



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 10:30 pm BST

PDB ID : 2WS9
Title : Equine Rhinitis A Virus at Low pH
Authors : Fry, E.E.; Tuthill, T.J.; Harlos, K.; Walter, T.S.; Knowles, N.J.; Gropelli, E.;
Rowlands, D.J.; Stuart, D.I.
Deposited on : 2009-09-04
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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	:	2.11
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)	:	2.11

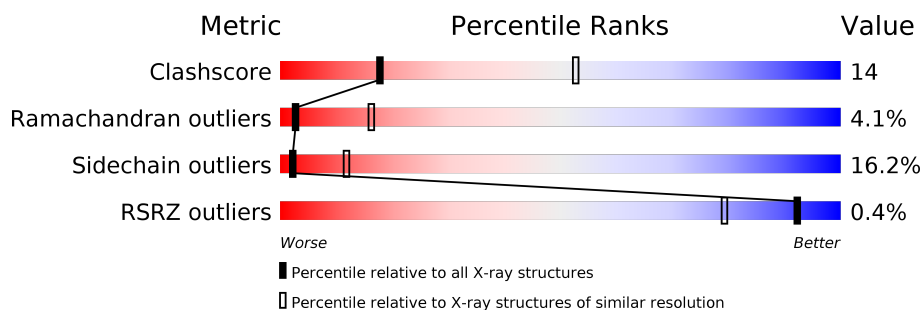
1 Overall quality at a glance

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 on 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	1	246	<div> <div></div> <div>65% 24% 9% .</div> </div>
2	2	230	<div> <div></div> <div>60% 17% 9% . 13%</div> </div>
3	3	226	<div> <div></div> <div>65% 26% 8% .</div> </div>
4	4	80	<div> <div></div> <div>15% 6% 5% 74%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5364 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 P1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	246	Total	C	N	O	S	0	0	0
			1928	1240	329	351	8			

- Molecule 2 is a protein called P1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	200	Total	C	N	O	S	0	0	0
			1553	997	266	283	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	85	SER	GLY	conflict	UNP B9VV85

- Molecule 3 is a protein called P1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	226	Total	C	N	O	S	0	0	0
			1718	1107	280	325	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	59	LYS	ARG	conflict	UNP B9VV85

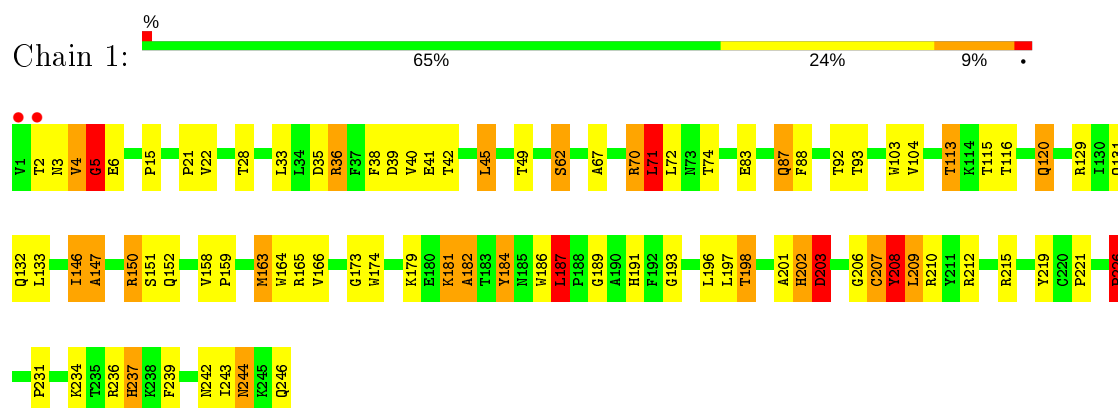
- Molecule 4 is a protein called P1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	21	Total	C	N	O	S	0	0	0
			165	101	28	35	1			

