



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 10, 2023 – 07:59 PM EDT

PDB ID : 1RHI  
Title : HUMAN RHINOVIRUS 3 COAT PROTEIN  
Authors : Zhao, R.; Rossmann, M.G.  
Deposited on : 1996-06-17  
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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  
Xtriage (Phenix) : 1.13  
EDS : 2.32.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.32.2

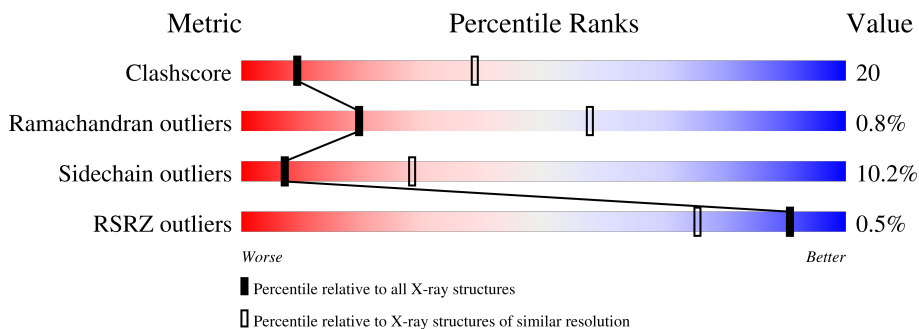
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	1	288	
2	2	262	
3	3	236	
4	4	68	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6288 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 HUMAN RHINOVIRUS 3 COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1	273	2163	1366	379	412	6	0	0	0

- Molecule 2 is a protein called HUMAN RHINOVIRUS 3 COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	2	255	1964	1239	335	377	13	0	0	0

- Molecule 3 is a protein called HUMAN RHINOVIRUS 3 COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	3	236	1835	1175	299	354	7	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	142	LYS	ARG	conflict	UNP Q82081
3	144	GLU	LYS	conflict	UNP Q82081

- Molecule 4 is a protein called HUMAN RHINOVIRUS 3 COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	4	43	325	206	50	67	2	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	26	TYR	PHE	conflict	UNP Q82081

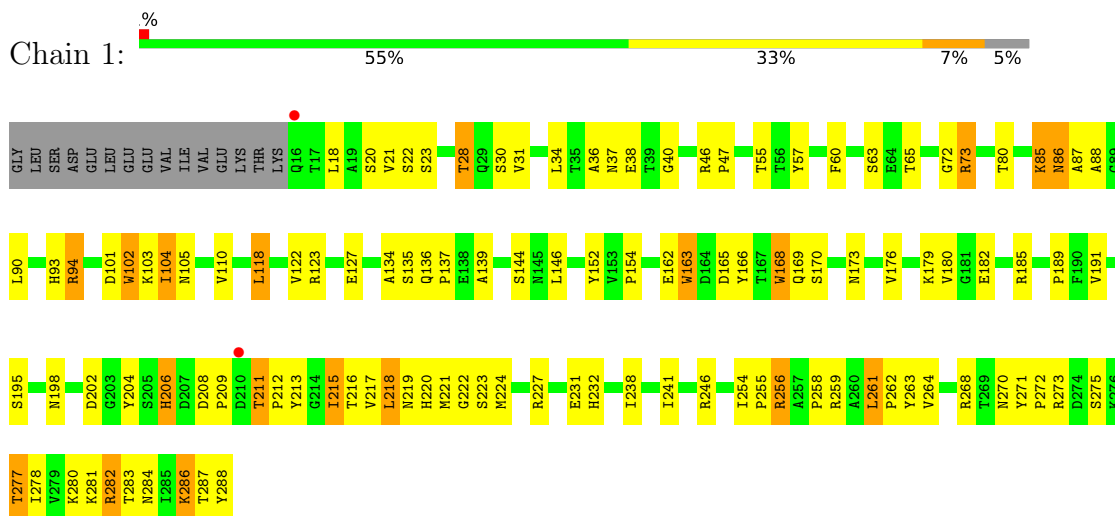
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	1	1	Total	Ca	0	0
			1	1		

