



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:18 AM UTC

PDB ID : 3C9I / pdb_00003c9i
Title : Structure of P22 Tail-Needle GP26 Bound to Xenon Gas
Authors : Cingolani, G.; Olia, A.S.
Deposited on : 2008-02-15
Resolution : 1.95 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:

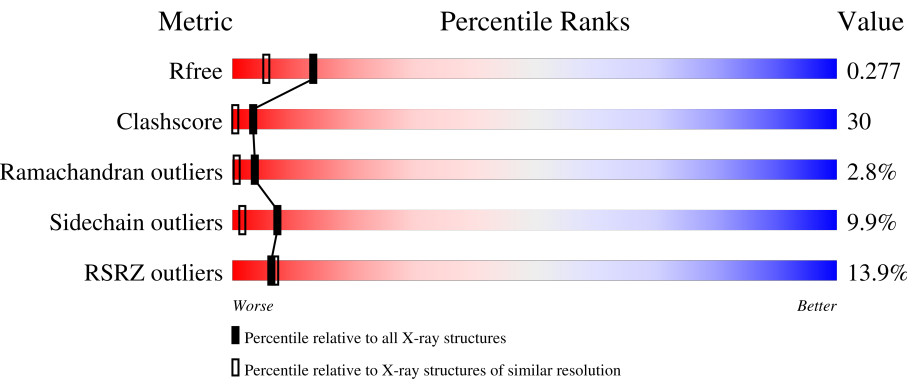
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	242	8% 62%26%7% . .
1	B	242	8% 67%28%5%
1	C	242	17% 54%31%8% . .
1	D	242	19% 45%35%10% . 9%
1	E	242	12% 55%31%7%7%

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Mol	Chain	Length	Quality of chain
1	F	242	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	XE	A	7	-	-	X	-
2	XE	D	11	-	-	X	-
2	XE	D	14	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11851 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 Tail needle protein gp26.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	0	0
			1738	1065	311	360	2			
1	B	242	Total	C	N	O	S	0	0	0
			1800	1103	325	370	2			
1	C	233	Total	C	N	O	S	0	0	0
			1735	1063	311	359	2			
1	D	221	Total	C	N	O	S	0	0	0
			1645	1009	297	337	2			
1	E	226	Total	C	N	O	S	0	0	0
			1681	1029	307	343	2			
1	F	221	Total	C	N	O	S	0	0	0
			1644	1005	298	339	2			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	992	GLY	-	expression tag	UNP P35837
A	993	ALA	-	expression tag	UNP P35837
A	994	LEU	-	expression tag	UNP P35837
A	995	VAL	-	expression tag	UNP P35837
A	996	PRO	-	expression tag	UNP P35837
A	997	ARG	-	expression tag	UNP P35837
A	998	GLY	-	expression tag	UNP P35837
A	999	SER	-	expression tag	UNP P35837
A	1000	HIS	-	expression tag	UNP P35837
A	1169	VAL	LEU	engineered mutation	UNP P35837
A	1222	MET	LEU	engineered mutation	UNP P35837
B	992	GLY	-	expression tag	UNP P35837
B	993	ALA	-	expression tag	UNP P35837
B	994	LEU	-	expression tag	UNP P35837
B	995	VAL	-	expression tag	UNP P35837
B	996	PRO	-	expression tag	UNP P35837
B	997	ARG	-	expression tag	UNP P35837

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Chain	Residue	Modelled	Actual	Comment	Reference
B	998	GLY	-	expression tag	UNP P35837
B	999	SER	-	expression tag	UNP P35837
B	1000	HIS	-	expression tag	UNP P35837
B	1169	VAL	LEU	engineered mutation	UNP P35837
B	1222	MET	LEU	engineered mutation	UNP P35837
C	992	GLY	-	expression tag	UNP P35837
C	993	ALA	-	expression tag	UNP P35837
C	994	LEU	-	expression tag	UNP P35837
C	995	VAL	-	expression tag	UNP P35837
C	996	PRO	-	expression tag	UNP P35837
C	997	ARG	-	expression tag	UNP P35837
C	998	GLY	-	expression tag	UNP P35837
C	999	SER	-	expression tag	UNP P35837
C	1000	HIS	-	expression tag	UNP P35837
C	1169	VAL	LEU	engineered mutation	UNP P35837
C	1222	MET	LEU	engineered mutation	UNP P35837
D	992	GLY	-	expression tag	UNP P35837
D	993	ALA	-	expression tag	UNP P35837
D	994	LEU	-	expression tag	UNP P35837
D	995	VAL	-	expression tag	UNP P35837
D	996	PRO	-	expression tag	UNP P35837
D	997	ARG	-	expression tag	UNP P35837
D	998	GLY	-	expression tag	UNP P35837
D	999	SER	-	expression tag	UNP P35837
D	1000	HIS	-	expression tag	UNP P35837
D	1169	VAL	LEU	engineered mutation	UNP P35837
D	1222	MET	LEU	engineered mutation	UNP P35837
E	992	GLY	-	expression tag	UNP P35837
E	993	ALA	-	expression tag	UNP P35837
E	994	LEU	-	expression tag	UNP P35837
E	995	VAL	-	expression tag	UNP P35837
E	996	PRO	-	expression tag	UNP P35837
E	997	ARG	-	expression tag	UNP P35837
E	998	GLY	-	expression tag	UNP P35837
E	999	SER	-	expression tag	UNP P35837
E	1000	HIS	-	expression tag	UNP P35837
E	1169	VAL	LEU	engineered mutation	UNP P35837
E	1222	MET	LEU	engineered mutation	UNP P35837
F	992	GLY	-	expression tag	UNP P35837
F	993	ALA	-	expression tag	UNP P35837
F	994	LEU	-	expression tag	UNP P35837
F	995	VAL	-	expression tag	UNP P35837

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Chain	Residue	Modelled	Actual	Comment	Reference
F	996	PRO	-	expression tag	UNP P35837
F	997	ARG	-	expression tag	UNP P35837
F	998	GLY	-	expression tag	UNP P35837
F	999	SER	-	expression tag	UNP P35837
F	1000	HIS	-	expression tag	UNP P35837
F	1169	VAL	LEU	engineered mutation	UNP P35837
F	1222	MET	LEU	engineered mutation	UNP P35837

- Molecule 2 is XENON (CCD ID: XE) (formula: Xe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	6	Total Xe 6 6	0	0
2	C	1	Total Xe 1 1	0	0
2	D	6	Total Xe 6 6	0	0
2	F	1	Total Xe 1 1	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0

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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	266	Total O 266 266	0	0

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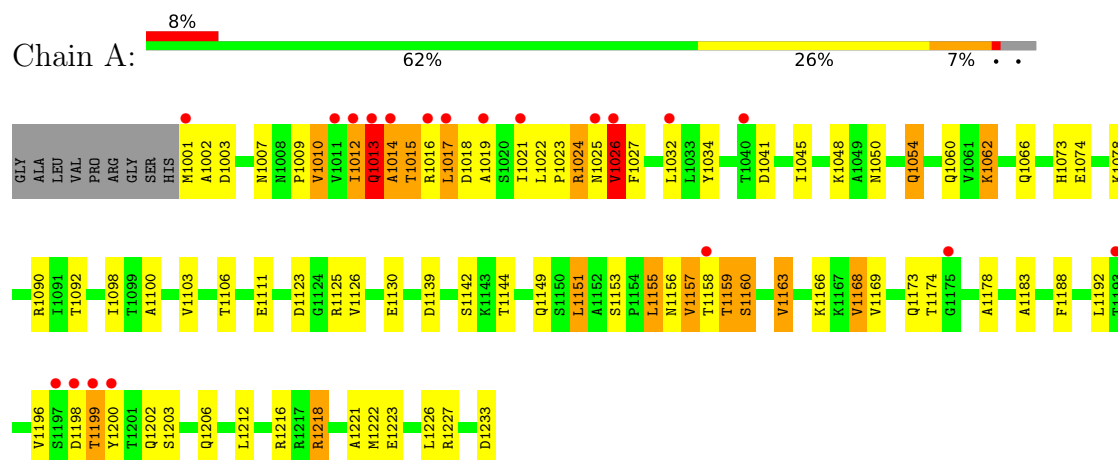
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	272	Total 272	O 272	0	0
5	C	277	Total 277	O 277	0	0
5	D	211	Total 211	O 211	0	0
5	E	275	Total 275	O 275	0	0
5	F	289	Total 289	O 289	0	0

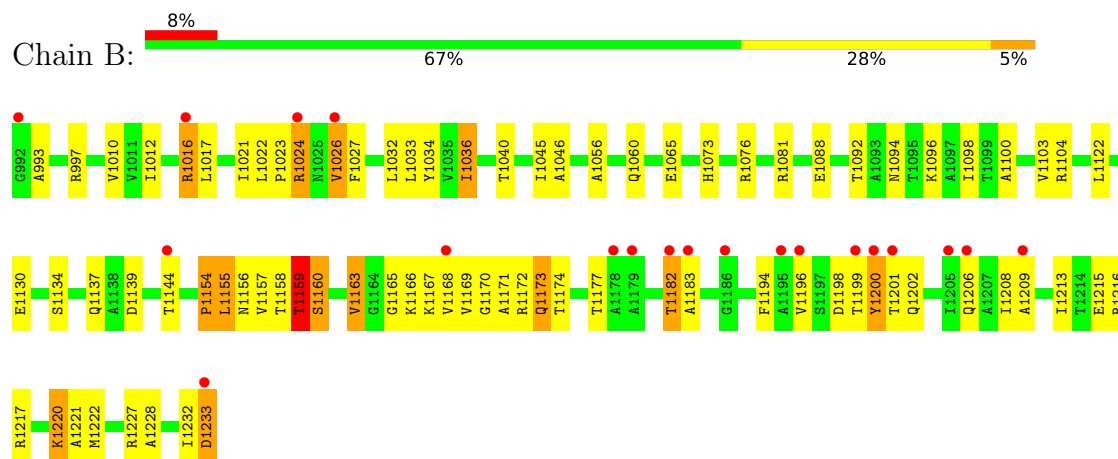
3 Residue-property plots

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 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.

