



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1H8T / pdb_00001h8t
Title : Echovirus 11
Authors : Stuart, A.; McKee, T.; Williams, P.A.; Harley, C.; Stuart, D.I.; Brown, T.D.K.;
Lea, S.M.
Deposited on : 2001-02-15
Resolution : 2.90 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

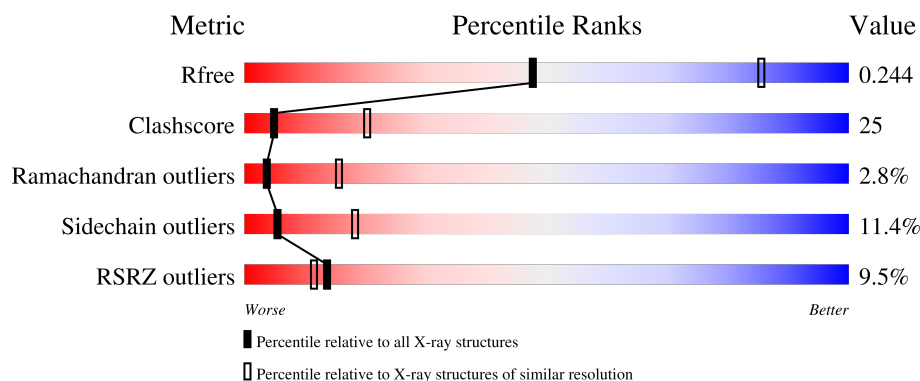
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	292	13% 55% 33% 8% • •
2	B	262	5% 57% 30% 7% • •
3	C	238	0% 60% 29% 8% •
4	D	68	40% 38% 32% 13% 6% 10%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6575 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 ECHOVIRUS 11 COAT PROTEIN VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	1
			2284	1439	399	435	11			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	VAL	MET	conflict	UNP P29813
A	78	GLU	GLY	conflict	UNP P29813
A	84	SER	THR	conflict	UNP P29813
A	131	THR	SER	conflict	UNP P29813
A	132	GLN	ARG	conflict	UNP P29813
A	161	THR	ALA	conflict	UNP P29813
A	267	SER	THR	conflict	UNP P29813
A	270	ASP	ASN	conflict	UNP P29813
A	271	ILE	VAL	conflict	UNP P29813
A	276	ASN	THR	conflict	UNP P29813
A	279	THR	ASN	conflict	UNP P29813
A	283	ASP	GLU	conflict	UNP P29813
A	289	VAL	LEU	conflict	UNP P29813
A	292	HIS	TYR	conflict	UNP P29813

- Molecule 2 is a protein called ECHOVIRUS 11 COAT PROTEIN VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	253	Total	C	N	O	S	0	0	1
			1964	1240	332	376	16			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1043	ARG	LYS	conflict	UNP P29813
B	1045	ASP	ASN	conflict	UNP P29813

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1073	LYS	ARG	conflict	UNP P29813
B	1108	ILE	LEU	conflict	UNP P29813
B	1136	THR	GLN	conflict	UNP P29813
B	1157	ALA	SER	conflict	UNP P29813
B	1159	GLY	SER	conflict	UNP P29813
B	1168	SER	THR	conflict	UNP P29813
B	1185	PHE	TYR	conflict	UNP P29813
B	1230	ASN	ASP	conflict	UNP P29813
B	1235	PHE	SER	conflict	UNP P29813
B	1260	ALA	SER	conflict	UNP P29813

- Molecule 3 is a protein called ECHOVIRUS 11 COAT PROTEIN VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	238	Total	C	N	O	S	0	0	0
			1819	1161	299	346	13			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2005	ILE	MET	conflict	UNP P29813
C	2059	ALA	GLU	conflict	UNP P29813
C	2061	ASN	LYS	conflict	UNP P29813
C	2063	GLU	ASP	conflict	UNP P29813
C	2066	ASP	GLU	conflict	UNP P29813
C	2067	ILE	VAL	conflict	UNP P29813
C	2080	SER	ASP	conflict	UNP P29813
C	2093	GLY	SER	conflict	UNP P29813
C	2107	TYR	PHE	conflict	UNP P29813
C	2144	SER	ASN	conflict	UNP P29813
C	2168	ILE	VAL	conflict	UNP P29813
C	2232	GLN	GLU	conflict	UNP P29813
C	2234	ALA	THR	conflict	UNP P29813

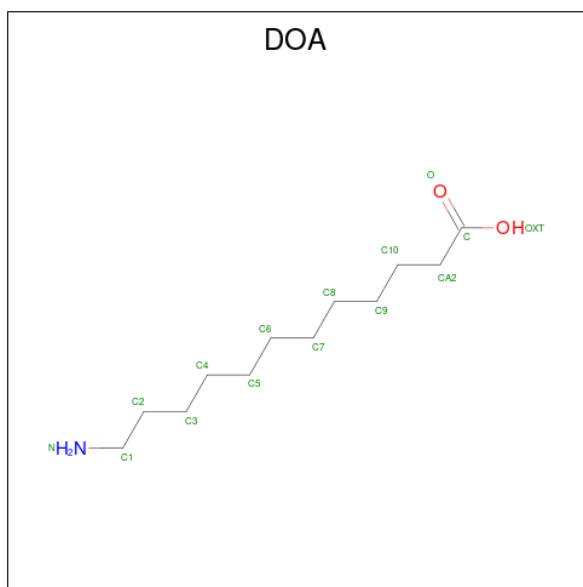
- Molecule 4 is a protein called ECHOVIRUS 11 COAT PROTEIN VP4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	61	Total	C	N	O	S	0	0	1
			467	289	82	95	1			

There are 4 discrepancies between the modelled and reference sequences:

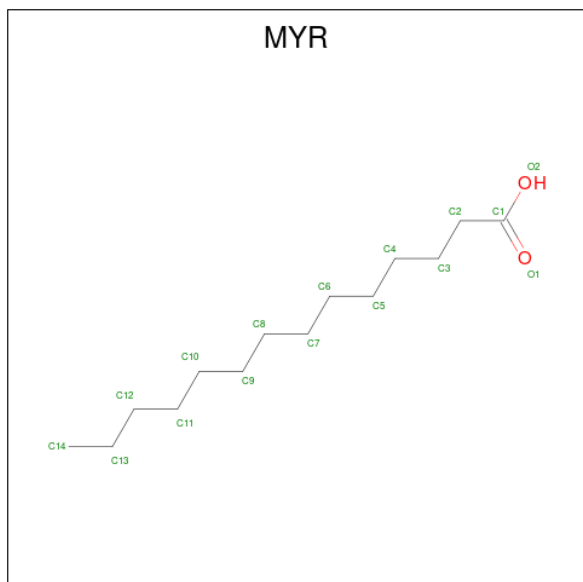
Chain	Residue	Modelled	Actual	Comment	Reference
D	3018	ARG	ASN	conflict	UNP P29813
D	3022	ASN	SER	conflict	UNP P29813
D	3045	ASP	GLU	conflict	UNP P29813
D	3047	THR	SER	conflict	UNP P29813

- Molecule 5 is 12-AMINO-DODECANOIC ACID (CCD ID: DOA) (formula: $C_{12}H_{25}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			15	12	1	2		