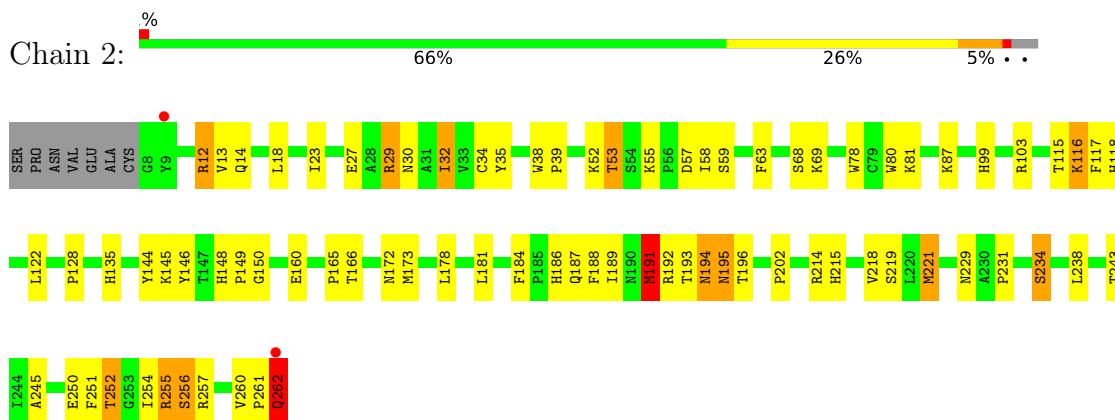
### 3 Residue-property plots [i](#)

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.

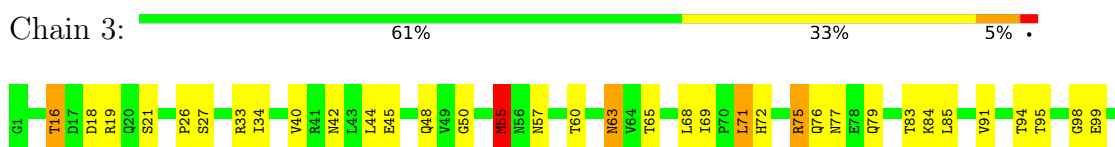
- Molecule 1: HUMAN RHINOVIRUS 3 COAT PROTEIN

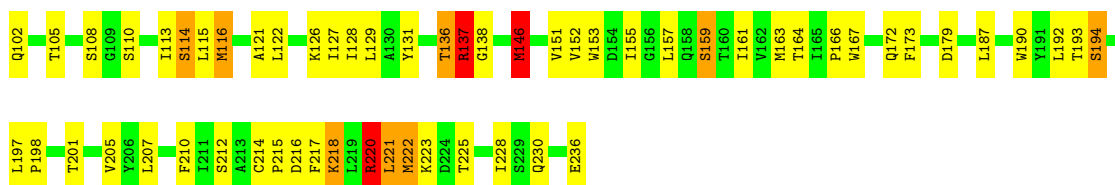


- Molecule 2: HUMAN RHINOVIRUS 3 COAT PROTEIN

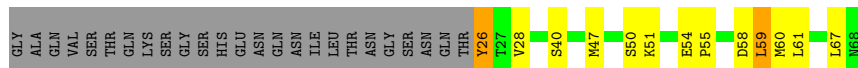


- Molecule 3: HUMAN RHINOVIRUS 3 COAT PROTEIN





- Molecule 4: HUMAN RHINOVIRUS 3 COAT PROTEIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	397.90Å 341.80Å 301.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 3.00 29.78 – 2.98	Depositor EDS
% Data completeness (in resolution range)	64.0 (5.00-3.00) 78.6 (29.78-2.98)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.54 (at 3.00Å)	Xtrriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.284 , 0.288 0.246 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.8	Xtrriage
Anisotropy	0.671	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 11.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.19$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.79	EDS
Total number of atoms	6288	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.49 % 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 3.7949e-03.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality i

### 5.1 Standard geometry i

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

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	0.63	3/2222 (0.1%)	0.97	7/3027 (0.2%)
2	2	0.65	2/2012 (0.1%)	0.99	7/2748 (0.3%)
3	3	0.57	1/1882 (0.1%)	0.99	9/2574 (0.3%)
4	4	0.57	0/332	0.91	1/447 (0.2%)
All	All	0.62	6/6448 (0.1%)	0.98	24/8796 (0.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	262	GLN	C-OXT	14.59	1.51	1.23
1	1	102	TRP	NE1-CE2	-5.59	1.30	1.37
3	3	167	TRP	NE1-CE2	-5.46	1.30	1.37
1	1	163	TRP	NE1-CE2	-5.38	1.30	1.37
1	1	168	TRP	NE1-CE2	-5.37	1.30	1.37
2	2	78	TRP	NE1-CE2	-5.07	1.30	1.37