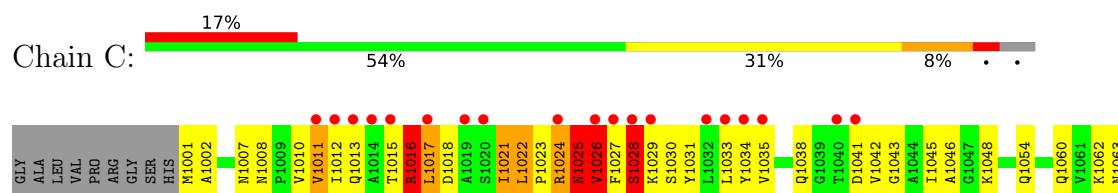
• Molecule 1: Tail needle protein gp26

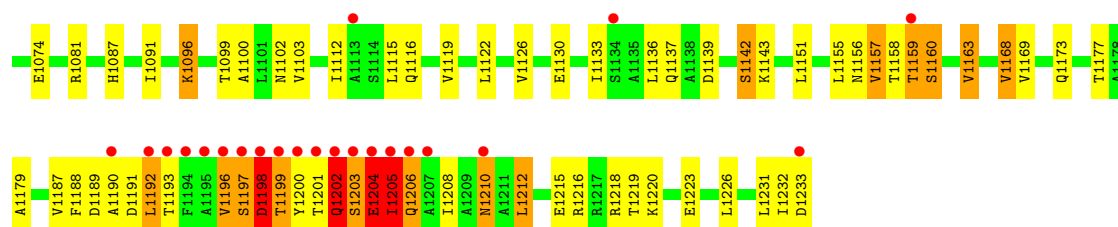


• Molecule 1: Tail needle protein gp26

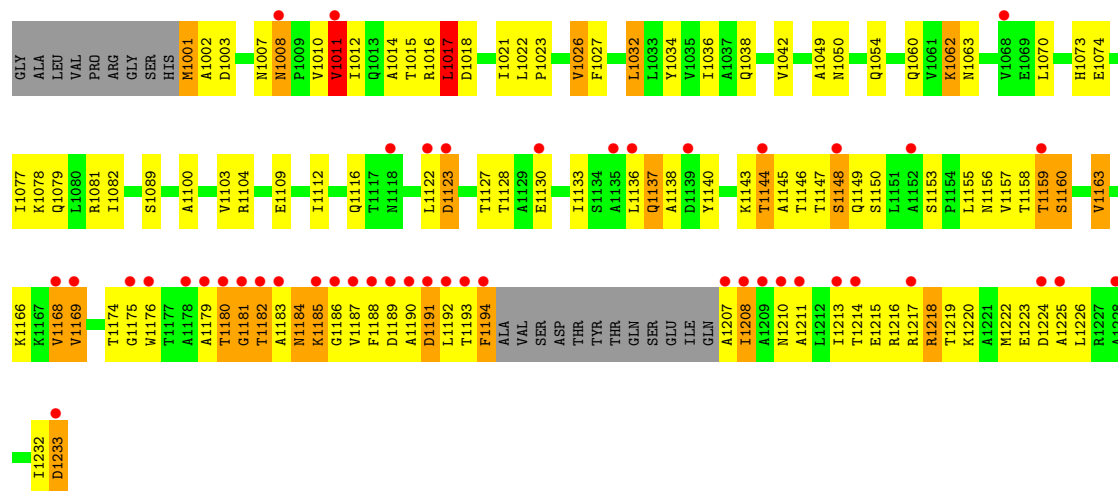


• Molecule 1: Tail needle protein gp26

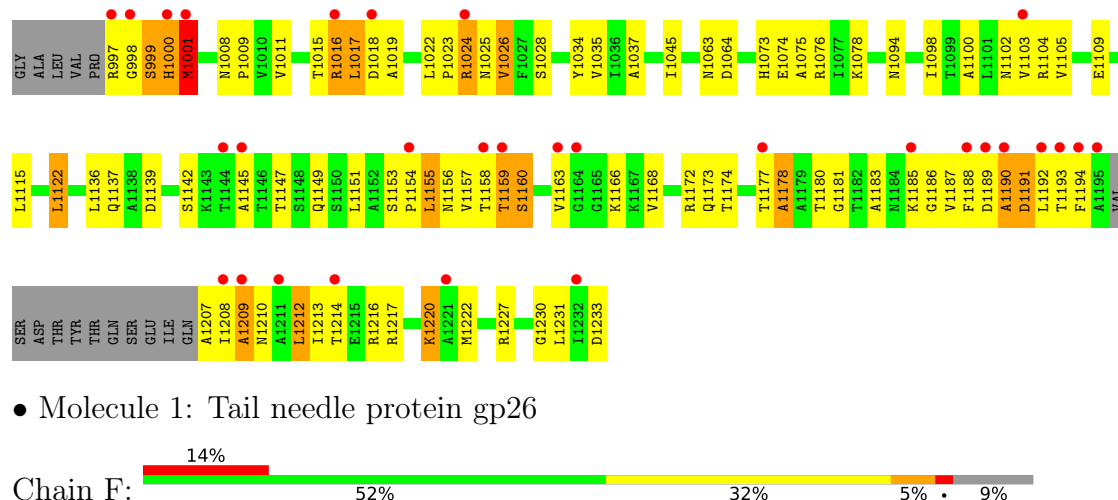




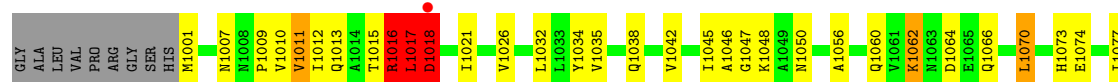
• Molecule 1: Tail needle protein gp26

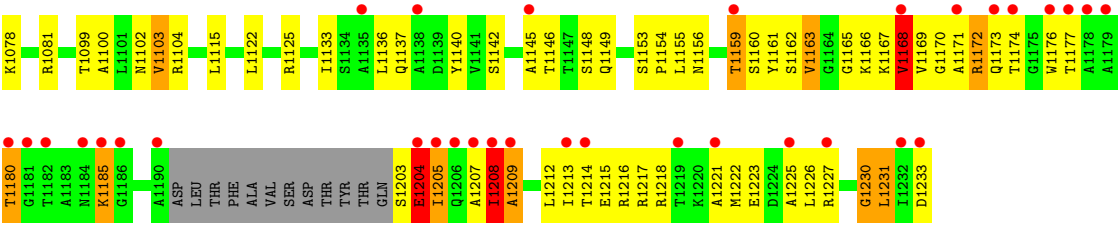


• Molecule 1: Tail needle protein gp26



• Molecule 1: Tail needle protein gp26





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	40.54Å 114.53Å 172.04Å 90.00° 91.01° 90.00°	Depositor
Resolution (Å)	20.00 – 1.95 20.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	92.5 (20.00-1.95) 91.2 (20.00-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.234 , 0.269 0.244 , 0.277	Depositor DCC
R_{free} test set	5233 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.828	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 76.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11851	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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: CA, CL, XE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.46	0/1755	0.89	2/2387 (0.1%)
1	B	0.43	0/1819	0.93	6/2474 (0.2%)
1	C	0.45	0/1752	1.15	16/2382 (0.7%)
1	D	0.63	3/1660 (0.2%)	1.02	15/2255 (0.7%)
1	E	0.42	0/1697	0.95	6/2304 (0.3%)
1	F	0.43	0/1658	0.89	5/2250 (0.2%)
All	All	0.47	3/10341 (0.0%)	0.97	50/14052 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1169	VAL	CA-CB	12.24	1.71	1.54
1	D	1169	VAL	CA-C	10.47	1.65	1.52
1	D	1169	VAL	C-O	8.09	1.32	1.23

