINOVIRUS SEROTYPE 2 (HRV2)
Authors : Verdaguer, N.; Blaas, D.; Fita, I.
Deposited on : 2000-08-31
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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

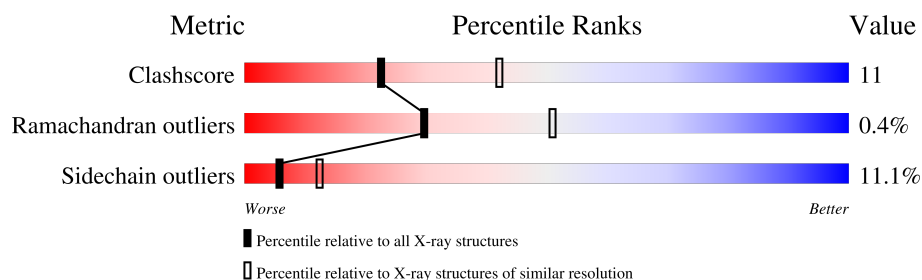
1 Overall quality at a glance

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))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	289	
2	2	261	
3	3	237	
4	4	68	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6316 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 COAT PROTEIN VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	269	Total	C	N	O	S	0	0	0
			2154	1356	378	409	11			

- Molecule 2 is a protein called COAT PROTEIN VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	250	Total	C	N	O	S	8	0	0
			1961	1245	339	369	8			

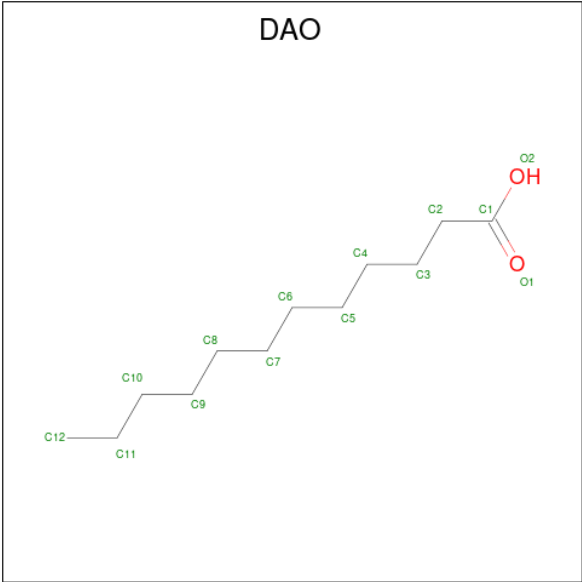
- Molecule 3 is a protein called COAT PROTEIN VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	237	Total	C	N	O	S	0	0	0
			1834	1172	304	346	12			

- Molecule 4 is a protein called COAT PROTEIN VP4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	4	25	Total	C	N	O	0	0	0
			194	122	35	37			

- Molecule 5 is LAURIC ACID (CCD ID: DAO) (formula: C₁₂H₂₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	1	1	Total	C	O	0	0
			14	12	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	1	51	Total	O	0	0
			51	51		
6	2	49	Total	O	0	0
			49	49		
6	3	56	Total	O	0	0
			56	56		
6	4	3	Total	O	0	0
			3	3		

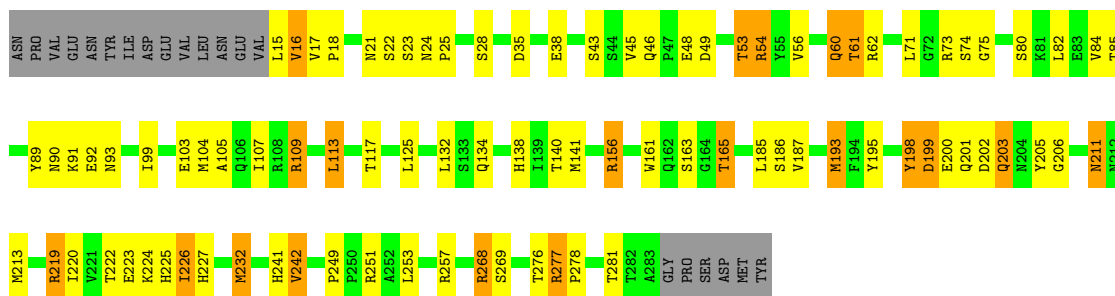
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