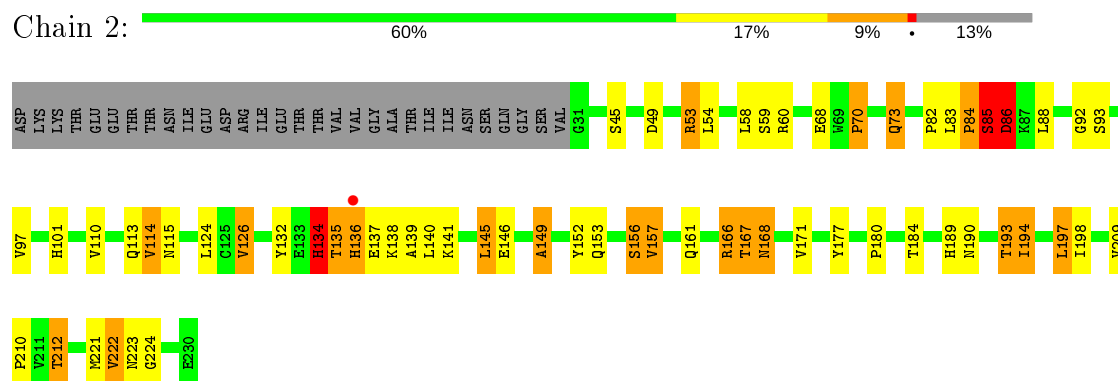
3 Residue-property plots [i](#)

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.

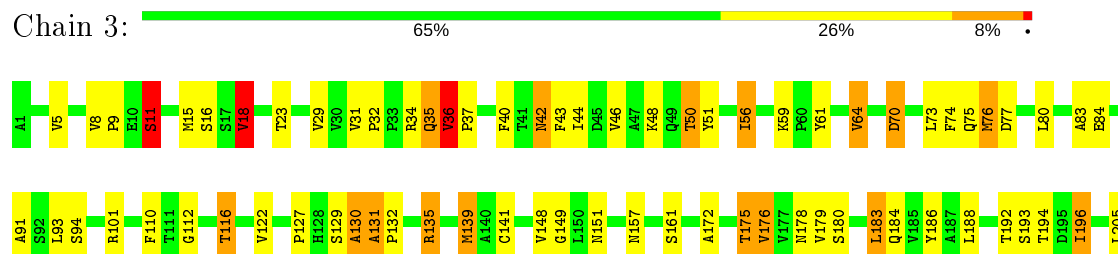
• Molecule 1: P1

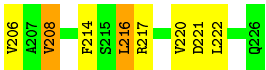


• Molecule 2: P1

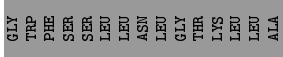
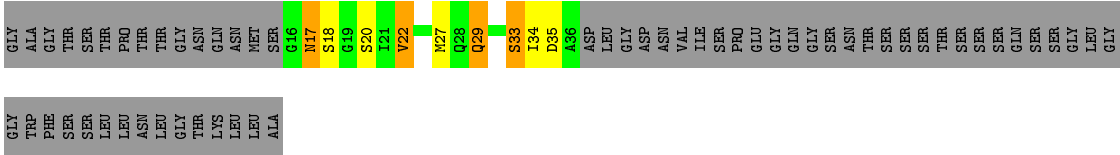


• Molecule 3: P1





● Molecule 4: P1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	344.80Å 531.40Å 488.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 74.97 – 3.00	Depositor EDS
% Data completeness (in resolution range)	37.1 (20.00-3.00) 41.1 (74.97-3.00)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.01Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.275 , (Not available) 0.248 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.68 , 25.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	5364	wwPDB-VP
Average B, all atoms (Å ²)	7.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.76	0/1992	1.12	17/2721 (0.6%)
2	2	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
3	3	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
4	4	0.72	0/167	0.94	1/224 (0.4%)
All	All	0.78	2/5534 (0.0%)	1.05	30/7573 (0.4%)

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
1	1	0	1
2	2	0	2
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	222	VAL	CB-CG1	-5.10	1.42	1.52
3	3	141	CYS	CB-SG	-5.08	1.73	1.81