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1205	ILE	N-CA-C	-23.25	91.05	112.43
1	D	1011	VAL	N-CA-C	10.44	117.38	106.21
1	D	1169	VAL	CA-C-O	8.54	130.04	120.90
1	E	1159	THR	N-CA-C	7.96	122.39	111.17
1	D	1138	ALA	N-CA-C	-7.92	102.90	114.39
1	E	1028	SER	N-CA-C	-7.44	101.25	110.41
1	B	1026	VAL	N-CA-C	7.24	123.95	113.16
1	D	1180	THR	N-CA-C	7.19	126.12	110.80
1	F	1209	ALA	N-CA-C	-7.19	104.13	113.12
1	C	1198	ASP	CA-C-N	7.05	131.03	120.17
1	C	1198	ASP	C-N-CA	7.05	131.03	120.17
1	B	1160	SER	N-CA-C	6.84	118.95	108.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1198	ASP	CB-CA-C	6.80	123.95	110.42
1	C	1022	LEU	CA-C-N	6.69	126.65	119.76
1	C	1022	LEU	C-N-CA	6.69	126.65	119.76
1	D	1225	ALA	N-CA-C	-6.48	104.30	111.82
1	D	1008	ASN	CA-C-N	6.45	126.47	119.90
1	D	1008	ASN	C-N-CA	6.45	126.47	119.90
1	D	1218	ARG	N-CA-C	-6.32	104.39	111.28
1	C	1028	SER	N-CA-C	6.08	123.74	110.80
1	C	1206	GLN	N-CA-C	-6.05	105.00	112.38
1	C	1139	ASP	N-CA-C	6.02	120.79	113.38
1	C	1021	ILE	N-CA-C	-6.02	107.26	113.10
1	B	1220	LYS	N-CA-C	-5.99	104.83	111.36
1	D	1168	VAL	N-CA-C	-5.88	108.12	113.71
1	F	1159	THR	N-CA-C	5.87	123.31	110.80
1	C	1197	SER	N-CA-C	5.87	117.45	108.30
1	A	1160	SER	N-CA-C	5.80	117.07	108.60
1	E	1001	MET	N-CA-C	5.66	120.71	111.37
1	D	1159	THR	N-CA-C	5.56	122.64	110.80
1	C	1177	THR	N-CA-C	-5.55	100.66	109.76
1	D	1168	VAL	CA-C-N	-5.52	113.59	122.25
1	D	1168	VAL	C-N-CA	-5.52	113.59	122.25
1	E	1212	LEU	N-CA-C	-5.47	105.23	111.14
1	C	1042	VAL	N-CA-C	-5.46	105.05	111.00
1	E	1209	ALA	N-CA-C	-5.41	105.78	112.38
1	C	1199	THR	N-CA-C	-5.38	104.62	113.50
1	B	1159	THR	N-CA-C	5.38	122.27	110.80
1	B	1024	ARG	N-CA-C	5.36	117.12	111.28
1	F	1230	GLY	N-CA-C	-5.32	107.35	115.00
1	B	1154	PRO	N-CA-C	-5.31	103.22	111.13
1	D	1017	LEU	N-CA-C	5.29	117.37	109.59
1	A	1218	ARG	N-CA-C	-5.24	106.74	113.23
1	F	1208	ILE	N-CA-C	-5.21	98.50	109.34
1	F	1161	TYR	N-CA-C	-5.16	101.47	109.72
1	C	1219	THR	N-CA-C	-5.15	105.75	111.36
1	C	1159	THR	N-CA-C	5.14	121.74	110.80
1	D	1184	ASN	N-CA-C	5.08	115.91	107.73
1	D	1232	ILE	N-CA-C	5.03	115.94	108.65
1	E	999	SER	N-CA-C	-5.01	106.47	112.59

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	1738	0	1728	127	0
1	B	1800	0	1791	106	0
1	C	1735	0	1722	149	0
1	D	1645	0	1643	154	0
1	E	1681	0	1676	114	0
1	F	1644	0	1642	131	0
2	A	6	0	0	2	0
2	C	1	0	0	1	0
2	D	6	0	0	4	0
2	F	1	0	0	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	A	266	0	0	13	0
5	B	272	0	0	7	0
5	C	277	0	0	15	0
5	D	211	0	0	12	0
5	E	275	0	0	15	0
5	F	289	0	0	20	0
All	All	11851	0	10202	615	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 30.