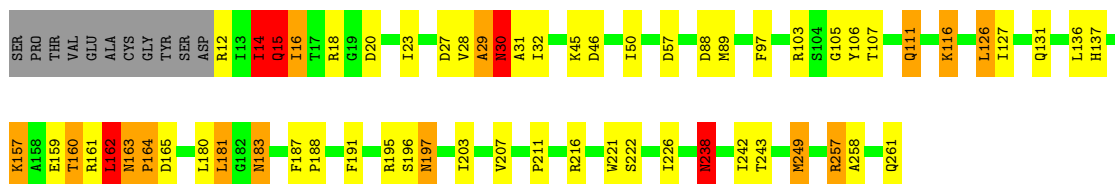
• Molecule 1: COAT PROTEIN VP1

Chain 1: 



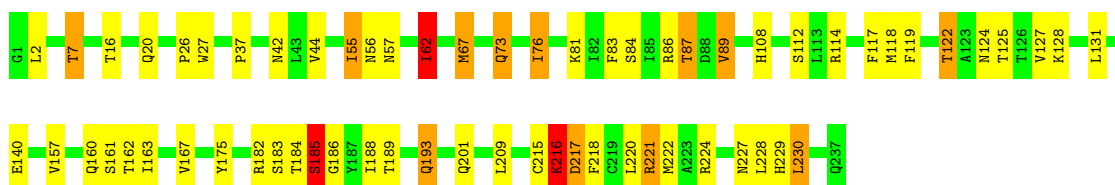
• Molecule 2: COAT PROTEIN VP2

Chain 2: 



• Molecule 3: COAT PROTEIN VP3

Chain 3: 



• Molecule 4: COAT PROTEIN VP4

Chain 4: 

GLY	A2	Q3	V4	S5	R6	Q7	ASN	VAL	GLY	THR	HIS	SER	THR	GLN	ASN	SER	VAL	SER	ASN	GLY	SER	SER	SER	LEU	N25	N28	Y31	F32	K33	L43	GLU	PHE	THR	GLN	ASP	PRO	SER	LYS	PHE	THR	ASP	PRO	VAL	LYS	ASP	VAL	LEU	GLU	LYS	GLY	ILE	PRO	THR	LEU	GLN
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	308.68Å 352.98Å 380.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.60)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6316	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DAO

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	1	0.90	3/2210 (0.1%)	1.15	23/3010 (0.8%)
2	2	0.80	2/2016 (0.1%)	1.31	27/2752 (1.0%)
3	3	0.81	2/1884 (0.1%)	1.18	17/2579 (0.7%)
4	4	0.90	0/196	1.18	1/261 (0.4%)
All	All	0.84	7/6306 (0.1%)	1.21	68/8602 (0.8%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	14	ILE	CA-CB	7.96	1.67	1.54
1	1	193	MET	SD-CE	-7.46	1.60	1.79
3	3	222	MET	SD-CE	-7.21	1.61	1.79
1	1	104	MET	SD-CE	-6.77	1.62	1.79
1	1	232	MET	SD-CE	-6.76	1.62	1.79
3	3	118	MET	SD-CE	-6.42	1.63	1.79
2	2	249	MET	SD-CE	-5.34	1.66	1.79