- Molecule 6 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			15	14	1		

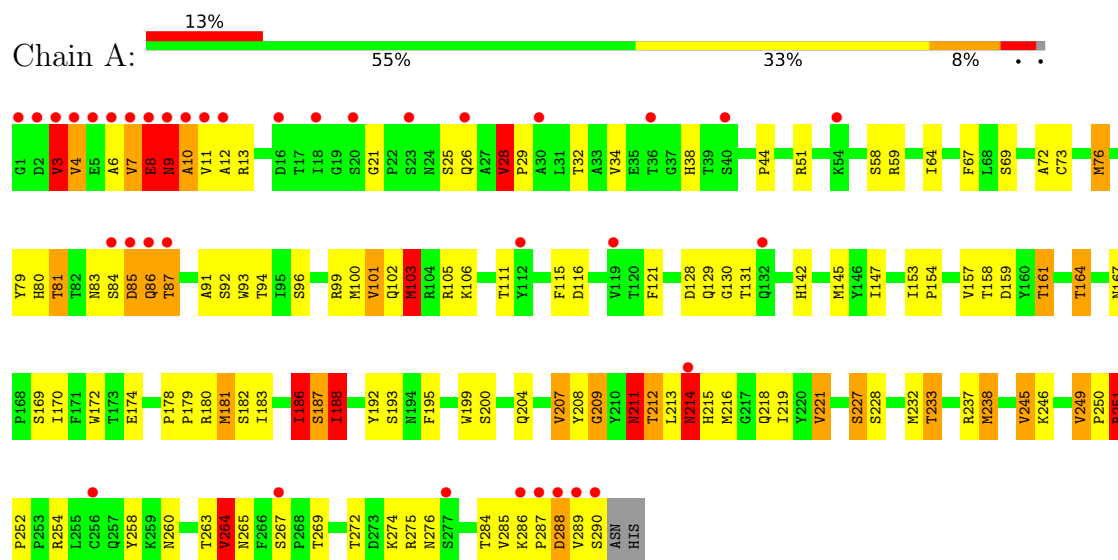
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	O	0	0
			2	2		
7	B	4	Total	O	0	0
			4	4		
7	C	5	Total	O	0	0
			5	5		

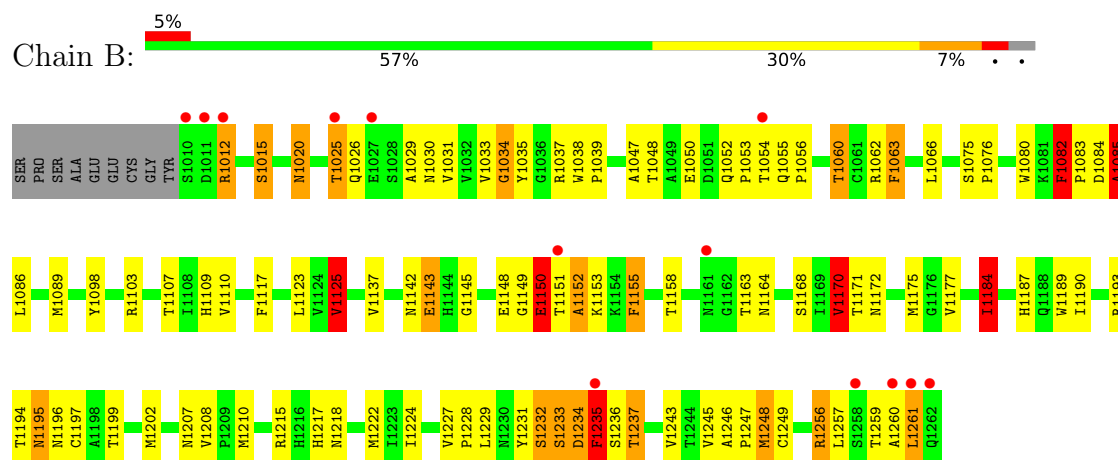
3 Residue-property plots [i](#)

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: ECHOVIRUS 11 COAT PROTEIN VP1

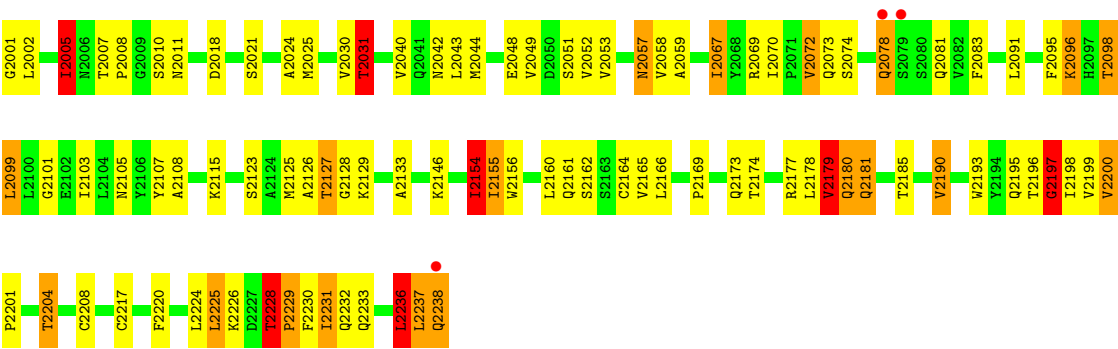


• Molecule 2: ECHOVIRUS 11 COAT PROTEIN VP2



• Molecule 3: ECHOVIRUS 11 COAT PROTEIN VP3





● Molecule 4: ECHOVIRUS 11 COAT PROTEIN VP4



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	300.85Å 300.85Å 1476.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.00 – 2.90 100.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	71.3 (100.00-2.90) 71.3 (100.00-2.90)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.86Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.246 , 0.255 0.247 , 0.244	Depositor DCC
R_{free} test set	2055 reflections (0.50%)	wwPDB-VP
Wilson B-factor (Å ²)	22.7	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.15	EDS
Total number of atoms	6575	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.04	8/2349 (0.3%)	1.35	25/3208 (0.8%)
2	B	0.98	4/2016 (0.2%)	1.52	38/2755 (1.4%)
3	C	0.93	3/1866 (0.2%)	1.38	29/2549 (1.1%)
4	D	1.19	4/475 (0.8%)	1.40	8/641 (1.2%)
All	All	1.01	19/6706 (0.3%)	1.41	100/9153 (1.1%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	MET	SD-CE	13.94	2.14	1.79
1	A	103	MET	SD-CE	8.13	1.99	1.79
1	A	3	VAL	CA-CB	7.91	1.65	1.54
2	B	1248	MET	SD-CE	-7.08	1.61	1.79
1	A	238	MET	SD-CE	-6.98	1.62	1.79
3	C	2067	ILE	CA-CB	6.23	1.62	1.54
1	A	7	VAL	CA-CB	6.22	1.62	1.54
3	C	2001	GLY	N-CA	5.98	1.55	1.45
4	D	3010	THR	CA-CB	-5.91	1.44	1.53
1	A	28	VAL	CA-CB	5.68	1.61	1.54
2	B	1085	ALA	N-CA	5.67	1.53	1.46
3	C	2197	GLY	CA-C	5.49	1.59	1.51
4	D	3013	HIS	N-CA	5.31	1.52	1.46
4	D	3054	THR	CA-CB	5.25	1.60	1.53
1	A	215	HIS	CA-C	-5.19	1.48	1.53
2	B	1015	SER	CA-C	5.12	1.58	1.52
4	D	3014	GLU	C-N	-5.09	1.26	1.33
1	A	8	GLU	CA-C	5.03	1.59	1.52
2	B	1261	LEU	C-N	-5.02	1.26	1.33