All (615) 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:D:1193:THR:HG21	1:F:1216:ARG:CD	1.60	1.32
1:A:1199:THR:HB	5:A:1472:HOH:O	1.45	1.16
1:C:1024:ARG:CD	1:C:1024:ARG:H	1.64	1.07
1:D:1193:THR:CG2	1:F:1216:ARG:HD2	1.86	1.06
1:C:1024:ARG:H	1:C:1024:ARG:HD2	1.00	1.05
1:C:1024:ARG:HD2	1:C:1024:ARG:N	1.64	1.05
1:F:1174:THR:HA	1:F:1233:ASP:HB2	1.44	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1158:THR:HG22	1:B:1159:THR:HG23	1.43	0.98
1:E:1174:THR:HA	1:E:1233:ASP:HB2	1.46	0.98
1:D:1207:ALA:HB1	1:D:1210:ASN:HD22	1.29	0.95
1:F:1010:VAL:H	1:F:1050:ASN:HD21	1.03	0.95
1:E:1024:ARG:HH11	1:E:1024:ARG:HB3	1.30	0.94
1:B:1024:ARG:HD2	1:B:1024:ARG:O	1.67	0.94
1:D:1156:ASN:HD21	1:F:1165:GLY:H	1.15	0.94
1:A:1023:PRO:HG3	1:C:1027:PHE:HB3	1.50	0.91
1:A:1023:PRO:CG	1:C:1027:PHE:HB3	2.02	0.90
1:C:1012:ILE:C	1:C:1013:GLN:HG2	1.97	0.90
1:B:1177:THR:HG22	5:B:1463:HOH:O	1.73	0.89
1:D:1193:THR:HG21	1:F:1216:ARG:HD2	0.90	0.86
1:C:1196:VAL:HG12	1:C:1197:SER:H	1.39	0.86
1:C:1204:GLU:HB2	5:C:1701:HOH:O	1.74	0.86
1:A:1017:LEU:C	1:A:1017:LEU:HD23	2.01	0.85
1:A:1142:SER:H	1:A:1149:GLN:HE22	1.23	0.85
1:A:1013:GLN:OE1	1:A:1013:GLN:HA	1.76	0.85
1:D:1193:THR:CG2	1:F:1216:ARG:CD	2.51	0.84
1:E:1183:ALA:HB2	1:E:1220:LYS:HE3	1.60	0.84
1:F:1017:LEU:O	1:F:1018:ASP:HB3	1.77	0.84
1:D:1191:ASP:O	1:D:1193:THR:HG23	1.78	0.84
1:E:1181:GLY:O	1:E:1220:LYS:HE2	1.76	0.84
1:A:1007:ASN:HD21	1:A:1054:GLN:NE2	1.75	0.83
1:C:1203:SER:O	1:C:1205:ILE:HG22	1.77	0.83
1:A:1007:ASN:HD21	1:A:1054:GLN:HE22	1.22	0.83
1:F:1015:THR:HG22	1:F:1016:ARG:CD	2.08	0.83
1:A:1168:VAL:HG12	1:A:1169:VAL:HG23	1.60	0.82
1:E:1142:SER:H	1:E:1149:GLN:HE22	1.23	0.82
1:D:1194:PHE:HA	1:D:1208:ILE:HG22	1.60	0.82
1:F:1015:THR:CG2	1:F:1016:ARG:HE	1.94	0.81
1:F:1010:VAL:H	1:F:1050:ASN:ND2	1.79	0.81
1:C:1159:THR:O	1:C:1160:SER:HB3	1.78	0.81
1:A:1016:ARG:HG2	5:A:1288:HOH:O	1.80	0.81
1:F:1015:THR:CG2	1:F:1016:ARG:NE	2.44	0.81
1:D:1089:SER:HA	5:D:1403:HOH:O	1.81	0.80
1:D:1185:LYS:HG3	1:F:1176:TRP:HA	1.61	0.80
1:D:1176:TRP:HB2	1:D:1233:ASP:C	2.07	0.80
1:C:1008:ASN:HB3	5:C:1704:HOH:O	1.81	0.79
1:E:1139:ASP:OD2	1:F:1142:SER:HB2	1.81	0.79
1:C:1212:LEU:HD22	1:C:1216:ARG:HD2	1.65	0.79
1:F:1015:THR:HG22	1:F:1016:ARG:HD2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1213:ILE:HD11	1:E:1194:PHE:CE1	2.18	0.78
5:B:1249:HOH:O	1:C:1196:VAL:HG11	1.83	0.78
1:E:1078:LYS:HD2	5:E:1656:HOH:O	1.84	0.78
1:D:1023:PRO:HB2	1:D:1026:VAL:HG22	1.65	0.78
1:C:1168:VAL:HG13	1:C:1169:VAL:HG23	1.66	0.77
1:E:997:ARG:HA	5:E:1628:HOH:O	1.85	0.76
1:A:1017:LEU:HD23	1:A:1017:LEU:O	1.86	0.76
1:D:1011:VAL:HG13	1:D:1011:VAL:O	1.86	0.76
1:E:1075:ALA:HA	5:E:1656:HOH:O	1.84	0.76
1:A:1169:VAL:HG11	1:C:1168:VAL:HG11	1.66	0.76
1:D:1179:ALA:HA	1:E:1188:PHE:HB3	1.68	0.75
1:E:1104:ARG:HH12	1:F:1102:ASN:ND2	1.85	0.75
1:C:1201:THR:O	1:C:1202:GLN:HB2	1.87	0.75
1:A:1007:ASN:ND2	1:A:1054:GLN:NE2	2.35	0.75
1:A:1174:THR:HA	1:A:1233:ASP:OD1	1.87	0.74
1:B:1134:SER:HA	1:B:1137:GLN:HE21	1.52	0.74
1:A:1034:TYR:CZ	1:B:1017:LEU:HG	2.23	0.74
1:B:1166:LYS:HE2	1:B:1166:LYS:HA	1.70	0.74
1:A:1157:VAL:HG13	1:A:1158:THR:O	1.88	0.74
1:C:1029:LYS:CG	1:C:1030:SER:H	2.01	0.74
1:F:1015:THR:HG22	1:F:1016:ARG:NE	2.02	0.74
1:C:1196:VAL:HG12	1:C:1197:SER:N	1.98	0.73
1:C:1015:THR:HG21	5:D:1410:HOH:O	1.88	0.73
2:D:11:XE:XE	1:F:1136:LEU:HD22	2.67	0.73
1:D:1183:ALA:HB1	1:D:1217:ARG:O	1.89	0.73
1:E:1016:ARG:NH2	5:E:1715:HOH:O	2.20	0.72
1:A:1198:ASP:O	1:A:1199:THR:HG23	1.88	0.72
1:F:1142:SER:H	1:F:1149:GLN:HE22	1.38	0.72
1:A:1126:VAL:O	1:A:1130:GLU:HG3	1.88	0.72
1:D:1208:ILE:HD11	2:D:14:XE:XE	2.68	0.72
1:C:1025:ASN:HA	5:C:1720:HOH:O	1.90	0.72
1:F:1162:SER:HB3	1:F:1167:LYS:HA	1.71	0.72
1:B:1100:ALA:O	1:B:1103:VAL:HG22	1.88	0.72
1:B:1104:ARG:HH12	1:C:1102:ASN:ND2	1.86	0.71
1:D:1176:TRP:NE1	1:E:1185:LYS:HD3	2.05	0.71
1:D:1136:LEU:HD11	1:E:1137:GLN:HG3	1.73	0.71
1:A:1155:LEU:HD23	1:A:1156:ASN:H	1.56	0.71
1:D:1163:VAL:HG23	1:E:1159:THR:HA	1.73	0.70
1:D:1183:ALA:HB2	1:D:1220:LYS:HG3	1.73	0.70
1:B:1016:ARG:NE	1:B:1016:ARG:H	1.89	0.70
1:D:1137:GLN:HA	1:D:1140:TYR:CD1	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1227:ARG:NH1	5:F:1496:HOH:O	2.23	0.70
5:B:1494:HOH:O	1:C:1208:ILE:HG12	1.90	0.70
1:D:1185:LYS:HA	1:D:1218:ARG:NH1	2.07	0.69
1:A:1017:LEU:HB2	1:C:1034:TYR:CE2	2.27	0.69
1:A:1073:HIS:HD2	5:C:1669:HOH:O	1.75	0.69
1:D:1226:LEU:HD21	1:F:1226:LEU:HD21	1.74	0.69
1:F:1209:ALA:O	1:F:1213:ILE:HG13	1.92	0.69
1:A:1157:VAL:HG21	1:B:1155:LEU:HB2	1.73	0.69
5:D:1260:HOH:O	1:F:1172:ARG:HA	1.92	0.69
1:C:1192:LEU:O	1:C:1192:LEU:HD22	1.93	0.69
1:C:1206:GLN:O	1:C:1210:ASN:HB2	1.93	0.69
1:D:1179:ALA:CB	1:D:1220:LYS:HD3	2.23	0.68
1:F:1077:ILE:HD11	5:F:1505:HOH:O	1.92	0.68
1:F:1208:ILE:HD13	1:F:1208:ILE:O	1.93	0.68
1:D:1122:LEU:HD21	1:E:1122:LEU:HB3	1.75	0.68
1:B:1183:ALA:HB1	1:B:1221:ALA:HB2	1.75	0.68
1:B:1032:LEU:O	1:B:1036:ILE:HG22	1.93	0.68
1:B:1200:TYR:CE2	1:C:1197:SER:OG	2.47	0.68
1:E:1074:GLU:HG3	1:E:1078:LYS:HE2	1.74	0.68
1:B:1073:HIS:HD2	5:C:1669:HOH:O	1.75	0.68
1:C:1013:GLN:HB2	1:D:1127:THR:HG21	1.76	0.68
1:C:1015:THR:HG22	1:D:1128:THR:OG1	1.94	0.68
1:D:1217:ARG:HH21	1:E:1191:ASP:HA	1.58	0.68
1:E:1212:LEU:O	1:E:1216:ARG:HG3	1.93	0.68
1:B:1168:VAL:HG13	1:B:1169:VAL:HG23	1.76	0.68
1:D:1155:LEU:HD11	1:E:1151:LEU:HD13	1.76	0.68
1:A:1009:PRO:HD3	5:A:1431:HOH:O	1.93	0.67
1:D:1156:ASN:HD21	1:F:1165:GLY:N	1.89	0.67
1:A:1012:ILE:O	1:A:1014:ALA:N	2.27	0.67