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	261	GLN	N-CA-CB	-16.02	83.27	110.50
3	3	62	ILE	N-CA-C	13.50	124.53	110.36
2	2	29	ALA	N-CA-C	-11.09	85.40	107.69
2	2	20	ASP	N-CA-C	-9.80	101.50	112.57
2	2	181	LEU	N-CA-C	-9.66	97.78	110.43
2	2	163	ASN	CA-C-N	9.52	131.73	119.84
2	2	163	ASN	C-N-CA	9.52	131.73	119.84
2	2	162	LEU	N-CA-C	9.21	123.91	109.81
1	1	105	ALA	N-CA-C	8.88	120.57	111.07
1	1	185	LEU	N-CA-C	8.78	123.99	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	200	GLU	N-CA-C	-8.24	103.20	113.18
3	3	216	LYS	CA-C-N	8.12	130.99	120.44
3	3	216	LYS	C-N-CA	8.12	130.99	120.44
1	1	242	VAL	N-CA-C	7.92	119.98	109.21
2	2	50	ILE	N-CA-C	7.75	119.53	112.17
2	2	30	ASN	N-CA-C	7.50	120.86	110.35
3	3	89	VAL	CB-CA-C	-7.47	101.14	112.05
3	3	182	ARG	N-CA-C	-7.45	100.32	110.68
1	1	16	VAL	N-CA-C	7.34	120.03	108.87
3	3	218	PHE	N-CA-C	7.21	120.83	110.24
1	1	113	LEU	N-CA-C	-7.20	104.47	113.18
2	2	165	ASP	N-CA-C	-7.01	104.47	113.16
1	1	89	TYR	N-CA-C	6.95	119.73	111.33
2	2	105	GLY	N-CA-C	-6.94	100.56	112.64
2	2	157	LYS	N-CA-C	-6.55	97.68	108.76
1	1	278	PRO	CA-C-N	-6.51	113.33	122.71
1	1	278	PRO	C-N-CA	-6.51	113.33	122.71
1	1	28	SER	N-CA-C	6.47	118.79	109.14
3	3	167	VAL	N-CA-C	-6.42	101.19	107.55
3	3	62	ILE	CA-C-N	-6.40	109.32	121.54
3	3	62	ILE	C-N-CA	-6.40	109.32	121.54
2	2	181	LEU	CA-C-N	-6.23	109.20	121.41
2	2	181	LEU	C-N-CA	-6.23	109.20	121.41
1	1	103	GLU	N-CA-C	6.18	120.82	113.28
1	1	186	SER	N-CA-C	6.13	118.62	110.53
1	1	211	ASN	N-CA-C	6.12	117.80	109.11
2	2	160	THR	N-CA-C	6.10	123.80	110.80
2	2	183	ASN	N-CA-C	-6.07	105.17	113.30
4	4	28	ASN	N-CA-C	6.05	117.91	107.93
3	3	89	VAL	N-CA-C	5.90	119.31	111.17
3	3	185	SER	N-CA-C	-5.87	105.77	113.17
2	2	242	ILE	N-CA-C	-5.85	99.11	107.77
2	2	89	MET	N-CA-C	5.78	118.50	107.75
1	1	278	PRO	O-C-N	5.70	129.35	122.23
2	2	127	ILE	N-CA-C	5.70	114.10	107.89
1	1	61	THR	N-CA-C	-5.65	102.16	110.52
2	2	57	ASP	CB-CA-C	-5.57	110.17	116.63
2	2	57	ASP	N-CA-C	5.52	117.42	108.08
1	1	198	TYR	N-CA-C	5.51	117.01	109.18
2	2	238	ASN	N-CA-C	5.48	119.66	112.92
3	3	217	ASP	N-CA-C	5.43	116.88	111.07
1	1	165	THR	CB-CA-C	5.39	116.12	109.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	73	GLN	N-CA-C	5.27	117.49	108.90
2	2	157	LYS	CA-C-N	-5.25	115.75	122.79
2	2	157	LYS	C-N-CA	-5.25	115.75	122.79
1	1	187	VAL	N-CA-C	-5.24	105.89	113.07
2	2	181	LEU	O-C-N	-5.22	116.64	122.75
1	1	220	ILE	N-CA-C	-5.20	100.28	108.23
3	3	7	THR	N-CA-CB	-5.18	103.76	110.03
2	2	136	LEU	N-CA-C	5.15	118.05	110.59
3	3	76	ILE	CB-CA-C	-5.14	105.06	111.08
2	2	15	GLN	N-CA-C	-5.14	99.45	107.93
3	3	86	ARG	N-CA-C	-5.14	103.75	110.53
3	3	230	LEU	N-CA-C	5.08	117.40	109.52
1	1	198	TYR	CA-C-N	5.07	129.97	120.95
1	1	198	TYR	C-N-CA	5.07	129.97	120.95
1	1	199	ASP	CB-CA-C	-5.05	98.39	110.02
1	1	206	GLY	N-CA-C	5.02	118.94	111.76