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1082	PHE	CA-C-N	-17.00	98.59	119.84
2	B	1082	PHE	C-N-CA	-17.00	98.59	119.84
1	A	101	VAL	N-CA-C	11.15	121.01	110.53
2	B	1082	PHE	N-CA-C	11.04	134.20	109.81
3	C	2070	ILE	CA-C-N	10.27	130.68	119.90
3	C	2070	ILE	C-N-CA	10.27	130.68	119.90
1	A	276	ASN	N-CA-C	9.52	121.25	111.07
4	D	3058	LYS	N-CA-C	-9.19	96.88	110.48
1	A	284	THR	N-CA-C	-8.87	96.01	109.94
2	B	1195	ASN	N-CA-CB	-8.81	95.12	111.52
3	C	2230	PHE	N-CA-C	8.75	123.51	113.01
3	C	2073	GLN	N-CA-C	8.46	121.56	108.96
1	A	251	ARG	CA-C-N	-8.40	113.53	119.66
1	A	251	ARG	C-N-CA	-8.40	113.53	119.66
2	B	1168	SER	N-CA-C	8.33	123.58	112.25
3	C	2197	GLY	N-CA-C	8.28	132.79	113.18
2	B	1012	ARG	N-CA-C	-8.26	101.53	111.69
1	A	211	ASN	N-CA-C	7.82	119.81	111.28
2	B	1055	GLN	CA-C-N	7.67	128.36	119.47
2	B	1055	GLN	C-N-CA	7.67	128.36	119.47
1	A	245	VAL	N-CA-C	7.62	121.16	109.12
3	C	2181	GLN	N-CA-C	7.52	120.85	110.24
2	B	1029	ALA	N-CA-C	-7.34	95.17	110.80
2	B	1232	SER	N-CA-C	7.29	119.05	108.34
3	C	2005	ILE	CB-CA-C	-7.27	99.72	110.33
4	D	3012	ALA	N-CA-C	7.22	126.18	110.80
3	C	2091	LEU	N-CA-C	7.05	122.31	112.93
3	C	2228	THR	CB-CA-C	-7.05	98.53	109.11
4	D	3066	PRO	N-CA-C	6.97	124.13	113.75
1	A	186	ILE	N-CA-C	6.95	119.71	112.83
1	A	153	ILE	N-CA-C	6.90	116.19	108.05
2	B	1224	ILE	CA-C-N	-6.66	112.91	119.90
2	B	1224	ILE	C-N-CA	-6.66	112.91	119.90
3	C	2096	LYS	N-CA-C	6.63	120.23	111.75
2	B	1143	GLU	N-CA-C	-6.53	104.25	111.82
2	B	1086	LEU	N-CA-C	-6.51	103.84	113.61
1	A	21	GLY	CA-C-N	6.51	126.43	119.85
1	A	21	GLY	C-N-CA	6.51	126.43	119.85
3	C	2078	GLN	N-CA-C	6.50	118.92	111.11
3	C	2155	ILE	N-CA-C	-6.45	98.45	107.80
2	B	1125	VAL	CB-CA-C	-6.42	100.42	110.69
4	D	3064	SER	N-CA-C	-6.32	97.33	110.80
4	D	3003	ALA	N-CA-C	6.31	119.79	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1137	VAL	N-CA-C	6.22	119.76	111.17
3	C	2154	ILE	CB-CA-C	-6.22	100.74	110.69
1	A	28	VAL	CA-C-N	6.19	126.09	119.28
1	A	28	VAL	C-N-CA	6.19	126.09	119.28
2	B	1035	TYR	N-CA-C	-6.07	97.86	110.80
2	B	1054	THR	N-CA-C	-6.03	99.88	109.59
2	B	1029	ALA	CA-C-N	-6.02	116.69	123.13
2	B	1029	ALA	C-N-CA	-6.02	116.69	123.13
2	B	1150	GLU	N-CA-C	-6.00	98.02	110.80
2	B	1037	ARG	N-CA-C	5.86	117.95	108.41
1	A	115	PHE	N-CA-C	5.84	117.36	108.07
2	B	1170	VAL	CB-CA-C	-5.84	101.71	111.29
3	C	2069	ARG	N-CA-C	5.80	118.19	108.73
3	C	2228	THR	CA-C-N	5.80	125.34	119.19
3	C	2228	THR	C-N-CA	5.80	125.34	119.19
2	B	1232	SER	O-C-N	-5.78	117.81	122.03
2	B	1155	PHE	N-CA-C	-5.75	103.11	110.53
1	A	187	SER	N-CA-C	5.70	118.53	110.50
1	A	209	GLY	N-CA-C	5.67	123.02	112.77
2	B	1063	PHE	N-CA-C	5.66	117.92	109.25
2	B	1184	ILE	CB-CA-C	-5.66	102.01	111.29
3	C	2053	VAL	N-CA-C	5.64	113.48	108.63
1	A	227	SER	N-CA-C	5.63	122.80	110.80
2	B	1050	GLU	N-CA-C	5.62	120.19	113.23
4	D	3063	LYS	CA-C-N	5.61	132.25	121.54
4	D	3063	LYS	C-N-CA	5.61	132.25	121.54
1	A	264	VAL	N-CA-C	-5.55	107.33	112.83
3	C	2128	GLY	N-CA-C	5.54	118.52	111.37
2	B	1208	VAL	N-CA-C	-5.54	104.65	109.19
3	C	2195	GLN	N-CA-C	-5.50	106.41	113.23
2	B	1107	THR	N-CA-C	-5.40	99.72	108.52
3	C	2204	THR	CA-C-N	5.40	125.32	119.76
3	C	2204	THR	C-N-CA	5.40	125.32	119.76
4	D	3013	HIS	N-CA-C	5.40	116.61	108.46
1	A	116	ASP	N-CA-C	-5.37	102.57	110.52
2	B	1026	GLN	N-CA-C	-5.35	106.76	113.72
1	A	188	ILE	N-CA-C	-5.35	104.27	111.44
1	A	51	ARG	N-CA-C	-5.32	102.11	110.36
3	C	2052	VAL	N-CA-C	5.32	115.91	108.89
2	B	1047	ALA	N-CA-C	5.31	118.77	110.32
3	C	2229	PRO	N-CA-C	-5.28	106.65	113.57
1	A	192	TYR	N-CA-C	-5.28	102.47	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1215	ARG	CG-CD-NE	5.28	123.61	112.00
3	C	2232	GLN	N-CA-C	5.24	115.45	108.38
1	A	25	SER	N-CA-C	5.22	114.93	108.19
2	B	1227	VAL	N-CA-C	-5.21	99.47	107.71
3	C	2165	VAL	N-CA-C	5.21	115.36	107.80
2	B	1228	PRO	N-CA-C	5.19	119.64	111.38
2	B	1237	THR	N-CA-C	-5.18	107.33	113.97
3	C	2237	LEU	N-CA-C	-5.15	99.83	110.80
2	B	1098	TYR	N-CA-C	5.14	119.41	113.18
1	A	85	ASP	N-CA-C	5.12	119.38	113.18
2	B	1125	VAL	N-CA-C	5.06	117.11	108.86
3	C	2179	VAL	N-CA-C	-5.05	104.78	111.09
1	A	9	ASN	N-CA-C	5.00	121.46	110.80
3	C	2031	THR	CA-C-N	5.00	125.00	119.90
3	C	2031	THR	C-N-CA	5.00	125.00	119.90

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	A	2284	0	2212	160	0
2	B	1964	0	1874	72	0
3	C	1819	0	1772	118	0
4	D	467	0	447	49	0
5	A	15	0	18	2	0
6	D	15	0	27	1	0
7	A	2	0	0	1	0
7	B	4	0	0	0	0
7	C	5	0	0	0	0
All	All	6575	0	6350	327	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 25.