1:D:1003:ASP:H	1:D:1060:GLN:NE2	1.93	0.67
1:E:1163:VAL:HG21	1:F:1171:ALA:HA	1.77	0.67
1:C:1012:ILE:C	1:C:1013:GLN:CG	2.67	0.67
1:D:1192:LEU:C	1:D:1193:THR:HG23	2.20	0.67
1:A:1206:GLN:HG2	1:B:1196:VAL:HG11	1.77	0.66
2:A:7:XE:XE	1:B:1208:ILE:HG21	2.73	0.66
1:B:1159:THR:O	1:B:1160:SER:HB3	1.95	0.66
1:A:1100:ALA:O	1:A:1103:VAL:HG22	1.96	0.66
1:C:1100:ALA:O	1:C:1103:VAL:HG22	1.96	0.66
1:D:1194:PHE:CA	1:D:1208:ILE:HG22	2.25	0.66
1:D:1002:ALA:HA	1:D:1060:GLN:HE21	1.60	0.66
1:E:1018:ASP:CG	1:E:1019:ALA:H	2.03	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1199:THR:C	1:C:1201:THR:H	2.04	0.66
5:D:1409:HOH:O	1:E:1001:MET:HE3	1.95	0.66
1:C:1192:LEU:O	1:C:1192:LEU:HD13	1.96	0.65
1:D:1063:ASN:ND2	1:F:1062:LYS:HG2	2.11	0.65
1:A:1168:VAL:HG11	1:B:1169:VAL:HG11	1.78	0.65
1:A:1202:GLN:O	1:A:1206:GLN:HG3	1.97	0.65
1:A:1153:SER:O	1:C:1157:VAL:HG22	1.97	0.65
1:A:1023:PRO:HG3	1:C:1027:PHE:CB	2.26	0.65
2:D:11:XE:XE	1:E:1136:LEU:HD22	2.75	0.65
1:A:1125:ARG:HD2	1:B:1130:GLU:OE1	1.96	0.65
1:C:1029:LYS:HG3	1:C:1030:SER:H	1.61	0.65
1:A:1142:SER:N	1:A:1149:GLN:HE22	1.94	0.64
1:A:1178:ALA:HA	1:A:1227:ARG:NH2	2.13	0.64
1:F:1159:THR:O	1:F:1160:SER:HB3	1.98	0.64
1:D:1207:ALA:HB1	1:D:1210:ASN:ND2	2.08	0.63
1:A:1155:LEU:HB2	1:C:1157:VAL:HG21	1.79	0.63
1:B:1045:ILE:HD11	1:C:1012:ILE:HG21	1.80	0.63
1:B:1024:ARG:O	1:B:1024:ARG:CD	2.43	0.63
1:D:1011:VAL:O	1:D:1011:VAL:CG1	2.47	0.63
1:A:1010:VAL:HG22	1:A:1050:ASN:OD1	1.99	0.63
1:B:1227:ARG:HD3	1:B:1233:ASP:O	1.99	0.63
1:C:1202:GLN:O	1:C:1203:SER:C	2.41	0.63
1:D:1003:ASP:H	1:D:1060:GLN:HE22	1.46	0.63
1:F:1172:ARG:HB2	1:F:1230:GLY:O	1.99	0.63
1:D:1073:HIS:HE1	1:E:1074:GLU:OE1	1.81	0.63
1:C:1001:MET:CE	1:C:1063:ASN:HD22	2.11	0.62
1:A:1023:PRO:HG2	1:C:1027:PHE:HB3	1.78	0.62
1:D:1185:LYS:CG	1:F:1176:TRP:HA	2.28	0.62
1:E:1024:ARG:HH11	1:E:1024:ARG:CB	2.09	0.62
1:D:1007:ASN:OD1	1:D:1054:GLN:HG3	2.00	0.62
1:A:1012:ILE:C	1:A:1014:ALA:H	2.07	0.62
1:A:1158:THR:C	5:A:1462:HOH:O	2.43	0.62
1:B:1092:THR:O	1:B:1096:LYS:HG2	2.01	0.61
1:A:1074:GLU:O	1:A:1078:LYS:HG2	2.00	0.61
1:A:1090:ARG:NH2	1:B:1088:GLU:OE2	2.33	0.61
1:E:1163:VAL:CG2	1:F:1171:ALA:HA	2.31	0.61
1:D:1163:VAL:HG13	1:D:1168:VAL:HG21	1.83	0.61
1:B:1183:ALA:HB2	1:B:1220:LYS:HG3	1.81	0.61
1:B:1200:TYR:CD1	1:C:1200:TYR:HB2	2.36	0.61
1:D:1012:ILE:HD11	1:F:1045:ILE:HD11	1.83	0.61
1:D:1185:LYS:HZ2	1:F:1176:TRP:CD1	2.19	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1159:THR:O	1:E:1160:SER:CB	2.48	0.61
1:D:1049:ALA:HB1	1:F:1048:LYS:HG3	1.82	0.61
1:A:1012:ILE:O	1:A:1012:ILE:HG12	2.00	0.61
1:A:1106:THR:HG22	1:E:998:GLY:HA2	1.82	0.61
1:A:1012:ILE:O	1:A:1012:ILE:CG1	2.47	0.60
1:C:1136:LEU:HD22	2:C:4:XE:XE	2.79	0.60
2:A:7:XE:XE	1:C:1208:ILE:HG21	2.78	0.60
1:E:1159:THR:O	1:E:1160:SER:HB2	2.01	0.60
1:A:1226:LEU:HD22	1:B:1222:MET:HE3	1.82	0.60
1:C:1038:GLN:HA	1:C:1041:ASP:OD2	2.01	0.60
1:F:1205:ILE:O	1:F:1208:ILE:HG22	2.01	0.60
1:A:1048:LYS:HB2	1:B:1010:VAL:HG21	1.82	0.60
1:A:1222:MET:HE2	1:C:1226:LEU:HD12	1.81	0.60
1:B:1209:ALA:O	1:B:1213:ILE:HG13	2.00	0.60
1:A:1012:ILE:HD12	1:A:1015:THR:OG1	2.01	0.60
1:D:1193:THR:HG22	1:F:1216:ARG:NH1	2.16	0.60
1:C:1023:PRO:HB2	1:C:1026:VAL:CG1	2.31	0.60
1:C:1029:LYS:CG	1:C:1030:SER:N	2.65	0.60
1:F:1073:HIS:HB3	5:F:1505:HOH:O	1.99	0.60
1:F:1133:ILE:O	1:F:1137:GLN:HG3	2.01	0.60
1:F:1168:VAL:HG13	1:F:1169:VAL:HG23	1.84	0.60
1:C:1007:ASN:OD1	1:C:1054:GLN:HG3	2.02	0.60
1:D:1123:ASP:OD2	1:F:1122:LEU:HD11	2.01	0.60
1:D:1183:ALA:HB2	1:D:1220:LYS:CG	2.31	0.60
1:E:1177:THR:O	1:E:1178:ALA:HB3	2.02	0.60
1:A:1142:SER:H	1:A:1149:GLN:NE2	1.97	0.59
1:F:1159:THR:O	1:F:1159:THR:HG22	2.02	0.59
1:F:1074:GLU:OE2	1:F:1078:LYS:HE3	2.02	0.59
1:B:1163:VAL:HA	1:C:1157:VAL:O	2.03	0.59
1:C:1015:THR:O	1:C:1016:ARG:C	2.45	0.59
1:D:1100:ALA:O	1:D:1103:VAL:HG22	2.02	0.59
1:B:1182:THR:HG22	1:C:1191:ASP:OD2	2.02	0.59
1:D:1185:LYS:HG3	1:F:1176:TRP:CG	2.38	0.59
1:E:1154:PRO:HG2	1:F:1148:SER:HB2	1.85	0.59
1:C:1203:SER:O	1:C:1204:GLU:C	2.45	0.59
1:F:1100:ALA:O	1:F:1103:VAL:HG13	2.01	0.59
1:F:1174:THR:HA	1:F:1233:ASP:CB	2.27	0.59
1:A:1169:VAL:HG11	1:C:1168:VAL:CG1	2.33	0.59
1:C:1001:MET:HE1	1:C:1063:ASN:HD22	1.68	0.58
1:F:1213:ILE:O	1:F:1217:ARG:HG3	2.03	0.58
1:A:1013:GLN:O	1:A:1014:ALA:CB	2.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1017:LEU:HB2	1:C:1034:TYR:CZ	2.38	0.58
1:B:1206:GLN:NE2	1:C:1196:VAL:HG21	2.19	0.58
1:A:1183:ALA:HB1	1:A:1221:ALA:HB2	1.86	0.58
1:D:1194:PHE:CD1	1:D:1194:PHE:N	2.58	0.58
1:E:1001:MET:HB2	5:E:1654:HOH:O	2.04	0.58
1:C:1168:VAL:CG1	1:C:1169:VAL:HG23	2.33	0.58
1:F:1168:VAL:CG1	1:F:1169:VAL:HG23	2.34	0.58
5:D:1260:HOH:O	1:F:1231:LEU:HA	2.02	0.58
1:E:1000:HIS:CD2	5:E:1452:HOH:O	2.56	0.58
1:A:1012:ILE:C	1:A:1014:ALA:N	2.60	0.58
1:D:1213:ILE:O	1:D:1217:ARG:HG2	2.03	0.58
1:D:1018:ASP:O	1:D:1021:ILE:HG12	2.04	0.58
1:A:1168:VAL:HG11	1:B:1169:VAL:CG1	2.34	0.57
1:B:1167:LYS:HZ1	1:B:1170:GLY:HA3	1.68	0.57
1:D:1163:VAL:CG2	1:E:1159:THR:HA	2.34	0.57
1:B:1024:ARG:HD2	1:B:1024:ARG:C	2.20	0.57
1:D:1136:LEU:HD21	1:E:1137:GLN:HG2	1.86	0.57
1:D:1179:ALA:HB3	1:D:1220:LYS:HD3	1.85	0.57
1:B:1012:ILE:O	1:B:1012:ILE:HG13	2.03	0.57
1:C:1024:ARG:O	1:C:1025:ASN:ND2	2.37	0.57
1:D:1179:ALA:HB3	1:D:1220:LYS:CD	2.34	0.57
1:D:1190:ALA:O	1:F:1216:ARG:HD3	2.04	0.57
1:B:1076:ARG:HH22	1:C:1074:GLU:CD	2.13	0.57
1:B:1155:LEU:HD21	1:C:1151:LEU:HD13	1.86	0.57
1:B:1016:ARG:H	1:B:1016:ARG:HE	1.50	0.57