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	1	2154	0	2077	66	0
2	2	1961	0	1902	38	0
3	3	1834	0	1817	48	0
4	4	194	0	180	2	0
5	1	14	0	23	1	0
6	1	51	0	0	0	0
6	2	49	0	0	0	0
6	3	56	0	0	1	0
6	4	3	0	0	0	0
All	All	6316	0	5999	128	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 11.

All (128) 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)
1:1:268:ARG:HH11	1:1:268:ARG:HB3	1.10	1.09
1:1:268:ARG:HH11	1:1:268:ARG:CB	1.69	1.04
3:3:87:THR:HG22	3:3:185:SER:HB2	1.47	0.97
1:1:199:ASP:HB3	1:1:201:GLN:H	1.32	0.94
1:1:268:ARG:HB3	1:1:268:ARG:NH1	1.87	0.90
1:1:48:GLU:HG3	1:1:53:THR:HG21	1.51	0.89
3:3:224:ARG:HH12	3:3:227:ASN:HD22	1.18	0.87
1:1:43:SER:HB3	3:3:114:ARG:HD2	1.56	0.87
1:1:85:THR:H	1:1:93:ASN:HD21	1.23	0.87
1:1:117:THR:OG1	1:1:193:MET:HE3	1.74	0.87
3:3:42:ASN:HD22	3:3:44:VAL:H	1.19	0.86
2:2:207:VAL:HG22	3:3:37:PRO:HG2	1.62	0.81
1:1:199:ASP:HB2	1:1:203:GLN:H	1.46	0.80
3:3:20:GLN:HE22	4:4:31:TYR:H	1.30	0.79
3:3:122:THR:CG2	3:3:124:ASN:H	1.98	0.77
1:1:195:TYR:H	2:2:131:GLN:HE21	1.33	0.74
2:2:203:ILE:HG23	2:2:249:MET:HE1	1.70	0.73
3:3:224:ARG:HH12	3:3:227:ASN:ND2	1.86	0.72
3:3:193:GLN:HE21	3:3:193:GLN:HA	1.53	0.72
3:3:87:THR:CG2	3:3:185:SER:HB2	2.22	0.69
3:3:184:THR:HG22	3:3:186:GLY:H	1.58	0.68
2:2:14:ILE:HB	2:2:28:VAL:HG11	1.74	0.68
1:1:23:SER:HB3	1:1:53:THR:H	1.58	0.68
2:2:197:ASN:HD22	2:2:197:ASN:N	1.91	0.68
3:3:42:ASN:ND2	3:3:44:VAL:H	1.90	0.67
1:1:21:ASN:O	1:1:53:THR:CG2	2.42	0.67
1:1:38:GLU:HA	2:2:191:PHE:HB2	1.76	0.66
3:3:122:THR:HG22	3:3:124:ASN:H	1.60	0.65
1:1:46:GLN:HG3	3:3:216:LYS:HE3	1.79	0.63
1:1:276:THR:CG2	3:3:62:ILE:HG13	2.29	0.62
2:2:12:ARG:O	2:2:28:VAL:HG22	1.99	0.61
2:2:162:LEU:C	2:2:164:PRO:CD	2.74	0.61
1:1:21:ASN:O	1:1:53:THR:HG23	2.01	0.61
2:2:162:LEU:C	2:2:164:PRO:HD3	2.25	0.61
1:1:18:PRO:HG2	3:3:216:LYS:HB2	1.83	0.60
2:2:238:ASN:HD22	2:2:238:ASN:H	1.49	0.60
3:3:122:THR:HG23	3:3:124:ASN:H	1.67	0.59
1:1:161:TRP:CE2	1:1:219:ARG:HG2	2.38	0.59
3:3:55:ILE:HD11	3:3:83:PHE:CE2	2.38	0.59
1:1:109:ARG:NH1	1:1:251:ARG:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:225:HIS:HD2	1:1:227:HIS:H	1.52	0.57
1:1:281:THR:O	3:3:81:LYS:HE2	2.05	0.57