All (327) 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:A:76:MET:SD	1:A:76:MET:CE	2.14	1.34
1:A:260:ASN:OD1	1:A:263:THR:HG22	1.49	1.09
3:C:2098:THR:HG22	3:C:2101:GLY:H	1.20	1.04
3:C:2233:GLN:NE2	3:C:2238:GLN:HG2	1.73	1.04
4:D:3054:THR:O	4:D:3055:GLU:HB2	1.51	1.04
1:A:101:VAL:HB	3:C:2238:GLN:OE1	1.60	1.01
2:B:1234:ASP:O	2:B:1236:SER:N	1.92	1.01
3:C:2196:THR:HG23	3:C:2196:THR:O	1.58	0.99
2:B:1025:THR:HG21	2:B:1197:CYS:SG	2.03	0.98
3:C:2233:GLN:CD	3:C:2238:GLN:HE21	1.74	0.95
1:A:101:VAL:HB	3:C:2238:GLN:CD	1.92	0.94
1:A:275:ARG:HE	3:C:2057:ASN:HD21	1.08	0.93
3:C:2233:GLN:HE22	3:C:2238:GLN:HG2	1.34	0.92
2:B:1082:PHE:O	2:B:1083:PRO:C	2.01	0.91
1:A:38:HIS:HD2	4:D:3055:GLU:HG3	1.39	0.85
2:B:1030:ASN:HD21	4:D:3059:ASP:HB2	1.42	0.84
3:C:2129:LYS:HB2	3:C:2196:THR:HG22	1.59	0.84
1:A:252:PRO:HD3	2:B:1184:ILE:HD11	1.57	0.84
3:C:2154:ILE:HD11	3:C:2166:LEU:HA	1.59	0.84
3:C:2233:GLN:HB3	3:C:2238:GLN:NE2	1.93	0.83
1:A:159:ASP:OD1	1:A:161:THR:HB	1.78	0.83
1:A:128:ASP:OD2	1:A:233:THR:HG22	1.77	0.83
1:A:219:ILE:CD1	1:A:238:MET:HE1	2.08	0.83
4:D:3002:GLY:N	6:D:3500:MYR:O1	2.13	0.82
1:A:101:VAL:HB	3:C:2238:GLN:NE2	1.95	0.81
4:D:3047:THR:HG22	4:D:3048:GLN:H	1.44	0.80
1:A:6:ALA:O	1:A:7:VAL:HG23	1.82	0.80
1:A:59:ARG:NH1	4:D:3048:GLN:HE22	1.79	0.80
3:C:2057:ASN:H	3:C:2057:ASN:HD22	1.27	0.79
1:A:83:ASN:ND2	1:A:84:SER:H	1.80	0.79
3:C:2042:ASN:HD22	3:C:2044:MET:H	1.28	0.79
3:C:2196:THR:O	3:C:2196:THR:CG2	2.29	0.79
4:D:3054:THR:O	4:D:3055:GLU:CB	2.31	0.79
2:B:1233:SER:O	2:B:1235:PHE:CD2	2.36	0.79
2:B:1193:ARG:HG3	2:B:1194:THR:HG23	1.63	0.78
3:C:2095:PHE:O	3:C:2098:THR:HB	1.82	0.78
3:C:2228:THR:HG22	3:C:2229:PRO:HD2	1.65	0.78
1:A:81:THR:HG21	1:A:232:MET:HB2	1.64	0.78
1:A:4:VAL:CG1	4:D:3036:ALA:HB1	2.14	0.78
1:A:99:ARG:C	3:C:2238:GLN:HB2	2.10	0.77
1:A:38:HIS:CD2	4:D:3055:GLU:HG3	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2057:ASN:HA	3:C:2067:ILE:HG13	1.67	0.76
2:B:1175:MET:HE2	2:B:1222:MET:HE1	1.65	0.76
1:A:186:ILE:HD11	3:C:2025:MET:HE1	1.66	0.75
1:A:128:ASP:OD2	1:A:233:THR:CG2	2.36	0.74
1:A:164:THR:HG21	1:A:169:SER:OG	1.87	0.74
4:D:3058:LYS:O	4:D:3059:ASP:HB2	1.86	0.74
2:B:1117:PHE:CD2	3:C:2204:THR:HG22	2.22	0.74
1:A:32:THR:HB	4:D:3063:LYS:HE3	1.70	0.74
2:B:1190:ILE:HA	2:B:1195:ASN:ND2	2.05	0.72
3:C:2057:ASN:HD22	3:C:2057:ASN:N	1.87	0.72
1:A:32:THR:HA	4:D:3063:LYS:HE2	1.71	0.72
1:A:3:VAL:HG23	1:A:3:VAL:O	1.90	0.70
1:A:269:THR:H	2:B:1172:ASN:HD21	1.39	0.70
1:A:81:THR:HG22	1:A:232:MET:O	1.92	0.70
1:A:101:VAL:CG1	3:C:2238:GLN:NE2	2.55	0.69
1:A:121:PHE:CE1	1:A:238:MET:HE3	2.27	0.69
2:B:1142:ASN:HB3	2:B:1145:GLY:H	1.55	0.69
1:A:209:GLY:O	1:A:212:THR:HG23	1.91	0.69
3:C:2173:GLN:HG2	3:C:2174:THR:HG23	1.74	0.69
3:C:2005:ILE:HD12	3:C:2005:ILE:H	1.58	0.69
3:C:2107:TYR:O	3:C:2226:LYS:HE3	1.92	0.69
3:C:2072:VAL:HG13	3:C:2198:ILE:CD1	2.23	0.68
4:D:3007:THR:HA	4:D:3026:HIS:HB3	1.73	0.68
3:C:2233:GLN:HB3	3:C:2238:GLN:HE21	1.57	0.68
1:A:99:ARG:O	3:C:2238:GLN:HB2	1.93	0.68
2:B:1151:THR:O	2:B:1152:ALA:HB2	1.93	0.68
1:A:4:VAL:HG12	4:D:3036:ALA:HB1	1.75	0.67
3:C:2236:LEU:C	3:C:2238:GLN:N	2.48	0.67
1:A:85:ASP:O	1:A:87:THR:N	2.25	0.67
4:D:3003:ALA:HB2	4:D:3030:ILE:HG12	1.77	0.67
1:A:6:ALA:HB1	4:D:3040:SER:OG	1.94	0.66
1:A:105:ARG:HD3	3:C:2231:ILE:HG12	1.76	0.66
2:B:1194:THR:HG21	3:C:2162:SER:HB3	1.78	0.66
1:A:100:MET:CA	3:C:2238:GLN:HG3	2.26	0.66
1:A:101:VAL:CB	3:C:2238:GLN:OE1	2.43	0.66
3:C:2180:GLN:O	3:C:2180:GLN:HG3	1.94	0.66
1:A:286:LYS:C	1:A:288:ASP:H	2.04	0.65
1:A:263:THR:HG23	1:A:265:ASN:H	1.61	0.65
3:C:2098:THR:HG22	3:C:2101:GLY:N	2.04	0.65
1:A:101:VAL:CB	3:C:2238:GLN:NE2	2.60	0.64
2:B:1084:ASP:O	2:B:1085:ALA:CB	2.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ALA:HB2	4:D:3046:PHE:HB3	1.80	0.64
3:C:2129:LYS:HB2	3:C:2196:THR:CG2	2.28	0.64
3:C:2200:VAL:HG22	3:C:2201:PRO:HD2	1.79	0.64
4:D:3055:GLU:H	4:D:3056:PRO:CD	2.11	0.64
1:A:286:LYS:HD2	1:A:289:VAL:HB	1.80	0.63
4:D:3066:PRO:O	4:D:3067:ALA:HB3	1.98	0.63
1:A:80:HIS:CD2	1:A:233:THR:HB	2.32	0.63
2:B:1184:ILE:HD12	2:B:1184:ILE:N	2.14	0.63
1:A:101:VAL:CG1	3:C:2238:GLN:HE22	2.10	0.63
1:A:181:MET:HE2	3:C:2024:ALA:HB2	1.79	0.63
1:A:145:MET:SD	1:A:164:THR:HG23	2.39	0.63
1:A:72:ALA:CB	1:A:103:MET:HG2	2.29	0.62
3:C:2044:MET:HE1	3:C:2220:PHE:CD1	2.34	0.62
1:A:81:THR:CG2	1:A:232:MET:H	2.12	0.62
2:B:1117:PHE:HD2	3:C:2204:THR:HG22	1.63	0.62
3:C:2072:VAL:HG13	3:C:2198:ILE:HD12	1.80	0.62
1:A:101:VAL:HG12	3:C:2238:GLN:NE2	2.15	0.62
1:A:101:VAL:HB	3:C:2238:GLN:HE22	1.65	0.62
4:D:3006:SER:O	4:D:3026:HIS:HB2	2.00	0.62
3:C:2228:THR:HG22	3:C:2229:PRO:CD	2.29	0.62
1:A:164:THR:HG22	1:A:167:ASN:HB2	1.82	0.62
3:C:2233:GLN:CD	3:C:2238:GLN:NE2	2.54	0.62
1:A:207:VAL:HG22	1:A:212:THR:HG22	1.82	0.61
1:A:219:ILE:HD12	1:A:238:MET:HE1	1.82	0.61
2:B:1056:PRO:HB2	2:B:1060:THR:HB	1.82	0.61
3:C:2018:ASP:OD2	4:D:3043:ARG:HD2	2.01	0.61
1:A:200:SER:HB3	1:A:207:VAL:HG13	1.83	0.61
4:D:3047:THR:HG22	4:D:3048:GLN:N	2.15	0.61