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	5	GLY	N-CA-C	10.73	139.92	113.10
1	1	207	CYS	N-CA-C	8.40	133.69	111.00
2	2	138	LYS	N-CA-C	-7.70	90.21	111.00
1	1	21	PRO	N-CA-C	7.60	131.86	112.10
2	2	86	ASP	CB-CA-C	7.00	124.40	110.40
3	3	130	ALA	N-CA-C	6.88	129.56	111.00
2	2	223	ASN	CB-CA-C	-6.58	97.25	110.40
1	1	87	GLN	N-CA-C	6.56	128.71	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	203	ASP	N-CA-C	-6.50	93.44	111.00
4	4	17	ASN	N-CA-C	6.42	128.32	111.00
1	1	146	ILE	CB-CA-C	-6.34	98.92	111.60
3	3	70	ASP	N-CA-C	6.20	127.75	111.00
2	2	134	HIS	N-CA-C	-6.16	94.36	111.00
2	2	85	SER	N-CA-C	6.16	127.62	111.00
3	3	216	LEU	CA-CB-CG	6.09	129.30	115.30
1	1	4	VAL	N-CA-C	6.05	127.35	111.00
1	1	151	SER	N-CA-C	-5.72	95.54	111.00
1	1	181	LYS	N-CA-C	-5.64	95.77	111.00
1	1	226	PRO	N-CA-C	5.56	126.56	112.10
1	1	186	TRP	N-CA-C	5.51	125.87	111.00
3	3	64	VAL	CB-CA-C	-5.50	100.95	111.40
3	3	18	VAL	CB-CA-C	-5.47	101.00	111.40
3	3	208	VAL	CB-CA-C	-5.47	101.01	111.40
1	1	242	ASN	CB-CA-C	-5.30	99.80	110.40
1	1	6	GLU	N-CA-C	5.22	125.09	111.00
1	1	70	ARG	N-CA-C	-5.17	97.04	111.00
1	1	62	SER	N-CA-C	5.13	124.86	111.00
1	1	4	VAL	C-N-CA	5.13	133.07	122.30
1	1	113	THR	N-CA-C	5.06	124.65	111.00
2	2	59	SER	N-CA-C	-5.03	97.41	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	208	TYR	Sidechain
2	2	177	TYR	Sidechain
2	2	86	ASP	Mainchain

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	1928	0	1864	68	0
2	2	1553	0	1523	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	3	1718	0	1677	48	0
4	4	165	0	146	5	0
All	All	5364	0	5210	144	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 14.