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	220	ARG	NE-CZ-NH2	8.04	124.32	120.30
2	2	12	ARG	NE-CZ-NH2	7.50	124.05	120.30
2	2	214	ARG	NE-CZ-NH2	7.49	124.05	120.30
3	3	137	ARG	NE-CZ-NH2	7.49	124.05	120.30
1	1	282	ARG	NE-CZ-NH2	7.48	124.04	120.30
2	2	257	ARG	NE-CZ-NH2	7.47	124.03	120.30
2	2	29	ARG	NE-CZ-NH2	7.37	123.99	120.30
3	3	33	ARG	NE-CZ-NH2	7.35	123.97	120.30
1	1	46	ARG	NE-CZ-NH2	7.34	123.97	120.30
3	3	75	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	1	227	ARG	NE-CZ-NH2	7.26	123.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	103	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	1	94	ARG	NE-CZ-NH2	7.24	123.92	120.30
1	1	73	ARG	NE-CZ-NH2	7.19	123.90	120.30
1	1	224	MET	CG-SD-CE	6.20	110.11	100.20
3	3	222	MET	CG-SD-CE	6.18	110.09	100.20
3	3	55	MET	CG-SD-CE	6.15	110.04	100.20
4	4	60	MET	CG-SD-CE	6.14	110.02	100.20
2	2	191	MET	CG-SD-CE	6.13	110.01	100.20
3	3	146	MET	CG-SD-CE	6.11	109.98	100.20
1	1	221	MET	CG-SD-CE	6.09	109.94	100.20
3	3	116	MET	CG-SD-CE	6.08	109.93	100.20
3	3	163	MET	CG-SD-CE	6.04	109.87	100.20
2	2	221	MET	CG-SD-CE	5.87	109.60	100.20

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2163	0	2100	108	0
2	2	1964	0	1930	101	0
3	3	1835	0	1832	83	0
4	4	325	0	315	13	0
5	1	1	0	0	0	0
All	All	6288	0	6177	248	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 20.