1:A:101:VAL:CB	3:C:2238:GLN:CD	2.71	0.60
1:A:105:ARG:HD3	3:C:2231:ILE:CG1	2.31	0.60
1:A:13:ARG:HH11	1:A:13:ARG:HG3	1.66	0.60
2:B:1151:THR:O	2:B:1152:ALA:CB	2.48	0.60
2:B:1184:ILE:HD12	2:B:1184:ILE:H	1.66	0.60
1:A:72:ALA:HB3	1:A:103:MET:HG2	1.83	0.59
3:C:2233:GLN:CB	3:C:2238:GLN:HE21	2.15	0.59
2:B:1020:ASN:HD21	2:B:1062:ARG:HH21	1.51	0.59
1:A:100:MET:HA	3:C:2238:GLN:HG3	1.82	0.59
1:A:180:ARG:C	1:A:181:MET:HG3	2.28	0.59
1:A:81:THR:HG21	1:A:232:MET:CB	2.32	0.59
1:A:81:THR:CG2	1:A:232:MET:HB2	2.31	0.58
2:B:1151:THR:OG1	2:B:1152:ALA:N	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2042:ASN:ND2	3:C:2044:MET:H	1.99	0.58
4:D:3055:GLU:H	4:D:3056:PRO:HD3	1.67	0.58
3:C:2057:ASN:H	3:C:2057:ASN:ND2	2.00	0.58
1:A:195:PHE:CE1	1:A:251:ARG:HD2	2.39	0.58
1:A:3:VAL:HG21	1:A:246:LYS:HG3	1.86	0.57
1:A:59:ARG:NH1	4:D:3048:GLN:NE2	2.50	0.57
1:A:85:ASP:O	1:A:85:ASP:OD1	2.22	0.57
3:C:2236:LEU:C	3:C:2238:GLN:H	2.11	0.57
1:A:252:PRO:HG2	2:B:1177:VAL:HG11	1.86	0.57
1:A:12:ALA:HB2	4:D:3046:PHE:CB	2.35	0.56
1:A:9:ASN:O	1:A:10:ALA:HB3	2.04	0.56
3:C:2233:GLN:CG	3:C:2238:GLN:HE21	2.18	0.56
1:A:44:PRO:HB3	3:C:2169:PRO:HB3	1.87	0.56
3:C:2107:TYR:CE2	3:C:2225:LEU:HD13	2.40	0.56
3:C:2049:VAL:HA	4:D:3054:THR:HG22	1.87	0.56
1:A:99:ARG:HA	3:C:2238:GLN:HB2	1.87	0.55
1:A:249:VAL:O	1:A:249:VAL:HG22	2.05	0.55
2:B:1012:ARG:HG3	2:B:1012:ARG:HH11	1.71	0.55
1:A:59:ARG:HH11	4:D:3048:GLN:NE2	2.05	0.55
1:A:272:THR:HG22	3:C:2067:ILE:HD11	1.88	0.55
4:D:3066:PRO:O	4:D:3067:ALA:CB	2.54	0.55
1:A:32:THR:CB	4:D:3063:LYS:HE3	2.37	0.54
2:B:1063:PHE:CD1	2:B:1246:ALA:HB2	2.41	0.54
2:B:1193:ARG:NH1	3:C:2123:SER:O	2.40	0.54
3:C:2154:ILE:HD11	3:C:2166:LEU:CA	2.35	0.54
3:C:2233:GLN:CD	3:C:2238:GLN:HG2	2.32	0.54
1:A:245:VAL:HG12	1:A:246:LYS:N	2.23	0.54
1:A:289:VAL:CG1	1:A:290:SER:N	2.70	0.54
1:A:99:ARG:O	3:C:2238:GLN:CG	2.56	0.54
1:A:83:ASN:ND2	1:A:84:SER:N	2.54	0.53
1:A:7:VAL:HG22	4:D:3027:TYR:OH	2.08	0.53
2:B:1033:VAL:O	2:B:1034:GLY:C	2.51	0.53
4:D:3062:VAL:HB	4:D:3065:LEU:HD13	1.91	0.53
2:B:1234:ASP:C	2:B:1236:SER:N	2.66	0.53
1:A:13:ARG:HG3	1:A:13:ARG:NH1	2.24	0.53
3:C:2107:TYR:O	3:C:2179:VAL:HG11	2.09	0.53
1:A:59:ARG:HH11	4:D:3048:GLN:HE22	1.55	0.52
1:A:275:ARG:HE	3:C:2057:ASN:ND2	1.92	0.52
1:A:93:TRP:O	1:A:218:GLN:HB2	2.08	0.52
2:B:1084:ASP:O	2:B:1085:ALA:HB2	2.09	0.52
2:B:1233:SER:O	2:B:1235:PHE:HD2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2180:GLN:O	3:C:2180:GLN:CG	2.57	0.52
1:A:28:VAL:HG13	1:A:28:VAL:O	2.10	0.52
2:B:1012:ARG:HG3	2:B:1012:ARG:NH1	2.24	0.52
3:C:2005:ILE:HD12	3:C:2005:ILE:N	2.25	0.52
2:B:1234:ASP:C	2:B:1236:SER:H	2.08	0.52
1:A:128:ASP:CG	1:A:233:THR:HG22	2.34	0.52
1:A:73:CYS:SG	1:A:100:MET:CE	2.98	0.52
1:A:79:TYR:OH	1:A:142:HIS:HD2	1.93	0.52
1:A:28:VAL:N	1:A:29:PRO:HD3	2.24	0.51
1:A:79:TYR:OH	1:A:142:HIS:CD2	2.63	0.51
1:A:99:ARG:O	3:C:2238:GLN:CB	2.57	0.51
1:A:183:ILE:HG12	5:A:1000:DOA:H31	1.92	0.51
3:C:2051:SER:HB3	3:C:2099:LEU:HD22	1.93	0.51
1:A:101:VAL:CB	3:C:2238:GLN:HE22	2.23	0.51
1:A:170:ILE:HD11	1:A:181:MET:HG2	1.92	0.51
4:D:3011:GLY:O	4:D:3013:HIS:N	2.41	0.51
1:A:99:ARG:CA	3:C:2238:GLN:HB2	2.41	0.50
1:A:129:GLN:NE2	1:A:130:GLY:H	2.10	0.50
2:B:1125:VAL:HG13	2:B:1187:HIS:HB3	1.93	0.50
1:A:81:THR:HG22	1:A:232:MET:C	2.37	0.50
1:A:99:ARG:HD3	3:C:2237:LEU:HA	1.92	0.50
1:A:172:TRP:CD1	1:A:179:PRO:HG3	2.47	0.50
1:A:64:ILE:HD12	3:C:2040:VAL:O	2.12	0.50
1:A:101:VAL:CG2	3:C:2231:ILE:HG13	2.42	0.50
1:A:286:LYS:O	1:A:288:ASP:N	2.44	0.50
1:A:250:PRO:HD3	3:C:2040:VAL:CG2	2.42	0.50
2:B:1232:SER:C	2:B:1234:ASP:H	2.19	0.50
1:A:111:THR:OG1	1:A:249:VAL:HG22	2.11	0.49
2:B:1148:GLU:OE2	2:B:1153:LYS:HE3	2.12	0.49
3:C:2044:MET:HE1	3:C:2220:PHE:HD1	1.77	0.49
1:A:157:VAL:HG23	1:A:158:THR:HG23	1.94	0.49
3:C:2133:ALA:O	3:C:2190:VAL:HA	2.13	0.49
1:A:154:PRO:HG3	1:A:161:THR:CG2	2.43	0.49
1:A:249:VAL:O	1:A:249:VAL:CG2	2.60	0.49
1:A:275:ARG:NE	3:C:2057:ASN:HD21	1.92	0.49
2:B:1052:GLN:HE21	2:B:1053:PRO:HD2	1.78	0.49
3:C:2173:GLN:HG2	3:C:2174:THR:N	2.28	0.49
4:D:3061:MET:HE3	4:D:3067:ALA:HB1	1.94	0.49
1:A:260:ASN:CG	1:A:263:THR:HG22	2.29	0.49
2:B:1080:TRP:CE2	2:B:1152:ALA:HB2	2.47	0.49
1:A:99:ARG:O	3:C:2238:GLN:HG3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1031:VAL:HB	4:D:3058:LYS:HG2	1.94	0.48
1:A:3:VAL:O	1:A:3:VAL:CG2	2.59	0.48
1:A:214:ASN:ND2	1:A:216:MET:HE2	2.29	0.48
2:B:1066:LEU:HD23	2:B:1089:MET:HE3	1.95	0.48
1:A:85:ASP:OD1	1:A:87:THR:HB	2.13	0.48
1:A:263:THR:HG21	1:A:265:ASN:HB2	1.96	0.48
3:C:2072:VAL:HG13	3:C:2198:ILE:HD11	1.94	0.48
2:B:1150:GLU:O	2:B:1151:THR:OG1	2.30	0.47
1:A:81:THR:HG23	1:A:232:MET:H	1.78	0.47
1:A:101:VAL:N	3:C:2238:GLN:CD	2.72	0.47
1:A:101:VAL:HG21	3:C:2231:ILE:HD12	1.94	0.47
1:A:264:VAL:HG23	7:A:2001:HOH:O	2.14	0.47
2:B:1062:ARG:HG3	2:B:1062:ARG:HH11	1.80	0.47
2:B:1020:ASN:HD21	2:B:1062:ARG:HE	1.62	0.47
2:B:1109:HIS:HD2	2:B:1199:THR:OG1	1.97	0.47
4:D:3010:THR:O	4:D:3010:THR:CG2	2.61	0.47
1:A:9:ASN:O	1:A:10:ALA:CB	2.63	0.47