All (144) 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)
1:1:115:THR:HG21	1:1:131:GLN:HB3	1.44	0.97
2:2:134:HIS:HD2	2:2:145:LEU:HD13	1.43	0.82
1:1:70:ARG:O	1:1:71:LEU:HB2	1.81	0.79
1:1:207:CYS:O	1:1:208:TYR:HB2	1.86	0.76
1:1:181:LYS:HE3	2:2:137:GLU:HB2	1.67	0.75
1:1:191:HIS:HD2	1:1:193:GLY:H	1.33	0.74
3:3:46:VAL:O	3:3:50:THR:HB	1.86	0.74
2:2:184:THR:HG21	2:2:189:HIS:ND1	2.03	0.74
2:2:157:VAL:HG23	3:3:50:THR:HG21	1.69	0.73
1:1:115:THR:CG2	1:1:131:GLN:HB3	2.19	0.72
1:1:150:ARG:H	1:1:150:ARG:HE	1.40	0.70
1:1:74:THR:HG21	3:3:43:PHE:HE2	1.57	0.69
2:2:134:HIS:CD2	2:2:145:LEU:HD13	2.26	0.69
1:1:92:THR:HG22	1:1:93:THR:H	1.57	0.68
1:1:87:GLN:HE21	1:1:210:ARG:HH22	1.39	0.68
2:2:82:PRO:HA	2:2:193:THR:HB	1.75	0.68
1:1:83:GLU:HB2	1:1:212:ARG:HB3	1.78	0.66
1:1:150:ARG:NE	1:1:150:ARG:H	1.93	0.66
1:1:103:TRP:HB2	1:1:198:THR:HG22	1.78	0.66
1:1:231:PRO:HG2	3:3:83:ALA:HB2	1.77	0.65
2:2:149:ALA:HA	2:2:152:TYR:CE2	2.33	0.63
2:2:132:TYR:HB3	2:2:193:THR:HG21	1.79	0.63
2:2:114:VAL:HG22	2:2:209:VAL:CG1	2.29	0.62
1:1:120:GLN:HG3	1:1:129:ARG:HG2	1.82	0.62
1:1:146:ILE:O	1:1:147:ALA:HB2	1.99	0.62
1:1:115:THR:HG22	1:1:131:GLN:OE1	2.01	0.61
1:1:115:THR:HG23	1:1:132:GLN:HB3	1.82	0.61
1:1:163:MET:CE	1:1:189:GLY:HA3	2.31	0.61
1:1:74:THR:O	1:1:74:THR:HG22	1.99	0.61
1:1:181:LYS:O	1:1:182:ALA:HB2	2.01	0.60
1:1:201:ALA:O	1:1:203:ASP:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:159:PRO:HB2	3:3:29:VAL:HG21	1.84	0.60
1:1:181:LYS:HE3	2:2:137:GLU:CB	2.31	0.60
1:1:159:PRO:CB	3:3:29:VAL:HG21	2.33	0.58
2:2:85:SER:HB2	2:2:190:ASN:HD21	1.67	0.58
1:1:5:GLY:HA3	1:1:15:PRO:HD3	1.85	0.58
2:2:114:VAL:HG22	2:2:209:VAL:HG12	1.86	0.58
2:2:97:VAL:O	2:2:101:HIS:HD2	1.87	0.57
2:2:132:TYR:HB3	2:2:193:THR:CG2	2.34	0.57
3:3:44:ILE:O	3:3:48:LYS:HG3	2.05	0.57
1:1:87:GLN:NE2	1:1:210:ARG:HH12	2.02	0.57
2:2:126:VAL:HG13	2:2:171:VAL:HG21	1.86	0.57
2:2:137:GLU:C	2:2:139:ALA:N	2.55	0.56
2:2:54:LEU:HD21	2:2:97:VAL:HG11	1.87	0.56
3:3:42:ASN:HD22	3:3:44:ILE:H	1.50	0.56
1:1:87:GLN:NE2	1:1:210:ARG:HH22	2.03	0.55
2:2:113:GLN:HB2	2:2:212:THR:HG22	1.88	0.55
2:2:126:VAL:HG22	2:2:171:VAL:HG11	1.89	0.54
2:2:134:HIS:O	2:2:136:HIS:N	2.36	0.54
1:1:159:PRO:CG	3:3:29:VAL:HG21	2.38	0.54
3:3:139:MET:O	3:3:139:MET:HG2	2.07	0.54
1:1:163:MET:HE1	1:1:189:GLY:HA3	1.88	0.53
2:2:137:GLU:O	2:2:139:ALA:N	2.41	0.53
3:3:220:VAL:HG12	3:3:221:ASP:N	2.23	0.53
1:1:33:LEU:O	1:1:36:ARG:HD2	2.08	0.53
2:2:83:LEU:HD11	2:2:194:ILE:HD12	1.91	0.53
3:3:56:ILE:HD12	3:3:74:PHE:CE1	2.43	0.53
3:3:135:ARG:HB3	3:3:186:TYR:CG	2.44	0.53
3:3:148:VAL:HG12	3:3:149:GLY:N	2.24	0.53
3:3:193:SER:HB3	3:3:196:ILE:HD12	1.90	0.52
1:1:45:LEU:HB2	1:1:202:HIS:HA	1.90	0.52
2:2:73:GLN:HA	2:2:73:GLN:NE2	2.25	0.52
2:2:167:THR:HB	2:2:168:ASN:ND2	2.25	0.52
1:1:173:GLY:O	1:1:184:TYR:O	2.28	0.51
2:2:101:HIS:CG	2:2:222:VAL:CG1	2.93	0.51
1:1:104:VAL:HG22	1:1:197:LEU:HD23	1.92	0.51
1:1:70:ARG:HH11	3:3:222:LEU:HD21	1.76	0.51
2:2:157:VAL:HG23	3:3:50:THR:CG2	2.39	0.51
3:3:132:PRO:HG2	3:3:184:GLN:HE22	1.76	0.51
1:1:237:HIS:HB3	1:1:239:PHE:CE1	2.45	0.51
1:1:115:THR:HG22	1:1:116:THR:N	2.24	0.50
2:2:84:PRO:CG	2:2:85:SER:H	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:191:HIS:CD2	1:1:193:GLY:H	2.21	0.50