All (248) 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)
1:1:36:ALA:CB	2:2:29:ARG:HH21	1.60	1.14
2:2:194:ASN:ND2	2:2:196:THR:O	1.81	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:36:ALA:HB2	2:2:29:ARG:NH2	1.72	1.03
2:2:53:THR:HG21	2:2:250:GLU:HG2	1.36	1.03
1:1:216:THR:HG21	1:1:218:LEU:HD12	1.39	1.02
2:2:29:ARG:HD2	4:4:67:LEU:HD11	1.40	1.02
1:1:36:ALA:HB2	2:2:29:ARG:HH21	0.88	1.01
1:1:36:ALA:HB1	2:2:29:ARG:HE	1.24	1.00
2:2:262:GLN:HA	2:2:262:GLN:OE1	1.63	0.95
2:2:12:ARG:HH22	3:3:157:LEU:HD22	1.29	0.95
2:2:255:ARG:HG2	2:2:255:ARG:HH11	1.31	0.94
2:2:32:ILE:HD13	2:2:186:HIS:O	1.69	0.93
2:2:53:THR:CG2	2:2:250:GLU:HG2	2.02	0.90
2:2:261:PRO:O	2:2:262:GLN:HB2	1.74	0.87
3:3:136:THR:HG23	3:3:137:ARG:O	1.75	0.87
2:2:29:ARG:HD2	4:4:67:LEU:CD1	2.05	0.86
1:1:36:ALA:HB1	2:2:29:ARG:NE	1.91	0.86
1:1:281:LYS:HD2	3:3:57:ASN:O	1.76	0.85
1:1:259:ARG:HD2	1:1:263:TYR:CE1	2.12	0.84
2:2:115:THR:HB	2:2:118:HIS:ND1	1.93	0.83
3:3:136:THR:HG23	3:3:137:ARG:N	1.94	0.80
2:2:29:ARG:NH1	2:2:193:THR:HG23	1.96	0.80
1:1:216:THR:CG2	1:1:218:LEU:HD12	2.11	0.78
2:2:53:THR:HG21	2:2:250:GLU:CG	2.14	0.78
1:1:36:ALA:CB	2:2:29:ARG:NH2	2.36	0.78
2:2:32:ILE:CD1	2:2:186:HIS:O	2.34	0.75
1:1:258:PRO:CB	3:3:99:GLU:HG2	2.17	0.74
3:3:79:GLN:HB2	3:3:190:TRP:CZ3	2.23	0.74
3:3:193:THR:O	3:3:194:SER:HB3	1.88	0.73
2:2:29:ARG:NH1	4:4:67:LEU:HD12	2.03	0.73
3:3:105:THR:HB	3:3:221:LEU:HB3	1.69	0.73
1:1:216:THR:HG21	1:1:218:LEU:CD1	2.19	0.72
1:1:87:ALA:HA	1:1:90:LEU:HD12	1.73	0.71
2:2:29:ARG:CD	4:4:67:LEU:HD11	2.20	0.71
1:1:284:ASN:HB3	1:1:287:THR:HG23	1.73	0.70
2:2:115:THR:HG22	2:2:117:PHE:H	1.56	0.70
1:1:134:ALA:HB2	1:1:180:VAL:HG11	1.73	0.70
2:2:115:THR:HB	2:2:118:HIS:CE1	2.26	0.69
1:1:38:GLU:HA	2:2:188:PHE:HB2	1.75	0.68
1:1:94:ARG:NH2	1:1:101:ASP:OD2	2.26	0.68
3:3:126:LYS:HB2	3:3:193:THR:OG1	1.93	0.68
4:4:59:LEU:HD21	4:4:61:LEU:HD13	1.76	0.67
2:2:260:VAL:HB	2:2:261:PRO:HD2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:29:ARG:HH11	2:2:193:THR:HG23	1.55	0.67
2:2:231:PRO:HG2	2:2:234:SER:HB2	1.77	0.66
1:1:277:THR:O	1:1:277:THR:OG1	2.14	0.66
3:3:197:LEU:HD13	3:3:201:THR:HG22	1.78	0.66
1:1:208:ASP:OD1	1:1:209:PRO:HD2	1.97	0.65
2:2:29:ARG:NH1	2:2:193:THR:CG2	2.60	0.65
2:2:29:ARG:HH11	4:4:67:LEU:HD12	1.62	0.64
1:1:261:LEU:HD12	1:1:271:TYR:CD2	2.31	0.64
1:1:208:ASP:HB3	1:1:211:THR:HG22	1.77	0.64
1:1:286:LYS:HG2	3:3:79:GLN:HG2	1.79	0.64
1:1:162:GLU:HB2	1:1:165:ASP:OD1	1.98	0.64
2:2:172:ASN:HD21	2:2:178:LEU:HA	1.63	0.64
3:3:164:THR:O	3:3:166:PRO:HD3	1.97	0.64
3:3:55:MET:CE	3:3:91:VAL:HG21	2.29	0.63
1:1:261:LEU:N	1:1:261:LEU:HD23	2.13	0.63
2:2:135:HIS:HD2	2:2:160:GLU:OE1	1.81	0.62
2:2:115:THR:C	2:2:117:PHE:H	2.03	0.62
3:3:173:PHE:CE1	3:3:220:ARG:HD2	2.34	0.62