2:B:1189:TRP:O	2:B:1195:ASN:ND2	2.47	0.47
3:C:2057:ASN:N	3:C:2057:ASN:ND2	2.59	0.47
1:A:172:TRP:CG	1:A:179:PRO:HG3	2.50	0.47
1:A:216:MET:HE1	5:A:1000:DOA:H101	1.96	0.46
1:A:274:LYS:HD2	3:C:2059:ALA:HB2	1.97	0.46
2:B:1103:ARG:HB2	2:B:1210:MET:HG2	1.96	0.46
3:C:2115:LYS:HG3	3:C:2217:CYS:SG	2.55	0.46
1:A:285:VAL:HG12	1:A:285:VAL:O	2.14	0.46
1:A:263:THR:HG23	1:A:265:ASN:N	2.30	0.46
2:B:1196:ASN:C	2:B:1196:ASN:OD1	2.59	0.46
3:C:2156:TRP:CD1	3:C:2164:CYS:HB2	2.50	0.46
1:A:103:MET:HE2	1:A:106:LYS:HE3	1.97	0.46
1:A:286:LYS:HD2	1:A:289:VAL:CB	2.45	0.46
3:C:2231:ILE:HD13	3:C:2231:ILE:HA	1.76	0.46
1:A:81:THR:CG2	1:A:232:MET:O	2.62	0.46
1:A:154:PRO:CA	1:A:161:THR:HG21	2.46	0.46
1:A:263:THR:CG2	1:A:265:ASN:HB2	2.46	0.46
1:A:101:VAL:O	1:A:102:GLN:C	2.59	0.46
3:C:2177:ARG:HG2	3:C:2185:THR:HB	1.98	0.46
2:B:1020:ASN:HD21	2:B:1062:ARG:NH2	2.14	0.46
2:B:1142:ASN:HB2	2:B:1164:ASN:HB3	1.98	0.45
3:C:2201:PRO:HG2	3:C:2204:THR:HG21	1.99	0.45
1:A:154:PRO:HG3	1:A:161:THR:HG21	1.99	0.45
1:A:267:SER:O	1:A:269:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ILE:HG21	1:A:188:ILE:HD13	1.62	0.45
3:C:2010:SER:O	3:C:2011:ASN:HB2	2.17	0.45
2:B:1020:ASN:C	2:B:1020:ASN:HD22	2.24	0.45
1:A:211:ASN:HD22	1:A:211:ASN:HA	1.53	0.45
3:C:2196:THR:O	3:C:2197:GLY:O	2.34	0.45
1:A:105:ARG:HG3	1:A:254:ARG:HB3	1.99	0.44
1:A:81:THR:CG2	1:A:232:MET:N	2.81	0.44
1:A:121:PHE:CZ	1:A:238:MET:CE	3.01	0.44
1:A:182:SER:C	1:A:183:ILE:HD12	2.43	0.44
1:A:252:PRO:HD3	2:B:1184:ILE:CD1	2.37	0.44
3:C:2083:PHE:C	3:C:2083:PHE:CD1	2.95	0.44
4:D:3063:LYS:CD	4:D:3067:ALA:HB2	2.48	0.44
1:A:99:ARG:C	3:C:2238:GLN:HG3	2.42	0.44
4:D:3068:LEU:O	4:D:3069:ASN:HB2	2.17	0.44
2:B:1202:MET:HE3	2:B:1202:MET:HB3	1.89	0.44
1:A:286:LYS:C	1:A:288:ASP:N	2.74	0.44
3:C:2129:LYS:CB	3:C:2196:THR:HG22	2.40	0.44
3:C:2044:MET:O	3:C:2048:GLU:HG3	2.18	0.43
1:A:193:SER:HB2	2:B:1207:ASN:ND2	2.33	0.43
2:B:1083:PRO:HD2	2:B:1217:HIS:HA	2.01	0.43
2:B:1193:ARG:HG3	2:B:1194:THR:CG2	2.42	0.43
3:C:2072:VAL:CG1	3:C:2198:ILE:HD11	2.49	0.43
1:A:92:SER:HA	1:A:219:ILE:O	2.17	0.43
1:A:187:SER:O	3:C:2031:THR:HG21	2.19	0.43
2:B:1248:MET:O	2:B:1249:CYS:HB2	2.18	0.43
1:A:93:TRP:O	1:A:218:GLN:CB	2.67	0.43
3:C:2007:THR:O	3:C:2008:PRO:C	2.62	0.43
3:C:2146:LYS:HE2	3:C:2146:LYS:HB2	1.68	0.43
3:C:2160:LEU:HD21	4:D:3069:ASN:H	1.82	0.43
4:D:3067:ALA:O	4:D:3068:LEU:HD23	2.18	0.43
3:C:2074:SER:HA	3:C:2198:ILE:O	2.19	0.43
1:A:199:TRP:CZ3	1:A:208:TYR:HB2	2.54	0.42
1:A:219:ILE:HD11	1:A:238:MET:HE1	1.98	0.42
2:B:1020:ASN:C	2:B:1020:ASN:ND2	2.77	0.42
2:B:1190:ILE:HA	2:B:1195:ASN:HD21	1.81	0.42
4:D:3010:THR:O	4:D:3010:THR:HG22	2.18	0.42
4:D:3061:MET:HE2	4:D:3063:LYS:HD3	2.00	0.42
1:A:245:VAL:CG1	1:A:246:LYS:N	2.82	0.42
2:B:1184:ILE:H	2:B:1184:ILE:CD1	2.28	0.42
1:A:12:ALA:O	1:A:58:SER:HA	2.19	0.42
3:C:2201:PRO:HG2	3:C:2204:THR:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ALA:HB3	1:A:221:VAL:HG13	2.01	0.42
1:A:204:GLN:NE2	2:B:1143:GLU:HG2	2.34	0.42
1:A:121:PHE:CZ	1:A:238:MET:HE3	2.54	0.42
1:A:142:HIS:HE1	1:A:174:GLU:OE1	2.02	0.42
3:C:2125:MET:HE3	3:C:2125:MET:HB3	1.89	0.42
2:B:1259:THR:HG22	2:B:1260:ALA:N	2.35	0.42
2:B:1256:ARG:HD2	2:B:1257:LEU:O	2.18	0.42
3:C:2193:TRP:CD1	3:C:2193:TRP:N	2.87	0.42
1:A:67:PHE:CG	3:C:2043:LEU:HD11	2.55	0.41
1:A:213:LEU:HA	1:A:213:LEU:HD23	1.61	0.41
3:C:2127:THR:HG22	3:C:2199:VAL:HB	2.02	0.41
4:D:3047:THR:CG2	4:D:3048:GLN:H	2.24	0.41
2:B:1075:SER:HA	2:B:1076:PRO:HD3	1.89	0.41
2:B:1231:TYR:CE1	2:B:1237:THR:HG22	2.55	0.41
1:A:129:GLN:NE2	1:A:130:GLY:N	2.68	0.41
4:D:3014:GLU:OE2	4:D:3014:GLU:HA	2.20	0.41
2:B:1083:PRO:HD3	2:B:1218:ASN:H	1.86	0.41
2:B:1233:SER:O	2:B:1235:PHE:N	2.53	0.41
1:A:145:MET:HE3	1:A:147:ILE:HD11	2.03	0.41
2:B:1038:TRP:CD1	2:B:1039:PRO:HD2	2.55	0.41
2:B:1256:ARG:HD3	2:B:1257:LEU:HD23	2.03	0.41
3:C:2161:GLN:NE2	4:D:3066:PRO:HB3	2.35	0.41
2:B:1155:PHE:HB3	2:B:1170:VAL:HG13	2.02	0.41
4:D:3003:ALA:HB2	4:D:3030:ILE:CG1	2.47	0.41
1:A:101:VAL:HG21	3:C:2231:ILE:CD1	2.50	0.41
2:B:1123:LEU:HB2	2:B:1189:TRP:CZ3	2.56	0.41
3:C:2108:ALA:C	3:C:2179:VAL:HG13	2.46	0.41
3:C:2018:ASP:OD1	4:D:3040:SER:HB2	2.20	0.41
2:B:1149:GLY:C	2:B:1150:GLU:O	2.63	0.40
2:B:1246:ALA:HA	2:B:1247:PRO:HD3	1.95	0.40
4:D:3008:GLN:HG3	4:D:3026:HIS:HA	2.04	0.40
3:C:2105:ASN:HB3	3:C:2228:THR:HG23	2.02	0.40
1:A:178:PRO:HA	1:A:179:PRO:HD3	1.83	0.40
2:B:1110:VAL:HG22	2:B:1243:VAL:HG22	2.03	0.40
3:C:2081:GLN:HB2	3:C:2193:TRP:CZ3	2.56	0.40
3:C:2115:LYS:HB2	3:C:2115:LYS:HE3	1.75	0.40
1:A:101:VAL:HG23	1:A:258:TYR:CE2	2.56	0.40
4:D:3003:ALA:CB	4:D:3030:ILE:HG12	2.49	0.40
1:A:129:GLN:HE21	1:A:130:GLY:N	2.20	0.40
3:C:2126:ALA:HA	3:C:2200:VAL:HG23	2.03	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	A	288/292 (99%)	259 (90%)	20 (7%)	9 (3%)	3	14
2	B	251/262 (96%)	220 (88%)	23 (9%)	8 (3%)	3	13
3	C	236/238 (99%)	224 (95%)	10 (4%)	2 (1%)	16	44
4	D	57/68 (84%)	44 (77%)	9 (16%)	4 (7%)	1	2
All	All	832/860 (97%)	747 (90%)	62 (8%)	23 (3%)	4	15