1:1:236:ARG:NH1	3:3:172:ALA:O	2.45	0.49
4:4:22:VAL:O	4:4:22:VAL:HG13	2.12	0.49
1:1:38:PHE:O	1:1:210:ARG:HA	2.12	0.49
1:1:88:PHE:HA	1:1:206:GLY:O	2.13	0.49
2:2:82:PRO:HB2	2:2:190:ASN:HD22	1.77	0.49
3:3:130:ALA:O	3:3:131:ALA:HB3	2.13	0.49
1:1:181:LYS:O	1:1:182:ALA:CB	2.61	0.48
2:2:86:ASP:HB3	2:2:141:LYS:HA	1.96	0.48
1:1:87:GLN:O	1:1:152:GLN:O	2.31	0.48
3:3:76:MET:HB2	3:3:84:GLU:HG2	1.96	0.48
1:1:174:TRP:CZ2	2:2:139:ALA:HB3	2.49	0.48
1:1:234:LYS:HD2	3:3:75:GLN:HB3	1.96	0.47
1:1:165:ARG:HG2	2:2:180:PRO:O	2.14	0.47
1:1:243:ILE:HG22	1:1:244:ASN:N	2.28	0.47
1:1:104:VAL:HG22	1:1:197:LEU:CD2	2.44	0.47
1:1:184:TYR:CE1	2:2:139:ALA:HB2	2.50	0.47
2:2:140:LEU:HD23	2:2:140:LEU:N	2.30	0.47
3:3:42:ASN:ND2	3:3:44:ILE:H	2.12	0.47
3:3:110:PHE:HE2	3:3:116:THR:HG22	1.80	0.47
4:4:29:GLN:HB3	4:4:34:ILE:HD11	1.98	0.46
1:1:191:HIS:HD2	1:1:193:GLY:N	2.08	0.46
4:4:20:SER:OG	4:4:22:VAL:HG12	2.15	0.46
1:1:207:CYS:O	1:1:208:TYR:CB	2.57	0.46
2:2:157:VAL:CG2	3:3:50:THR:HG21	2.43	0.46
3:3:36:VAL:HA	3:3:37:PRO:HD3	1.64	0.45
2:2:85:SER:HB2	2:2:190:ASN:ND2	2.31	0.45
1:1:164:TRP:CE2	1:1:187:LEU:HD13	2.51	0.45
1:1:115:THR:OG1	1:1:133:LEU:HB2	2.16	0.45
1:1:174:TRP:CE2	1:1:179:LYS:HB3	2.51	0.45
3:3:61:TYR:HB3	3:3:205:LEU:HD23	1.97	0.45
1:1:35:ASP:OD2	1:1:212:ARG:HD3	2.16	0.45
1:1:209:LEU:HD22	1:1:209:LEU:HA	1.74	0.45
1:1:87:GLN:HE21	1:1:210:ARG:NH2	2.12	0.44
3:3:9:PRO:C	3:3:11:SER:H	2.20	0.44
2:2:53:ARG:HG2	2:2:221:MET:CE	2.48	0.44
2:2:83:LEU:HA	2:2:84:PRO:HA	1.60	0.44
2:2:84:PRO:CD	2:2:85:SER:H	2.31	0.44
2:2:156:SER:HB2	3:3:51:TYR:O	2.18	0.44
1:1:67:ALA:O	1:1:70:ARG:O	2.35	0.44
2:2:53:ARG:HG2	2:2:221:MET:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:165:ARG:HA	3:3:32:PRO:HG2	2.00	0.43
2:2:124:LEU:HD23	2:2:198:ILE:HA	2.00	0.43
1:1:219:TYR:CD1	3:3:36:VAL:HG22	2.53	0.43
1:1:74:THR:HG21	3:3:43:PHE:CE2	2.45	0.43
2:2:166:ARG:HB3	3:3:112:GLY:O	2.19	0.43
3:3:74:PHE:HE2	3:3:183:LEU:HD13	1.84	0.43
2:2:86:ASP:CB	2:2:141:LYS:HA	2.49	0.42
1:1:215:ARG:NH1	4:4:33:SER:OG	2.52	0.42
1:1:231:PRO:HG2	3:3:83:ALA:CB	2.48	0.42
3:3:34:ARG:NH2	4:4:35:ASP:OD1	2.52	0.42
2:2:152:TYR:HB3	2:2:197:LEU:HD11	2.02	0.42
2:2:70:PRO:HG2	2:2:73:GLN:HB2	2.02	0.42
3:3:175:THR:HG23	3:3:176:VAL:N	2.34	0.42
2:2:152:TYR:CB	2:2:197:LEU:HD11	2.49	0.42
3:3:44:ILE:HD12	3:3:44:ILE:HA	1.88	0.42
1:1:72:LEU:HA	1:1:72:LEU:HD23	1.82	0.42
3:3:76:MET:HG3	3:3:76:MET:O	2.18	0.42
2:2:149:ALA:O	2:2:153:GLN:HG3	2.20	0.42
1:1:221:PRO:HD3	3:3:40:PHE:CD2	2.54	0.42
3:3:110:PHE:CD2	3:3:148:VAL:HG11	2.55	0.41
3:3:148:VAL:CG1	3:3:149:GLY:N	2.83	0.41
1:1:212:ARG:NH2	3:3:18:VAL:O	2.46	0.41
3:3:127:PRO:HD3	3:3:180:SER:O	2.21	0.41
1:1:74:THR:O	1:1:74:THR:CG2	2.68	0.41
2:2:115:ASN:HB3	2:2:210:PRO:HG2	2.02	0.41
3:3:101:ARG:O	3:3:214:PHE:HA	2.21	0.41
3:3:91:ALA:O	3:3:94:SER:HB2	2.21	0.41
3:3:84:GLU:H	3:3:84:GLU:CD	2.23	0.41
1:1:174:TRP:CH2	2:2:139:ALA:HB3	2.55	0.40
2:2:68:GLU:O	2:2:70:PRO:HD3	2.21	0.40
3:3:29:VAL:O	3:3:29:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	10
2	2	198/230 (86%)	183 (92%)	7 (4%)	8 (4%)	3	17
3	3	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	26
4	4	19/80 (24%)	19 (100%)	0	0	100	100
All	All	685/782 (88%)	612 (89%)	45 (7%)	28 (4%)	3	16