1:A:1017:LEU:C	1:A:1017:LEU:CD2	2.74	0.57
1:A:1139:ASP:OD1	1:B:1144:THR:HG22	2.05	0.57
1:A:1173:GLN:NE2	1:B:1228:ALA:HB3	2.20	0.57
1:A:1222:MET:HE1	1:C:1223:GLU:HA	1.87	0.57
1:D:1215:GLU:OE2	1:F:1216:ARG:HA	2.05	0.57
1:C:1023:PRO:CB	1:C:1026:VAL:HG11	2.35	0.56
1:D:1077:ILE:HD11	5:F:1505:HOH:O	2.05	0.56
1:F:1204:GLU:OE1	1:F:1204:GLU:N	2.39	0.56
1:B:1206:GLN:HE21	1:B:1206:GLN:HA	1.70	0.56
5:B:1446:HOH:O	1:C:1187:VAL:HG23	2.05	0.56
1:C:1023:PRO:HB3	1:C:1026:VAL:HG11	1.86	0.56
1:E:1210:ASN:O	1:E:1214:THR:HG23	2.05	0.56
5:A:1462:HOH:O	1:B:1154:PRO:HA	2.06	0.56
1:A:1158:THR:O	1:A:1160:SER:N	2.39	0.56
1:D:1157:VAL:HG12	1:D:1158:THR:N	2.20	0.56
1:F:1204:GLU:HG3	5:F:1447:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1002:ALA:HA	1:C:1060:GLN:HE21	1.69	0.55
1:F:1204:GLU:HA	5:F:1447:HOH:O	2.05	0.55
1:B:1036:ILE:HD12	5:B:1349:HOH:O	2.05	0.55
1:A:1159:THR:HB	5:A:1462:HOH:O	2.05	0.55
1:A:1212:LEU:HD13	1:A:1216:ARG:HD3	1.87	0.55
1:A:1163:VAL:HG21	1:B:1171:ALA:HA	1.89	0.55
1:B:1104:ARG:HH12	1:C:1102:ASN:HD21	1.53	0.55
1:B:1139:ASP:OD2	1:C:1142:SER:HB2	2.07	0.55
1:B:1168:VAL:HG22	1:C:1231:LEU:HD23	1.87	0.55
1:E:1078:LYS:HE3	5:E:1680:HOH:O	2.07	0.55
1:F:1207:ALA:O	1:F:1208:ILE:HB	2.07	0.55
1:F:1203:SER:N	5:F:1272:HOH:O	2.39	0.55
1:B:1157:VAL:CG1	1:B:1158:THR:N	2.70	0.55
1:A:1018:ASP:O	1:A:1019:ALA:HB3	2.07	0.55
1:A:1027:PHE:CE2	1:B:1027:PHE:HZ	2.25	0.55
1:D:1215:GLU:OE1	1:F:1216:ARG:HG2	2.06	0.55
1:E:1194:PHE:HD2	1:E:1208:ILE:HG21	1.71	0.55
5:A:1433:HOH:O	1:C:1062:LYS:HE3	2.07	0.54
1:A:1155:LEU:HD23	1:A:1156:ASN:N	2.21	0.54
1:A:1198:ASP:O	1:A:1199:THR:CG2	2.55	0.54
1:D:1070:LEU:HD21	1:F:1070:LEU:HD13	1.89	0.54
1:A:1013:GLN:OE1	1:A:1013:GLN:CA	2.54	0.54
1:A:1222:MET:HB3	1:B:1222:MET:HE1	1.90	0.54
1:C:1143:LYS:HE3	5:C:1634:HOH:O	2.07	0.54
1:A:1023:PRO:HB2	1:A:1026:VAL:CG1	2.37	0.54
1:A:1173:GLN:HE22	1:B:1228:ALA:CB	2.21	0.54
1:D:1008:ASN:HB2	5:D:1398:HOH:O	2.06	0.54
1:E:1192:LEU:HD22	1:E:1194:PHE:CE2	2.43	0.54
1:D:1155:LEU:HD12	1:E:1149:GLN:O	2.08	0.54
1:E:1155:LEU:HD23	1:E:1156:ASN:H	1.73	0.54
1:C:1202:GLN:HA	1:C:1202:GLN:NE2	2.23	0.53
1:D:1022:LEU:HD11	1:D:1036:ILE:HD11	1.90	0.53
1:E:1037:ALA:HB1	1:F:1013:GLN:HB2	1.90	0.53
1:B:1206:GLN:HE21	1:C:1196:VAL:HG21	1.71	0.53
1:C:1024:ARG:CD	1:C:1024:ARG:N	2.41	0.53
1:D:1208:ILE:HD11	1:F:1208:ILE:HD12	1.91	0.53
1:F:1217:ARG:HD2	5:F:1299:HOH:O	2.08	0.53
1:A:1003:ASP:H	1:A:1060:GLN:NE2	2.06	0.53
1:D:1185:LYS:HD3	1:D:1185:LYS:N	2.23	0.53
1:E:1073:HIS:HE1	1:F:1074:GLU:OE1	1.92	0.53
1:D:1222:MET:O	1:D:1226:LEU:HG	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1204:GLU:CD	1:F:1204:GLU:H	2.17	0.53
1:A:1169:VAL:CG1	1:C:1168:VAL:HG11	2.38	0.53
1:C:1202:GLN:HA	1:C:1202:GLN:HE21	1.74	0.53
1:E:1018:ASP:CG	1:E:1019:ALA:N	2.66	0.53
1:A:1048:LYS:HB2	1:B:1010:VAL:CG2	2.39	0.52
1:B:1217:ARG:HA	1:C:1190:ALA:HB1	1.91	0.52
1:C:1029:LYS:HG3	1:C:1030:SER:N	2.23	0.52
1:C:1159:THR:O	1:C:1160:SER:CB	2.50	0.52
1:A:1198:ASP:O	1:A:1198:ASP:OD1	2.27	0.52
1:B:1200:TYR:HE2	1:C:1197:SER:HG	1.46	0.52
1:D:1112:ILE:O	1:D:1116:GLN:HG3	2.09	0.52
1:A:1222:MET:HE1	1:C:1223:GLU:CA	2.38	0.52
1:C:1232:ILE:O	1:C:1233:ASP:C	2.53	0.52
1:E:999:SER:O	1:E:1000:HIS:C	2.51	0.52
1:F:1214:THR:HG22	5:F:1299:HOH:O	2.08	0.52
1:A:1212:LEU:HD12	1:B:1194:PHE:CE1	2.45	0.52
1:C:1212:LEU:O	1:C:1216:ARG:HG2	2.10	0.52
1:E:1142:SER:H	1:E:1149:GLN:NE2	1.99	0.52
1:D:1217:ARG:NH2	1:E:1191:ASP:HA	2.24	0.52
1:B:1155:LEU:HD23	1:B:1156:ASN:N	2.24	0.52
1:E:1214:THR:HA	1:E:1217:ARG:HG3	1.92	0.52
1:A:1203:SER:HA	1:A:1206:GLN:OE1	2.09	0.52
1:D:1001:MET:SD	1:D:1001:MET:N	2.82	0.52
1:D:1185:LYS:CB	1:F:1176:TRP:CE3	2.93	0.52
1:E:1173:GLN:HG3	1:F:1225:ALA:HB1	1.92	0.52
1:C:1041:ASP:O	1:C:1045:ILE:HG13	2.09	0.52
1:F:1155:LEU:HD22	1:F:1156:ASN:H	1.74	0.52
1:F:1185:LYS:HG3	1:F:1221:ALA:HB1	1.92	0.52
1:B:1157:VAL:HG12	1:B:1158:THR:N	2.24	0.51
1:D:1179:ALA:O	1:D:1180:THR:OG1	2.21	0.51
1:D:1213:ILE:CD1	1:E:1194:PHE:CE1	2.93	0.51
1:D:1217:ARG:HA	1:D:1220:LYS:HB3	1.92	0.51
1:A:1023:PRO:HB2	1:A:1026:VAL:HG11	1.91	0.51
1:D:1010:VAL:HG12	1:D:1050:ASN:HD21	1.74	0.51
1:B:1056:ALA:O	1:B:1060:GLN:HG3	2.11	0.51
1:D:1233:ASP:C	1:D:1233:ASP:OD1	2.54	0.51
1:A:1200:TYR:HA	1:C:1200:TYR:CE2	2.46	0.51
1:E:1213:ILE:O	1:E:1217:ARG:HG2	2.10	0.51
1:C:1012:ILE:O	1:C:1013:GLN:C	2.52	0.51
1:D:1159:THR:O	1:D:1160:SER:HB3	2.10	0.51
1:D:1215:GLU:CD	1:F:1215:GLU:HG3	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1167:LYS:HG2	1:F:1168:VAL:N	2.26	0.51
1:A:1157:VAL:CG1	1:A:1158:THR:O	2.58	0.50
1:A:1166:LYS:HE2	1:B:1172:ARG:HB3	1.93	0.50
1:E:1154:PRO:HG2	1:F:1148:SER:CB	2.41	0.50
1:E:1157:VAL:CG1	1:E:1158:THR:N	2.75	0.50
1:F:1169:VAL:HG12	1:F:1170:GLY:N	2.26	0.50
1:C:1038:GLN:HG3	5:C:1474:HOH:O	2.10	0.50
1:C:1199:THR:O	1:C:1200:TYR:HB3	2.11	0.50
1:E:1076:ARG:NH2	1:F:1074:GLU:OE1	2.40	0.50
1:F:1159:THR:O	1:F:1159:THR:CG2	2.60	0.50
1:D:1213:ILE:CD1	1:E:1194:PHE:HE1	2.24	0.50
1:B:1081:ARG:O	1:B:1081:ARG:HD3	2.11	0.50
1:E:1104:ARG:HH12	1:F:1102:ASN:HD21	1.56	0.50
1:E:1189:ASP:OD2	1:E:1192:LEU:HD12	2.11	0.50
1:D:1143:LYS:HE3	1:F:1140:TYR:O	2.12	0.50
1:A:1045:ILE:HG22	1:C:1045:ILE:HG21	1.94	0.50
1:A:1198:ASP:O	1:A:1199:THR:OG1	2.29	0.50
1:C:1112:ILE:O	1:C:1116:GLN:HG3	2.12	0.50
1:D:1073:HIS:HD2	5:F:1234:HOH:O	1.95	0.50
1:D:1192:LEU:C	1:D:1193:THR:CG2	2.85	0.50
1:F:1001:MET:HB3	1:F:1064:ASP:OD1	2.12	0.50
1:C:1023:PRO:CB	1:C:1026:VAL:CG1	2.90	0.49