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	9	ASN
1	A	214	ASN
1	A	228	SER
2	B	1152	ALA
2	B	1234	ASP
2	B	1235	PHE
2	B	1261	LEU
3	C	2197	GLY
4	D	3012	ALA
4	D	3055	GLU
4	D	3064	SER
1	A	227	SER
2	B	1034	GLY
2	B	1085	ALA
3	C	2236	LEU
4	D	3063	LYS
1	A	10	ALA
2	B	1150	GLU
1	A	86	GLN
2	B	1082	PHE
1	A	4	VAL
1	A	287	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	259/262 (99%)	229 (88%)	30 (12%)	5	18
2	B	217/225 (96%)	201 (93%)	16 (7%)	13	38
3	C	204/204 (100%)	175 (86%)	29 (14%)	3	11
4	D	51/56 (91%)	43 (84%)	8 (16%)	2	9
All	All	731/747 (98%)	648 (89%)	83 (11%)	5	18

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	8	GLU
1	A	11	VAL
1	A	26	GLN
1	A	28	VAL
1	A	34	VAL
1	A	69	SER
1	A	81	THR
1	A	86	GLN
1	A	87	THR
1	A	94	THR
1	A	96	SER
1	A	103	MET
1	A	131	THR
1	A	161	THR
1	A	164	THR
1	A	181	MET
1	A	186	ILE
1	A	188	ILE
1	A	207	VAL
1	A	211	ASN
1	A	212	THR
1	A	214	ASN
1	A	221	VAL