2:2:255:ARG:HH11	2:2:255:ARG:CG	2.08	0.62
1:1:36:ALA:CB	2:2:29:ARG:HE	2.08	0.61
1:1:123:ARG:HD2	1:1:195:SER:O	2.01	0.61
1:1:261:LEU:CD2	1:1:278:ILE:HG13	2.30	0.61
2:2:87:LYS:HE2	2:2:150:GLY:HA2	1.82	0.61
3:3:98:GLY:O	3:3:102:GLN:HG3	2.00	0.61
3:3:55:MET:HE2	3:3:83:THR:HB	1.83	0.61
2:2:29:ARG:HH11	2:2:193:THR:CG2	2.14	0.60
2:2:23:ILE:HD11	2:2:243:THR:HG21	1.83	0.60
1:1:261:LEU:HD22	1:1:278:ILE:HG13	1.83	0.60
1:1:152:TYR:O	1:1:154:PRO:HD3	2.02	0.60
1:1:85:LYS:O	1:1:232:HIS:HB3	2.02	0.60
1:1:36:ALA:HB1	2:2:29:ARG:CZ	2.32	0.59
1:1:93:HIS:HD2	1:1:163:TRP:H	1.49	0.59
1:1:206:HIS:HD2	1:1:211:THR:HG21	1.67	0.59
2:2:262:GLN:OE1	2:2:262:GLN:CA	2.40	0.58
1:1:258:PRO:CG	3:3:99:GLU:HG2	2.33	0.58
1:1:264:VAL:CG1	1:1:272:PRO:HD3	2.33	0.58
1:1:40:GLY:HA3	2:2:32:ILE:HD11	1.86	0.58
3:3:55:MET:HE3	3:3:91:VAL:HG11	1.85	0.58
3:3:69:ILE:HB	3:3:207:LEU:HB2	1.84	0.58
1:1:47:PRO:HD3	3:3:164:THR:HG21	1.85	0.57
3:3:18:ASP:OD2	4:4:40:SER:HB2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:95:THR:O	3:3:99:GLU:HB2	2.04	0.57
3:3:146:MET:HG2	3:3:146:MET:O	2.05	0.57
1:1:259:ARG:HD2	1:1:263:TYR:CZ	2.38	0.57
1:1:110:VAL:HG22	3:3:230:GLN:OE1	2.04	0.57
3:3:76:GLN:O	3:3:77:ASN:HB2	2.05	0.57
1:1:258:PRO:HG2	3:3:99:GLU:HG2	1.85	0.57
2:2:145:LYS:HE2	2:2:146:TYR:CZ	2.40	0.56
2:2:38:TRP:CD1	2:2:39:PRO:HD2	2.40	0.56
1:1:72:GLY:O	1:1:246:ARG:HD2	2.06	0.55
3:3:214:CYS:HB3	3:3:215:PRO:HD2	1.88	0.55
3:3:50:GLY:HA2	3:3:212:SER:HB3	1.88	0.55
1:1:220:HIS:CE1	1:1:222:GLY:HA2	2.42	0.55
1:1:288:TYR:O	3:3:84:LYS:HE3	2.07	0.55
2:2:63:PHE:CD1	2:2:245:ALA:HB2	2.43	0.54
3:3:173:PHE:CD1	3:3:220:ARG:HD2	2.43	0.54
1:1:137:PRO:CG	1:1:238:ILE:HD12	2.37	0.54
1:1:37:ASN:HB2	3:3:116:MET:CE	2.38	0.54
1:1:165:ASP:H	1:1:168:TRP:HD1	1.54	0.54
1:1:256:ARG:HB3	2:2:184:PHE:HZ	1.73	0.54
1:1:204:TYR:CE2	1:1:213:TYR:HB2	2.43	0.54
3:3:108:SER:HB3	3:3:218:LYS:HG3	1.89	0.54
1:1:86:ASN:ND2	1:1:88:ALA:H	2.06	0.54
3:3:113:ILE:CD1	3:3:187:LEU:HD21	2.37	0.53
3:3:136:THR:CG2	3:3:137:ARG:N	2.62	0.53
1:1:273:ARG:NH2	2:2:160:GLU:OE1	2.41	0.53
1:1:220:HIS:HE1	1:1:222:GLY:HA2	1.73	0.53
1:1:282:ARG:HG3	3:3:57:ASN:HB3	1.89	0.53
2:2:29:ARG:CZ	4:4:67:LEU:HG	2.38	0.53
2:2:34:CYS:HB2	2:2:202:PRO:HD2	1.91	0.53
2:2:145:LYS:HD2	2:2:262:GLN:HE22	1.74	0.53
2:2:115:THR:HG22	2:2:117:PHE:HB2	1.90	0.52
2:2:118:HIS:CE1	2:2:231:PRO:HD2	2.44	0.52
1:1:36:ALA:HB1	2:2:29:ARG:NH2	2.24	0.52
3:3:55:MET:HE1	3:3:91:VAL:HG21	1.91	0.52
3:3:198:PRO:O	3:3:201:THR:HB	2.09	0.52
1:1:166:TYR:O	1:1:169:GLN:HB2	2.10	0.52
1:1:256:ARG:HB3	2:2:184:PHE:CZ	2.45	0.52
3:3:71:LEU:CB	3:3:205:VAL:HG23	2.39	0.52
3:3:63:ASN:OD1	3:3:65:THR:HB	2.09	0.52
1:1:216:THR:C	1:1:218:LEU:H	2.12	0.51
1:1:211:THR:OG1	1:1:212:PRO:HD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:206:HIS:CD2	1:1:211:THR:HG21	2.45	0.51