1:A:1198:ASP:O	1:A:1199:THR:CB	2.60	0.49
1:E:1189:ASP:OD1	1:E:1189:ASP:N	2.45	0.49
1:E:1208:ILE:C	1:E:1210:ASN:N	2.69	0.49
1:D:1014:ALA:HB3	5:F:1303:HOH:O	2.12	0.49
1:D:1183:ALA:CB	1:D:1217:ARG:O	2.59	0.49
1:E:1153:SER:HB2	1:F:1146:THR:O	2.12	0.49
1:B:1155:LEU:HD22	1:B:1157:VAL:HG23	1.93	0.49
1:A:1023:PRO:HG3	5:C:1522:HOH:O	2.11	0.49
1:D:1185:LYS:HG3	1:F:1176:TRP:CD2	2.47	0.49
1:A:1012:ILE:CD1	1:A:1015:THR:OG1	2.60	0.49
1:D:1026:VAL:HG23	1:D:1027:PHE:CD2	2.48	0.49
1:D:1176:TRP:CE2	1:E:1185:LYS:HD3	2.46	0.49
1:E:1208:ILE:C	1:E:1208:ILE:HD12	2.38	0.49
1:B:1122:LEU:HD21	1:C:1122:LEU:HB3	1.94	0.49
1:D:1179:ALA:HB1	1:D:1220:LYS:HD3	1.92	0.49
1:E:1186:GLY:HA3	5:E:1614:HOH:O	2.13	0.49
1:C:1208:ILE:N	1:C:1208:ILE:HD12	2.27	0.49
5:A:1462:HOH:O	1:B:1154:PRO:HG3	2.12	0.49
1:C:1197:SER:N	5:C:1678:HOH:O	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1157:VAL:HG13	1:A:1158:THR:N	2.27	0.49
1:A:1157:VAL:O	1:C:1163:VAL:HA	2.13	0.49
1:A:1045:ILE:HD11	1:B:1046:ALA:HB2	1.95	0.48
1:B:1103:VAL:HG23	1:B:1104:ARG:N	2.28	0.48
1:E:1142:SER:N	1:E:1149:GLN:HE22	2.00	0.48
1:B:1215:GLU:HG3	1:C:1215:GLU:OE2	2.13	0.48
1:E:1210:ASN:ND2	5:E:1651:HOH:O	2.46	0.48
1:B:1199:THR:O	1:B:1200:TYR:C	2.57	0.48
1:C:1012:ILE:O	1:C:1013:GLN:CG	2.61	0.48
1:C:1205:ILE:O	1:C:1205:ILE:HG12	2.12	0.48
1:E:1000:HIS:HD2	5:E:1452:HOH:O	1.94	0.48
1:F:1001:MET:SD	5:F:1467:HOH:O	2.60	0.48
1:A:1027:PHE:CE2	1:B:1027:PHE:CZ	3.02	0.48
1:C:1087:HIS:O	1:C:1091:ILE:HG13	2.13	0.48
1:D:1023:PRO:HB2	1:D:1026:VAL:CG2	2.40	0.48
1:D:1163:VAL:HA	1:E:1157:VAL:O	2.13	0.48
2:D:14:XE:XE	5:E:1595:HOH:O	3.10	0.48
1:C:1188:PHE:CD1	1:C:1218:ARG:HD2	2.49	0.48
1:D:1186:GLY:HA2	1:F:1177:THR:HB	1.94	0.48
1:C:1022:LEU:O	1:C:1024:ARG:NH1	2.47	0.48
1:C:1233:ASP:CG	1:C:1233:ASP:O	2.56	0.48
1:D:1214:THR:OG1	1:F:1216:ARG:NH2	2.46	0.48
1:E:1025:ASN:O	1:E:1025:ASN:CG	2.55	0.48
1:E:1173:GLN:O	1:E:1233:ASP:N	2.47	0.48
1:F:1099:THR:HG21	5:F:1414:HOH:O	2.14	0.48
1:F:1162:SER:HB2	1:F:1166:LYS:O	2.13	0.48
1:D:1181:GLY:O	1:D:1182:THR:HB	2.14	0.47
1:D:1032:LEU:O	1:D:1036:ILE:HG12	2.14	0.47
1:B:1017:LEU:CD2	1:B:1021:ILE:HD11	2.45	0.47
1:C:1015:THR:O	1:C:1016:ARG:O	2.31	0.47
1:C:1200:TYR:CD1	1:C:1200:TYR:C	2.92	0.47
1:E:1100:ALA:O	1:E:1103:VAL:HG22	2.14	0.47
1:C:1199:THR:C	1:C:1201:THR:N	2.71	0.47
1:A:1206:GLN:HG2	1:B:1196:VAL:CG1	2.43	0.47
1:E:1155:LEU:HD23	1:E:1156:ASN:N	2.30	0.47
1:F:1159:THR:O	1:F:1160:SER:CB	2.63	0.47
1:A:1173:GLN:HE22	1:B:1228:ALA:HB1	1.78	0.47
5:A:1462:HOH:O	1:B:1154:PRO:CA	2.60	0.47
1:D:1179:ALA:HB3	1:D:1220:LYS:HE2	1.96	0.47
1:B:1206:GLN:NE2	1:B:1206:GLN:HA	2.30	0.47
1:C:1200:TYR:CD1	1:C:1200:TYR:O	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:997:ARG:NH2	5:E:1688:HOH:O	2.48	0.47
1:E:1019:ALA:HA	1:E:1022:LEU:HD12	1.96	0.47
1:F:1012:ILE:HD11	5:F:1400:HOH:O	2.15	0.47
1:F:1212:LEU:O	1:F:1216:ARG:HG3	2.14	0.47
5:D:1260:HOH:O	1:E:1168:VAL:HG13	2.14	0.47
1:E:1008:ASN:HB2	5:E:1721:HOH:O	2.14	0.47
1:E:1189:ASP:O	1:E:1190:ALA:C	2.57	0.47
1:A:1041:ASP:OD1	1:B:1012:ILE:HA	2.15	0.47
1:E:1157:VAL:HG12	1:E:1158:THR:N	2.29	0.47
1:A:1022:LEU:HD23	1:C:1031:TYR:CD1	2.49	0.46
1:C:1010:VAL:O	1:C:1010:VAL:CG1	2.63	0.46
1:E:1153:SER:HB3	1:F:1145:ALA:O	2.15	0.46
1:C:1115:LEU:O	1:C:1119:VAL:HG23	2.15	0.46
1:A:1166:LYS:CE	1:B:1172:ARG:HB3	2.46	0.46
1:E:1227:ARG:HD3	1:E:1233:ASP:O	2.16	0.46
5:D:1241:HOH:O	1:F:1180:THR:HG23	2.15	0.46
1:B:1045:ILE:CD1	1:C:1046:ALA:HB2	2.46	0.46
1:D:1063:ASN:CG	1:F:1062:LYS:HG2	2.40	0.46
1:C:1205:ILE:O	1:C:1205:ILE:CG1	2.63	0.46
1:A:1151:LEU:O	1:C:1158:THR:HG23	2.16	0.46
1:B:1167:LYS:NZ	1:B:1170:GLY:HA3	2.30	0.46
1:B:1094:ASN:O	1:B:1098:ILE:HG12	2.15	0.46
1:D:1074:GLU:OE2	1:D:1078:LYS:HE3	2.16	0.46
1:D:1153:SER:HB3	1:E:1145:ALA:O	2.15	0.46
1:E:1163:VAL:HG23	1:E:1163:VAL:O	2.15	0.46
1:F:1222:MET:HE3	1:F:1222:MET:HB2	1.86	0.46
1:B:1033:LEU:O	1:B:1036:ILE:HG23	2.16	0.46
1:C:1010:VAL:O	1:C:1010:VAL:HG13	2.15	0.46
1:E:1105:VAL:O	1:E:1109:GLU:HG3	2.15	0.45
1:C:1099:THR:HB	5:C:1665:HOH:O	2.15	0.45
1:B:1034:TYR:CD1	1:B:1034:TYR:C	2.95	0.45
1:B:1200:TYR:CG	1:C:1200:TYR:HB2	2.50	0.45
1:D:1103:VAL:HG23	1:D:1104:ARG:N	2.31	0.45
1:E:1034:TYR:CZ	1:F:1017:LEU:HG	2.52	0.45
1:A:1021:ILE:HB	1:C:1030:SER:HB2	1.98	0.45
1:D:1163:VAL:HG13	1:D:1168:VAL:CG2	2.45	0.45
1:A:1045:ILE:CD1	1:B:1046:ALA:HB2	2.46	0.45
1:D:1123:ASP:CG	1:F:1122:LEU:HD11	2.41	0.45
1:E:1000:HIS:NE2	1:E:1064:ASP:OD1	2.49	0.45
1:E:1172:ARG:HG3	1:E:1230:GLY:O	2.17	0.45
1:A:1024:ARG:O	1:A:1025:ASN:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1062:LYS:O	1:A:1066:GLN:HG3	2.15	0.45
1:A:1158:THR:HG22	1:A:1159:THR:N	2.32	0.45
1:B:1200:TYR:HE2	1:C:1197:SER:OG	1.93	0.45
1:C:1096:LYS:NZ	5:C:1694:HOH:O	2.48	0.45
1:D:1034:TYR:CE2	1:E:1017:LEU:HG	2.52	0.45
1:A:1218:ARG:O	1:A:1222:MET:HG3	2.17	0.45
1:D:1017:LEU:HD13	1:D:1036:ILE:HD13	1.97	0.45
1:D:1144:THR:HA	5:D:1379:HOH:O	2.16	0.45
1:D:1188:PHE:CE2	1:D:1190:ALA:HA	2.51	0.45
1:F:1007:ASN:O	1:F:1009:PRO:HD3	2.17	0.45
1:B:1076:ARG:NH2	1:C:1074:GLU:OE1	2.50	0.45
1:D:1002:ALA:HA	1:D:1060:GLN:NE2	2.28	0.45
1:F:1227:ARG:HD3	5:F:1440:HOH:O	2.17	0.45
1:D:1062:LYS:HG2	1:E:1063:ASN:CG	2.42	0.45
1:D:1215:GLU:OE2	1:F:1215:GLU:HG3	2.17	0.45
1:B:1040:THR:HA	5:B:1482:HOH:O	2.17	0.45
1:D:1109:GLU:OE1	1:F:1104:ARG:HD2	2.17	0.45
1:D:1150:SER:HA	1:F:1156:ASN:O	2.17	0.45
1:D:1214:THR:HA	1:D:1217:ARG:HD2	1.98	0.45
1:B:1073:HIS:HE1	1:C:1074:GLU:OE1	2.00	0.44