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	2	THR
1	1	5	GLY
1	1	41	GLU
1	1	202	HIS
1	1	244	ASN
2	2	84	PRO
2	2	85	SER
2	2	134	HIS
2	2	135	THR
3	3	11	SER
3	3	36	VAL
1	1	22	VAL
1	1	71	LEU
1	1	147	ALA
1	1	182	ALA
1	1	184	TYR
2	2	92	GLY
2	2	224	GLY
3	3	15	MET
3	3	35	GLN
3	3	70	ASP
1	1	3	ASN
1	1	187	LEU
1	1	208	TYR
2	2	149	ALA
3	3	131	ALA
2	2	60	ARG
1	1	226	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	1	208/208 (100%)	184 (88%)	24 (12%)	5	24
2	2	176/203 (87%)	150 (85%)	26 (15%)	3	14
3	3	190/190 (100%)	150 (79%)	40 (21%)	1	5
4	4	18/65 (28%)	12 (67%)	6 (33%)	0	1
All	All	592/666 (89%)	496 (84%)	96 (16%)	2	12

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	4	VAL
1	1	28	THR
1	1	36	ARG
1	1	39	ASP
1	1	40	VAL
1	1	42	THR
1	1	45	LEU
1	1	49	THR
1	1	62	SER
1	1	71	LEU
1	1	113	THR
1	1	120	GLN
1	1	150	ARG
1	1	158	VAL
1	1	163	MET
1	1	166	VAL
1	1	187	LEU
1	1	196	LEU
1	1	198	THR
1	1	203	ASP
1	1	209	LEU
1	1	226	PRO
1	1	237	HIS
1	1	246	GLN