1:1:255:PRO:HD3	3:3:40:VAL:CG2	2.41	0.51
3:3:85:LEU:HD12	3:3:131:TYR:HE1	1.75	0.51
1:1:146:LEU:HB2	1:1:180:VAL:HG21	1.93	0.51
3:3:136:THR:CG2	3:3:137:ARG:O	2.56	0.51
1:1:37:ASN:CB	3:3:116:MET:HE3	2.41	0.51
3:3:16:THR:HG23	3:3:16:THR:O	2.10	0.51
1:1:136:GLN:HE22	1:1:144:SER:H	1.57	0.51
1:1:36:ALA:CB	2:2:29:ARG:CZ	2.88	0.50
2:2:145:LYS:HD2	2:2:262:GLN:NE2	2.26	0.50
2:2:231:PRO:HG2	2:2:234:SER:CB	2.40	0.50
3:3:72:HIS:HB2	3:3:75:ARG:HG3	1.94	0.50
1:1:37:ASN:HB2	3:3:116:MET:HE3	1.94	0.50
3:3:116:MET:HG3	3:3:159:SER:OG	2.12	0.50
4:4:54:GLU:N	4:4:55:PRO:HD3	2.27	0.50
1:1:262:PRO:HG2	1:1:272:PRO:HG3	1.93	0.50
2:2:122:LEU:HB2	2:2:189:ILE:HB	1.92	0.50
2:2:13:VAL:O	2:2:14:GLN:HG3	2.12	0.50
1:1:179:LYS:HB2	1:1:182:GLU:HG3	1.94	0.49
1:1:259:ARG:NH2	1:1:271:TYR:HB3	2.28	0.49
2:2:255:ARG:CG	2:2:255:ARG:NH1	2.72	0.49
1:1:60:PHE:CE2	3:3:218:LYS:HB3	2.48	0.49
2:2:255:ARG:HG2	2:2:255:ARG:NH1	2.10	0.49
3:3:57:ASN:ND2	3:3:91:VAL:HG13	2.28	0.48
3:3:55:MET:HE3	3:3:91:VAL:HG21	1.95	0.48
1:1:31:VAL:HG11	1:1:34:LEU:HD12	1.96	0.48
1:1:47:PRO:CD	3:3:164:THR:HG21	2.44	0.48
2:2:115:THR:HG23	2:2:117:PHE:HD1	1.79	0.48
1:1:216:THR:C	1:1:218:LEU:N	2.67	0.48
2:2:32:ILE:HD12	2:2:187:GLN:NE2	2.29	0.48
2:2:80:TRP:O	2:2:219:SER:HA	2.14	0.48
2:2:99:HIS:HB3	2:2:252:THR:O	2.14	0.48
2:2:178:LEU:O	2:2:181:LEU:HB2	2.15	0.47
1:1:127:GLU:HB3	1:1:246:ARG:HB3	1.95	0.47
3:3:18:ASP:O	3:3:19:ARG:HD2	2.14	0.47
3:3:71:LEU:HB3	3:3:205:VAL:HG23	1.96	0.47
1:1:102:TRP:O	1:1:223:SER:HA	2.14	0.47
1:1:18:LEU:HD23	1:1:57:TYR:CE1	2.49	0.47
1:1:273:ARG:HH21	2:2:135:HIS:HA	1.79	0.47
1:1:273:ARG:NH2	2:2:166:THR:HG22	2.30	0.46
3:3:42:ASN:O	3:3:45:GLU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:195:SER:OG	3:3:34:ILE:HG23	2.15	0.46
2:2:18:LEU:HD12	2:2:18:LEU:HA	1.84	0.46
2:2:260:VAL:HB	2:2:261:PRO:CD	2.45	0.46
3:3:65:THR:HA	3:3:68:LEU:HD12	1.98	0.46
2:2:165:PRO:HB2	2:2:173:MET:HE2	1.97	0.46
3:3:79:GLN:HB2	3:3:190:TRP:CE3	2.50	0.46
1:1:73:ARG:HD2	3:3:222:MET:CE	2.46	0.46
2:2:12:ARG:NH2	3:3:157:LEU:HD22	2.12	0.46
2:2:115:THR:C	2:2:117:PHE:N	2.69	0.45
3:3:152:VAL:HG13	3:3:192:LEU:HD22	1.98	0.45
3:3:210:PHE:N	3:3:210:PHE:CD1	2.85	0.45
1:1:282:ARG:HG3	3:3:57:ASN:CB	2.47	0.45
1:1:170:SER:OG	1:1:173:ASN:O	2.35	0.45
3:3:44:LEU:O	3:3:48:GLN:HG3	2.18	0.44
3:3:113:ILE:CD1	3:3:187:LEU:CD2	2.95	0.44
1:1:261:LEU:HD22	1:1:278:ILE:CG1	2.47	0.44
1:1:273:ARG:HH22	2:2:160:GLU:CD	2.20	0.44
2:2:172:ASN:ND2	2:2:181:LEU:HD22	2.33	0.44
3:3:127:ILE:HG22	3:3:128:ILE:N	2.32	0.44
2:2:191:MET:CE	2:2:191:MET:HA	2.47	0.44
1:1:28:THR:HB	1:1:30:SER:H	1.83	0.44
2:2:87:LYS:HE2	2:2:150:GLY:CA	2.48	0.44
2:2:29:ARG:CD	4:4:67:LEU:CD1	2.87	0.44
2:2:34:CYS:HB2	2:2:202:PRO:CD	2.47	0.44