2:2:106:TYR:C	2:2:249:MET:HE2	2.30	0.57
2:2:16:ILE:HD12	2:2:23:ILE:HB	1.87	0.56
1:1:202:ASP:OD2	2:2:216:ARG:NH2	2.38	0.56
3:3:122:THR:HG22	3:3:124:ASN:N	2.20	0.56
1:1:276:THR:HG22	3:3:62:ILE:HG13	1.86	0.56
2:2:97:PHE:HE2	2:2:216:ARG:HG3	1.71	0.56
1:1:24:ASN:HB3	1:1:25:PRO:HD2	1.88	0.56
1:1:38:GLU:HG2	2:2:197:ASN:HD21	1.71	0.55
2:2:197:ASN:N	2:2:197:ASN:ND2	2.54	0.55
2:2:18:ARG:NH1	2:2:107:THR:OG1	2.40	0.55
1:1:80:SER:C	1:1:232:MET:CE	2.80	0.55
1:1:249:PRO:HB3	2:2:183:ASN:HB3	1.89	0.54
3:3:119:PHE:CD1	3:3:157:VAL:HG11	2.42	0.54
3:3:62:ILE:HA	3:3:67:MET:HE3	1.89	0.54
1:1:268:ARG:CB	1:1:268:ARG:NH1	2.54	0.54
1:1:80:SER:O	1:1:232:MET:HE3	2.08	0.53
1:1:80:SER:C	1:1:232:MET:HE3	2.34	0.53
3:3:62:ILE:HD13	3:3:62:ILE:O	2.09	0.52
1:1:211:ASN:HA	1:1:213:MET:HE2	1.91	0.52
2:2:162:LEU:O	2:2:164:PRO:N	2.41	0.52
1:1:23:SER:CB	1:1:53:THR:HG22	2.40	0.52
1:1:46:GLN:HA	1:1:46:GLN:OE1	2.09	0.51
1:1:277:ARG:HD3	3:3:57:ASN:OD1	2.10	0.51
3:3:227:ASN:ND2	3:3:227:ASN:H	2.07	0.51
1:1:71:LEU:HD12	1:1:242:VAL:HG11	1.91	0.51
1:1:268:ARG:HH11	1:1:268:ARG:CA	2.23	0.51
2:2:238:ASN:HD22	2:2:238:ASN:N	2.07	0.50
1:1:85:THR:N	1:1:93:ASN:HD21	2.03	0.50
2:2:162:LEU:C	2:2:164:PRO:N	2.68	0.50
3:3:62:ILE:HD13	3:3:67:MET:HE1	1.92	0.49
1:1:138:HIS:O	1:1:222:THR:HG21	2.12	0.49
3:3:20:GLN:NE2	6:3:5133:HOH:O	2.45	0.49
1:1:17:VAL:HG21	1:1:60:GLN:NE2	2.27	0.49
1:1:15:LEU:O	1:1:61:THR:HA	2.14	0.48
1:1:35:ASP:O	3:3:162:THR:HB	2.13	0.48
2:2:111:GLN:HG2	2:2:243:THR:O	2.13	0.48
3:3:193:GLN:HA	3:3:193:GLN:NE2	2.27	0.48
1:1:18:PRO:CG	3:3:216:LYS:HB2	2.43	0.48
4:4:6:ARG:O	4:4:6:ARG:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:90:ASN:OD1	1:1:156:ARG:NH1	2.47	0.48
1:1:225:HIS:CD2	1:1:227:HIS:H	2.31	0.47
3:3:26:PRO:O	3:3:27:TRP:HB2	2.13	0.47
1:1:18:PRO:HG2	3:3:216:LYS:HD3	1.96	0.47
1:1:84:VAL:HA	1:1:93:ASN:ND2	2.29	0.47
1:1:195:TYR:H	2:2:131:GLN:NE2	2.06	0.46
1:1:161:TRP:CD2	1:1:219:ARG:HG2	2.50	0.46
3:3:112:SER:H	3:3:217:ASP:HB3	1.80	0.46
1:1:99:ILE:CG2	5:1:6001:DAO:H81	2.45	0.46
2:2:126:LEU:HD22	2:2:221:TRP:HB3	1.96	0.46
1:1:73:ARG:HG2	3:3:16:THR:HG22	1.97	0.46
1:1:199:ASP:HB3	1:1:201:GLN:N	2.13	0.45