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Mol	Chain	Res	Type
2	2	45	SER
2	2	49	ASP
2	2	53	ARG
2	2	58	LEU
2	2	70	PRO
2	2	73	GLN
2	2	86	ASP
2	2	88	LEU
2	2	93	SER
2	2	110	VAL
2	2	114	VAL
2	2	126	VAL
2	2	135	THR
2	2	136	HIS
2	2	145	LEU
2	2	146	GLU
2	2	156	SER
2	2	157	VAL
2	2	161	GLN
2	2	166	ARG
2	2	167	THR
2	2	168	ASN
2	2	193	THR
2	2	194	ILE
2	2	197	LEU
2	2	212	THR
3	3	5	VAL
3	3	8	VAL
3	3	11	SER
3	3	16	SER
3	3	18	VAL
3	3	23	THR
3	3	31	VAL
3	3	35	GLN
3	3	36	VAL
3	3	42	ASN
3	3	50	THR
3	3	56	ILE
3	3	59	LYS
3	3	64	VAL
3	3	73	LEU
3	3	76	MET

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Mol	Chain	Res	Type
3	3	77	ASP
3	3	80	LEU
3	3	93	LEU
3	3	116	THR
3	3	122	VAL
3	3	129	SER
3	3	135	ARG
3	3	139	MET
3	3	151	ASN
3	3	157	ASN
3	3	161	SER
3	3	175	THR
3	3	176	VAL
3	3	178	ASN
3	3	179	VAL
3	3	183	LEU
3	3	188	LEU
3	3	192	THR
3	3	194	THR
3	3	196	ILE
3	3	206	VAL
3	3	208	VAL
3	3	216	LEU
3	3	217	ARG
4	4	17	ASN
4	4	18	SER
4	4	22	VAL
4	4	27	MET
4	4	29	GLN
4	4	33	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	47	ASN
1	1	87	GLN
1	1	191	HIS
1	1	217	ASN
2	2	73	GLN
2	2	77	HIS
2	2	95	HIS
2	2	101	HIS

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Mol	Chain	Res	Type
2	2	134	HIS
2	2	136	HIS
2	2	168	ASN
2	2	190	ASN
3	3	35	GLN
3	3	42	ASN
3	3	75	GLN
3	3	157	ASN
3	3	178	ASN
3	3	184	GLN
4	4	17	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 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	1	246/246 (100%)	-0.68	2 (0%) 86 65	2, 3, 29, 91	0
2	2	200/230 (86%)	-0.63	1 (0%) 91 75	2, 3, 32, 86	0
3	3	226/226 (100%)	-0.77	0 100 100	2, 3, 16, 31	0
4	4	21/80 (26%)	-0.64	0 100 100	7, 23, 31, 41	0
All	All	693/782 (88%)	-0.70	3 (0%) 92 79	2, 3, 28, 91	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1	1	VAL	2.9
1	1	2	THR	2.3
2	2	136	HIS	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.