2:2:53:THR:HG22	2:2:55:LYS:HZ1	1.82	0.44
2:2:115:THR:O	2:2:117:PHE:N	2.51	0.44
2:2:115:THR:CG2	2:2:117:PHE:HB2	2.48	0.44
1:1:18:LEU:HD23	1:1:57:TYR:CD1	2.53	0.43
2:2:53:THR:HG22	2:2:55:LYS:NZ	2.32	0.43
4:4:26:TYR:CE2	4:4:28:VAL:HG23	2.53	0.43
3:3:114:SER:HA	3:3:161:ILE:O	2.18	0.43
2:2:57:ASP:O	2:2:59:SER:N	2.51	0.43
2:2:189:ILE:HG22	2:2:189:ILE:O	2.17	0.43
2:2:255:ARG:CG	2:2:256:SER:N	2.80	0.43
1:1:20:SER:O	1:1:55:THR:HA	2.19	0.43
1:1:261:LEU:N	1:1:261:LEU:CD2	2.82	0.43
3:3:57:ASN:ND2	3:3:91:VAL:CG1	2.82	0.43
3:3:71:LEU:HB2	3:3:205:VAL:HG23	2.00	0.43
1:1:38:GLU:O	2:2:187:GLN:HG3	2.19	0.43
1:1:165:ASP:N	1:1:168:TRP:HD1	2.17	0.43
2:2:27:GLU:CB	2:2:195:ASN:HB2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:16:THR:O	3:3:16:THR:CG2	2.65	0.43
1:1:264:VAL:HG12	1:1:272:PRO:HD3	2.00	0.42
1:1:198:ASN:O	1:1:219:ASN:OD1	2.36	0.42
2:2:99:HIS:CG	2:2:251:PHE:HB3	2.55	0.42
3:3:85:LEU:HD12	3:3:131:TYR:CE1	2.52	0.42
3:3:113:ILE:HD12	3:3:187:LEU:HD21	2.00	0.42
3:3:151:VAL:HG11	3:3:161:ILE:HD11	2.00	0.42
1:1:21:VAL:HG12	1:1:22:SER:N	2.35	0.42
1:1:118:LEU:HD12	1:1:118:LEU:HA	1.95	0.42
2:2:115:THR:HG22	2:2:117:PHE:N	2.29	0.42
1:1:86:ASN:C	1:1:86:ASN:HD22	2.22	0.42
1:1:216:THR:HB	1:1:218:LEU:HB2	2.02	0.42
2:2:30:ASN:HD21	4:4:58:ASP:HB2	1.85	0.42
2:2:115:THR:CG2	2:2:117:PHE:HD1	2.33	0.42
2:2:148:HIS:N	2:2:149:PRO:CD	2.82	0.42
1:1:189:PRO:O	1:1:191:VAL:HG13	2.20	0.41
1:1:215:ILE:H	1:1:215:ILE:HG12	1.52	0.41
3:3:26:PRO:O	3:3:27:SER:HB2	2.20	0.41
2:2:23:ILE:HD11	2:2:243:THR:CG2	2.50	0.41
2:2:116:LYS:HB3	3:3:122:LEU:HG	2.02	0.41
1:1:288:TYR:CE2	3:3:138:GLY:HA3	2.55	0.41
1:1:204:TYR:CZ	2:2:144:TYR:HA	2.55	0.41
1:1:80:THR:HG22	1:1:241:ILE:HB	2.01	0.41
1:1:86:ASN:HD22	1:1:87:ALA:N	2.19	0.41
1:1:254:ILE:HG23	2:2:35:TYR:OH	2.19	0.41
1:1:268:ARG:HD3	1:1:270:ASN:ND2	2.36	0.41
3:3:75:ARG:O	3:3:194:SER:HB2	2.20	0.41
1:1:38:GLU:HG3	3:3:116:MET:HE1	2.02	0.41
1:1:73:ARG:HD2	3:3:222:MET:HE2	2.01	0.41
3:3:45:GLU:OE2	4:4:47:MET:HA	2.21	0.41
3:3:126:LYS:HA	3:3:153:TRP:O	2.21	0.41
1:1:18:LEU:CD2	1:1:57:TYR:CE1	3.04	0.41
1:1:152:TYR:CE2	1:1:154:PRO:HG3	2.56	0.40
2:2:128:PRO:HA	2:2:218:VAL:HG12	2.03	0.40
2:2:118:HIS:CE1	2:2:231:PRO:CD	3.04	0.40
2:2:181:LEU:HA	2:2:181:LEU:HD12	1.84	0.40
2:2:116:LYS:HG2	3:3:121:ALA:HB3	2.04	0.40
3:3:110:SER:H	3:3:216:ASP:HB3	1.86	0.40
1:1:202:ASP:O	2:2:215:HIS:HD2	2.04	0.40
3:3:152:VAL:CG1	3:3:192:LEU:HD22	2.51	0.40
1:1:103:LYS:O	1:1:104:ILE:C	2.60	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	271/288 (94%)	249 (92%)	19 (7%)	3 (1%)	14	50
2	2	253/262 (97%)	232 (92%)	19 (8%)	2 (1%)	19	57
3	3	234/236 (99%)	220 (94%)	13 (6%)	1 (0%)	34	72
4	4	41/68 (60%)	35 (85%)	6 (15%)	0	100	100
All	All	799/854 (94%)	736 (92%)	57 (7%)	6 (1%)	19	57