1:1:226:ILE:O	1:1:226:ILE:HG13	2.16	0.45
1:1:46:GLN:OE1	3:3:215:CYS:HB3	2.16	0.45
2:2:14:ILE:HD12	2:2:30:ASN:ND2	2.31	0.44
2:2:257:ARG:HG2	2:2:258:ALA:N	2.33	0.44
1:1:45:VAL:HG13	1:1:49:ASP:HB2	2.00	0.43
1:1:253:LEU:O	3:3:229:HIS:HE1	2.01	0.43
2:2:45:LYS:HE3	2:2:46:ASP:OD2	2.19	0.43
1:1:202:ASP:CG	2:2:216:ARG:HH22	2.26	0.43
2:2:116:LYS:O	3:3:122:THR:HG23	2.19	0.43
1:1:75:GLY:HA3	1:1:107:ILE:HD11	2.01	0.43
2:2:180:LEU:C	2:2:181:LEU:O	2.58	0.42
3:3:83:PHE:C	3:3:83:PHE:CD2	2.97	0.42
3:3:108:HIS:HB2	3:3:221:ARG:HG3	2.00	0.42
3:3:84:SER:HB2	3:3:189:THR:HG22	2.01	0.42
1:1:17:VAL:HG12	1:1:62:ARG:NE	2.35	0.42
1:1:277:ARG:NH2	3:3:84:SER:O	2.49	0.42
2:2:15:GLN:HA	2:2:23:ILE:O	2.20	0.42
2:2:103:ARG:HD2	2:2:211:PRO:O	2.20	0.42
1:1:17:VAL:HG12	1:1:62:ARG:CZ	2.50	0.42
3:3:117:PHE:O	3:3:162:THR:HG23	2.20	0.42
3:3:122:THR:HG22	3:3:125:THR:N	2.34	0.41
1:1:54:ARG:HD3	1:1:56:VAL:HG22	2.02	0.41
3:3:162:THR:HG22	3:3:163:ILE:N	2.34	0.41
2:2:195:ARG:HD3	3:3:161:SER:OG	2.21	0.41
2:2:29:ALA:O	2:2:30:ASN:C	2.61	0.41
3:3:127:VAL:HG22	3:3:128:LYS:N	2.36	0.41
1:1:140:THR:H	1:1:222:THR:HG23	1.85	0.41
1:1:198:TYR:CE1	1:1:205:TYR:HB2	2.56	0.41
1:1:92:GLU:HB3	1:1:93:ASN:H	1.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:238:ASN:H	2:2:238:ASN:ND2	2.18	0.41
1:1:60:GLN:HG2	3:3:175:TYR:OH	2.21	0.41
2:2:137:HIS:CD2	2:2:137:HIS:H	2.39	0.41
2:2:187:PHE:O	2:2:188:PRO:C	2.64	0.41
1:1:141:MET:HE3	1:1:141:MET:HB3	1.91	0.40
2:2:196:SER:HB2	2:2:197:ASN:HD22	1.86	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	1	267/289 (92%)	256 (96%)	11 (4%)	0	100	100
2	2	248/261 (95%)	228 (92%)	17 (7%)	3 (1%)	10	23
3	3	235/237 (99%)	222 (94%)	13 (6%)	0	100	100
4	4	21/68 (31%)	21 (100%)	0	0	100	100
All	All	771/855 (90%)	727 (94%)	41 (5%)	3 (0%)	30	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	160	THR
2	2	31	ALA
2	2	164	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	1	237/257 (92%)	211 (89%)	26 (11%)	6	13
2	2	216/226 (96%)	196 (91%)	20 (9%)	8	18
3	3	210/210 (100%)	185 (88%)	25 (12%)	5	10
4	4	19/59 (32%)	14 (74%)	5 (26%)	0	1
All	All	682/752 (91%)	606 (89%)	76 (11%)	6	12