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Mol	Chain	Res	Type
1	A	233	THR
1	A	237	ARG
1	A	249	VAL
1	A	251	ARG
1	A	264	VAL
1	A	288	ASP
2	B	1015	SER
2	B	1020	ASN
2	B	1025	THR
2	B	1048	THR
2	B	1060	THR
2	B	1125	VAL
2	B	1158	THR
2	B	1163	THR
2	B	1170	VAL
2	B	1171	THR
2	B	1184	ILE
2	B	1229	LEU
2	B	1233	SER
2	B	1235	PHE
2	B	1245	VAL
2	B	1256	ARG
3	C	2002	LEU
3	C	2005	ILE
3	C	2021	SER
3	C	2030	VAL
3	C	2031	THR
3	C	2057	ASN
3	C	2058	VAL
3	C	2072	VAL
3	C	2078	GLN
3	C	2096	LYS
3	C	2098	THR
3	C	2099	LEU
3	C	2103	ILE
3	C	2127	THR
3	C	2154	ILE
3	C	2155	ILE
3	C	2178	LEU
3	C	2179	VAL
3	C	2180	GLN
3	C	2181	GLN

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Mol	Chain	Res	Type
3	C	2190	VAL
3	C	2200	VAL
3	C	2208	CYS
3	C	2224	LEU
3	C	2225	LEU
3	C	2228	THR
3	C	2231	ILE
3	C	2236	LEU
3	C	2238	GLN
4	D	3010	THR
4	D	3014	GLU
4	D	3025	ILE
4	D	3028	THR
4	D	3063	LYS
4	D	3066	PRO
4	D	3068	LEU
4	D	3069	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	80	HIS
1	A	86	GLN
1	A	129	GLN
1	A	142	HIS
1	A	190	ASN
1	A	201	HIS
1	A	204	GLN
1	A	211	ASN
1	A	214	ASN
2	B	1020	ASN
2	B	1030	ASN
2	B	1052	GLN
2	B	1109	HIS
2	B	1119	GLN
2	B	1172	ASN
2	B	1195	ASN
2	B	1253	ASN
3	C	2012	GLN
3	C	2035	ASN
3	C	2042	ASN

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Mol	Chain	Res	Type
3	C	2056	ASN
3	C	2057	ASN
3	C	2088	GLN
3	C	2105	ASN
3	C	2140	ASN
3	C	2189	ASN
3	C	2238	GLN
4	D	3029	ASN
4	D	3044	GLN
4	D	3048	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](#)

2 ligands are 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	$\# Z > 2$
6	MYR	D	3500	-	13,14,15	0.55	0	12,13,15	1.06	1 (8%)
5	DOA	A	1000	-	14,14,14	0.86	1 (7%)	14,14,14	1.50	4 (28%)

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	MYR	D	3500	-	-	3/12/12/13	-
5	DOA	A	1000	-	-	4/12/12/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1000	DOA	CA2-C	2.33	1.56	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1000	DOA	C5-C4-C3	-2.88	99.83	114.37
5	A	1000	DOA	C7-C6-C5	-2.57	101.36	114.37
6	D	3500	MYR	C7-C6-C5	-2.47	101.89	114.37
5	A	1000	DOA	C10-C9-C8	-2.29	102.80	114.37
5	A	1000	DOA	OXT-C-CA2	2.00	120.33	114.00

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	3500	MYR	C5-C6-C7-C8
5	A	1000	DOA	C7-C8-C9-C10
6	D	3500	MYR	C2-C3-C4-C5
5	A	1000	DOA	C9-C10-CA2-C
6	D	3500	MYR	C10-C11-C12-C13
5	A	1000	DOA	O-C-CA2-C10
5	A	1000	DOA	OXT-C-CA2-C10

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	3500	MYR	1	0
5	A	1000	DOA	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	290/292 (99%)	0.97	37 (12%) 7 6	1, 12, 71, 119	0
2	B	253/262 (96%)	0.53	13 (5%) 33 26	2, 9, 37, 85	0
3	C	238/238 (100%)	0.35	3 (1%) 75 67	1, 8, 29, 75	0
4	D	61/68 (89%)	2.33	27 (44%) 0 0	6, 40, 83, 106	0
All	All	842/860 (97%)	0.76	80 (9%) 14 11	1, 10, 60, 119	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	290	SER	11.5
1	A	1	GLY	11.4
4	D	3015	THR	11.0
4	D	3023	SER	10.9
1	A	289	VAL	9.9
1	A	5	GLU	9.7
1	A	2	ASP	9.2
1	A	3	VAL	8.0
4	D	3069	ASN	7.6
1	A	8	GLU	6.7
4	D	3068	LEU	6.5
1	A	10	ALA	6.4
1	A	288	ASP	5.4
1	A	4	VAL	5.4
4	D	3064	SER	5.4
4	D	3063	LYS	5.3
4	D	3013	HIS	5.2
4	D	3012	ALA	5.2
1	A	9	ASN	5.1
2	B	1262	GLN	5.0
4	D	3049	ASP	5.0

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Mol	Chain	Res	Type	RSRZ
4	D	3067	ALA	4.8
4	D	3047	THR	4.7
1	A	7	VAL	4.6
1	A	6	ALA	4.3
2	B	1010	SER	4.3
1	A	11	VAL	4.3
1	A	267	SER	4.2
1	A	85	ASP	4.0
4	D	3045	ASP	3.9
2	B	1261	LEU	3.9
1	A	23	SER	3.9
2	B	1011	ASP	3.8
2	B	1235	PHE	3.8
4	D	3024	ILE	3.7
4	D	3065	LEU	3.6
2	B	1161	ASN	3.6
1	A	40	SER	3.5
4	D	3014	GLU	3.4
4	D	3050	PRO	3.4
2	B	1151	THR	3.4
1	A	287	PRO	3.3
4	D	3046	PHE	3.3
4	D	3051	GLY	3.3
3	C	2079	SER	3.3
1	A	214	ASN	3.0
1	A	86	GLN	3.0
1	A	30	ALA	2.9
1	A	256	CYS	2.9
2	B	1260	ALA	2.8
1	A	84	SER	2.7
1	A	26	GLN	2.7
4	D	3062	VAL	2.7
1	A	54	LYS	2.7
4	D	3006	SER	2.5
1	A	87	THR	2.5
1	A	16	ASP	2.5
4	D	3054	THR	2.4
1	A	119	VAL	2.4
4	D	3048	GLN	2.4
2	B	1012	ARG	2.4
2	B	1258	SER	2.4
4	D	3056	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	12	ALA	2.3
1	A	286	LYS	2.3
4	D	3025	ILE	2.3
1	A	36	THR	2.3
4	D	3057	VAL	2.3
4	D	3066	PRO	2.3
3	C	2078	GLN	2.2
3	C	2238	GLN	2.2
1	A	20	SER	2.2
1	A	277	SER	2.2
2	B	1054	THR	2.1
1	A	132	GLN	2.1
4	D	3010	THR	2.1
2	B	1025	THR	2.1
1	A	112	TYR	2.0
1	A	18	ILE	2.0
2	B	1027	GLU	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	MYR	D	3500	15/16	0.85	0.28	24,51,73,75	0
5	DOA	A	1000	15/15	0.90	0.20	7,19,41,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.