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	58	ILE
1	1	139	ALA
2	2	116	LYS
3	3	194	SER
1	1	231	GLU
1	1	104	ILE

### 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	239/253 (94%)	215 (90%)	24 (10%)	7	29
2	2	223/229 (97%)	204 (92%)	19 (8%)	10	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	3	207/207 (100%)	182 (88%)	25 (12%)	5	21
4	4	36/57 (63%)	32 (89%)	4 (11%)	6	25
All	All	705/746 (94%)	633 (90%)	72 (10%)	7	28

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	23	SER
1	1	28	THR
1	1	63	SER
1	1	65	THR
1	1	85	LYS
1	1	86	ASN
1	1	105	ASN
1	1	118	LEU
1	1	122	VAL
1	1	135	SER
1	1	176	VAL
1	1	185	ARG
1	1	206	HIS
1	1	211	THR
1	1	215	ILE
1	1	217	VAL
1	1	218	LEU
1	1	256	ARG
1	1	261	LEU
1	1	275	SER
1	1	277	THR
1	1	280	LYS
1	1	283	THR
1	1	286	LYS
2	2	32	ILE
2	2	52	LYS
2	2	53	THR
2	2	68	SER
2	2	69	LYS
2	2	81	LYS
2	2	191	MET
2	2	192	ARG
2	2	194	ASN
2	2	195	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	2	221	MET
2	2	229	ASN
2	2	234	SER
2	2	238	LEU
2	2	252	THR
2	2	254	ILE
2	2	255	ARG
2	2	256	SER
2	2	262	GLN
3	3	16	THR
3	3	21	SER
3	3	55	MET
3	3	60	THR
3	3	63	ASN
3	3	71	LEU
3	3	94	THR
3	3	114	SER
3	3	115	LEU
3	3	129	LEU
3	3	136	THR
3	3	137	ARG
3	3	146	MET
3	3	155	ILE
3	3	159	SER
3	3	172	GLN
3	3	179	ASP
3	3	217	PHE
3	3	218	LYS
3	3	220	ARG
3	3	221	LEU
3	3	223	LYS
3	3	225	THR
3	3	228	ILE
3	3	236	GLU
4	4	26	TYR
4	4	50	SER
4	4	51	LYS
4	4	59	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	59	HIS
1	1	86	ASN
1	1	93	HIS
1	1	136	GLN
1	1	206	HIS
1	1	219	ASN
2	2	135	HIS
2	2	172	ASN
2	2	195	ASN
2	2	217	ASN
2	2	229	ASN
3	3	204	GLN
3	3	226	GLN
4	4	43	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1	273/288 (94%)	-0.62	2 (0%) 87 69	15, 15, 15, 15	0
2	2	255/262 (97%)	-0.67	2 (0%) 86 65	15, 15, 15, 15	0
3	3	236/236 (100%)	-0.72	0 100 100	15, 15, 15, 15	0
4	4	43/68 (63%)	0.02	0 100 100	15, 15, 15, 15	0
All	All	807/854 (94%)	-0.63	4 (0%) 91 75	15, 15, 15, 15	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	2	262	GLN	3.3
1	1	210	ASP	2.3
1	1	16	GLN	2.3
2	2	9	TYR	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CA	1	289	1/1	0.99	0.40	15,15,15,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.