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	16	VAL
1	1	22	SER
1	1	53	THR
1	1	54	ARG
1	1	60	GLN
1	1	74	SER
1	1	82	LEU
1	1	91	LYS
1	1	109	ARG
1	1	113	LEU
1	1	125	LEU
1	1	132	LEU
1	1	134	GLN
1	1	156	ARG
1	1	163	SER
1	1	165	THR
1	1	203	GLN
1	1	219	ARG
1	1	223	GLU
1	1	224	LYS
1	1	226	ILE
1	1	241	HIS
1	1	257	ARG
1	1	268	ARG
1	1	269	SER
1	1	277	ARG
2	2	14	ILE
2	2	15	GLN
2	2	16	ILE
2	2	27	ASP

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Mol	Chain	Res	Type
2	2	30	ASN
2	2	32	ILE
2	2	88	ASP
2	2	111	GLN
2	2	116	LYS
2	2	126	LEU
2	2	157	LYS
2	2	159	GLU
2	2	161	ARG
2	2	162	LEU
2	2	163	ASN
2	2	197	ASN
2	2	222	SER
2	2	226	ILE
2	2	238	ASN
2	2	257	ARG
3	3	2	LEU
3	3	7	THR
3	3	55	ILE
3	3	56	ASN
3	3	62	ILE
3	3	67	MET
3	3	73	GLN
3	3	76	ILE
3	3	87	THR
3	3	89	VAL
3	3	122	THR
3	3	131	LEU
3	3	140	GLU
3	3	160	GLN
3	3	183	SER
3	3	185	SER
3	3	188	ILE
3	3	193	GLN
3	3	201	GLN
3	3	209	LEU
3	3	216	LYS
3	3	220	LEU
3	3	221	ARG
3	3	228	LEU
3	3	230	LEU
4	4	3	GLN

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Mol	Chain	Res	Type
4	4	4	VAL
4	4	6	ARG
4	4	33	LYS
4	4	43	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	93	ASN
1	1	162	GLN
1	1	209	ASN
1	1	211	ASN
1	1	225	HIS
2	2	15	GLN
2	2	30	ASN
2	2	40	HIS
2	2	111	GLN
2	2	131	GLN
2	2	193	ASN
2	2	197	ASN
2	2	219	ASN
2	2	238	ASN
3	3	20	GLN
3	3	42	ASN
3	3	48	GLN
3	3	193	GLN
3	3	227	ASN
3	3	229	HIS
4	4	30	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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	DAO	1	6001	-	13,13,13	2.18	5 (38%)	13,13,13	0.97	1 (7%)

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	DAO	1	6001	-	-	5/11/11/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	6001	DAO	C2-C1	5.32	1.62	1.50
5	1	6001	DAO	O1-C1	2.46	1.30	1.22
5	1	6001	DAO	C3-C2	2.21	1.60	1.52
5	1	6001	DAO	C9-C8	2.16	1.62	1.51
5	1	6001	DAO	C10-C9	2.15	1.62	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	6001	DAO	O2-C1-C2	2.41	121.61	114.00

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	1	6001	DAO	C1-C2-C3-C4
5	1	6001	DAO	C6-C7-C8-C9
5	1	6001	DAO	C5-C6-C7-C8
5	1	6001	DAO	O2-C1-C2-C3
5	1	6001	DAO	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1	6001	DAO	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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.