1:D:1081:ARG:O	1:D:1081:ARG:HD3	2.17	0.44
1:A:1155:LEU:CD2	1:A:1156:ASN:N	2.80	0.44
1:A:1188:PHE:CD1	1:A:1218:ARG:HD2	2.52	0.44
1:C:1126:VAL:O	1:C:1130:GLU:HG3	2.18	0.44
1:D:1176:TRP:CD1	1:E:1185:LYS:HD3	2.51	0.44
1:E:1155:LEU:CD2	1:E:1156:ASN:N	2.80	0.44
1:F:1205:ILE:O	1:F:1205:ILE:HG13	2.16	0.44
1:A:1212:LEU:CD1	1:A:1216:ARG:HD3	2.47	0.44
1:B:1165:GLY:H	1:C:1156:ASN:HD21	1.66	0.44
1:F:1001:MET:HA	5:F:1421:HOH:O	2.18	0.44
1:F:1047:GLY:HA2	5:F:1283:HOH:O	2.17	0.44
1:C:1025:ASN:ND2	1:C:1025:ASN:O	2.42	0.44
1:D:1159:THR:O	1:D:1160:SER:CB	2.64	0.44
1:C:1133:ILE:O	1:C:1137:GLN:HG3	2.17	0.44
1:D:1017:LEU:HG	1:F:1034:TYR:CZ	2.52	0.44
1:B:1045:ILE:HD13	1:C:1046:ALA:HB2	2.00	0.44
5:D:1288:HOH:O	1:F:1154:PRO:HD3	2.17	0.44
1:F:1215:GLU:O	1:F:1218:ARG:HB3	2.18	0.44
1:D:1157:VAL:HG12	1:D:1158:THR:H	1.81	0.44
1:D:1185:LYS:HB3	1:F:1176:TRP:CE3	2.52	0.44
1:D:1194:PHE:C	1:D:1208:ILE:HG22	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1207:ALA:C	1:E:1209:ALA:H	2.26	0.44
1:A:1223:GLU:OE1	1:A:1227:ARG:NH2	2.46	0.44
1:C:1200:TYR:O	1:C:1201:THR:C	2.59	0.44
1:D:1185:LYS:HB3	1:F:1176:TRP:CZ3	2.53	0.44
1:D:1213:ILE:HD13	1:D:1216:ARG:HD3	2.00	0.44
1:B:1173:GLN:O	1:B:1232:ILE:HA	2.18	0.43
1:D:1168:VAL:CG1	1:E:1231:LEU:HD23	2.48	0.43
1:A:1002:ALA:HA	1:A:1060:GLN:HE21	1.83	0.43
1:B:1200:TYR:CD1	1:C:1200:TYR:HD2	2.36	0.43
1:E:1180:THR:HG22	1:E:1181:GLY:N	2.32	0.43
1:B:1173:GLN:HG3	5:B:1334:HOH:O	2.17	0.43
1:E:1045:ILE:CD1	1:F:1046:ALA:HB2	2.48	0.43
1:E:1045:ILE:HD11	1:F:1046:ALA:HB2	2.00	0.43
1:A:1026:VAL:HG22	1:A:1027:PHE:CD2	2.53	0.43
1:A:1016:ARG:HA	1:A:1016:ARG:HD3	1.71	0.43
1:D:1193:THR:HB	1:D:1211:ALA:CB	2.49	0.43
1:F:1017:LEU:HD11	1:F:1035:VAL:HG12	1.99	0.43
1:A:1001:MET:N	5:A:1424:HOH:O	2.51	0.43
1:A:1015:THR:O	1:A:1016:ARG:HB2	2.19	0.43
1:A:1163:VAL:CG2	1:B:1171:ALA:HA	2.48	0.43
1:D:1174:THR:HG22	1:D:1175:GLY:N	2.33	0.43
1:D:1222:MET:HE3	1:E:1222:MET:CE	2.48	0.43
1:A:1212:LEU:HD13	1:A:1212:LEU:C	2.44	0.43
1:C:1013:GLN:HB3	5:C:1675:HOH:O	2.18	0.43
1:C:1081:ARG:O	1:C:1081:ARG:HD3	2.18	0.43
1:D:1190:ALA:O	1:D:1191:ASP:C	2.61	0.43
1:C:1017:LEU:CD1	1:C:1035:VAL:HG13	2.48	0.43
1:D:1145:ALA:O	1:F:1153:SER:HB3	2.19	0.43
1:D:1217:ARG:O	1:D:1220:LYS:HB3	2.17	0.43
1:E:1076:ARG:HH22	1:F:1074:GLU:CD	2.24	0.43
1:C:1034:TYR:CD1	1:C:1034:TYR:C	2.97	0.43
1:D:1082:ILE:HG12	5:D:1375:HOH:O	2.19	0.43
1:D:1146:THR:O	1:F:1153:SER:HB2	2.18	0.43
1:F:1015:THR:HG21	1:F:1016:ARG:NE	2.32	0.43
1:F:1169:VAL:CG1	1:F:1170:GLY:N	2.82	0.43
1:A:1015:THR:HB	1:A:1016:ARG:H	1.35	0.42
1:D:1157:VAL:O	1:F:1163:VAL:HA	2.19	0.42
1:E:997:ARG:HG3	1:E:999:SER:HB2	2.01	0.42
1:A:1098:ILE:HG12	1:B:1098:ILE:CD1	2.48	0.42
1:C:1196:VAL:CG1	1:C:1197:SER:N	2.71	0.42
1:D:1179:ALA:HB3	1:D:1220:LYS:CE	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1073:HIS:HD2	5:F:1234:HOH:O	2.01	0.42
1:E:1094:ASN:O	1:E:1098:ILE:HG13	2.19	0.42
1:A:1168:VAL:CG1	1:A:1169:VAL:HG23	2.40	0.42
1:D:1015:THR:O	1:D:1016:ARG:C	2.62	0.42
1:D:1183:ALA:HA	1:D:1217:ARG:HB2	2.00	0.42
1:E:1208:ILE:C	1:E:1210:ASN:H	2.28	0.42
5:A:1249:HOH:O	1:E:1000:HIS:HB2	2.19	0.42
1:B:1216:ARG:CZ	1:C:1192:LEU:HD11	2.49	0.42
1:D:1194:PHE:HB3	5:D:1417:HOH:O	2.18	0.42
1:F:1038:GLN:O	1:F:1042:VAL:HG23	2.19	0.42
1:F:1081:ARG:O	1:F:1081:ARG:HD3	2.19	0.42
1:C:1029:LYS:HG2	1:C:1030:SER:H	1.82	0.42
1:F:1017:LEU:HD23	1:F:1021:ILE:HD11	2.01	0.42
1:F:1167:LYS:NZ	5:F:1510:HOH:O	2.48	0.42
1:A:1200:TYR:HD1	1:C:1200:TYR:CD2	2.37	0.42
5:A:1255:HOH:O	1:E:998:GLY:HA3	2.19	0.42
1:B:997:ARG:O	1:B:997:ARG:HG3	2.17	0.42
1:B:1232:ILE:O	1:B:1233:ASP:C	2.62	0.42
1:D:1104:ARG:NH1	1:E:1102:ASN:OD1	2.51	0.42
1:E:1190:ALA:O	1:E:1191:ASP:CB	2.67	0.42
1:A:1013:GLN:O	1:A:1014:ALA:HB3	2.20	0.42
1:F:1056:ALA:O	1:F:1060:GLN:HG3	2.19	0.42
1:A:1010:VAL:HG13	1:C:1048:LYS:HB2	2.02	0.42
1:A:1222:MET:CB	1:B:1222:MET:HE1	2.49	0.42
1:A:1222:MET:CE	1:C:1223:GLU:HA	2.50	0.42
1:D:1191:ASP:HB3	1:F:1217:ARG:HE	1.85	0.42
1:D:1189:ASP:O	1:D:1190:ALA:C	2.63	0.42
1:A:1073:HIS:CD2	5:C:1669:HOH:O	2.60	0.41
1:D:1017:LEU:HD23	1:D:1021:ILE:HD11	2.01	0.41
1:D:1130:GLU:CD	1:F:1125:ARG:HH21	2.28	0.41
1:A:1218:ARG:HG3	1:A:1218:ARG:HH11	1.84	0.41
1:C:1024:ARG:O	1:C:1025:ASN:CG	2.64	0.41
1:F:1066:GLN:O	1:F:1070:LEU:HB2	2.19	0.41
1:C:1013:GLN:CB	1:D:1127:THR:HG21	2.48	0.41
1:C:1017:LEU:HD23	1:C:1021:ILE:HD11	2.02	0.41
1:B:1027:PHE:HB2	1:B:1032:LEU:HD13	2.02	0.41
1:C:1011:VAL:HA	5:C:1516:HOH:O	2.21	0.41
1:D:1157:VAL:HG22	1:E:1151:LEU:HD22	2.01	0.41
1:C:1023:PRO:HD2	1:C:1027:PHE:CZ	2.55	0.41
1:E:1213:ILE:O	1:E:1217:ARG:CG	2.68	0.41
1:C:1028:SER:HB2	1:C:1029:LYS:H	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1197:SER:OG	1:C:1198:ASP:N	2.47	0.41
1:D:1038:GLN:O	1:D:1042:VAL:HG23	2.21	0.41
1:C:1173:GLN:HB3	5:C:1520:HOH:O	2.20	0.41
1:D:1133:ILE:O	1:D:1136:LEU:N	2.54	0.41
1:E:1008:ASN:HD22	1:E:1009:PRO:HD2	1.84	0.41
1:E:1023:PRO:HB2	1:E:1026:VAL:HG22	2.03	0.41
1:E:1115:LEU:HD23	5:E:1559:HOH:O	2.20	0.41
1:F:1174:THR:HG23	5:F:1259:HOH:O	2.20	0.41
1:F:1176:TRP:CE3	1:F:1223:GLU:OE1	2.74	0.41
1:A:1196:VAL:HG23	1:A:1196:VAL:O	2.21	0.41
1:B:1022:LEU:HA	1:B:1023:PRO:HD3	1.85	0.41
1:C:1012:ILE:CD1	1:C:1043:GLY:HA2	2.51	0.41
1:D:1219:THR:HG23	1:E:1222:MET:HE2	2.02	0.41
1:F:1204:GLU:N	1:F:1204:GLU:CD	2.79	0.41
1:A:1024:ARG:NH2	5:A:1450:HOH:O	2.53	0.41
1:D:1027:PHE:HB2	1:D:1032:LEU:CD1	2.51	0.41
1:D:1156:ASN:ND2	1:F:1165:GLY:H	1.98	0.41
1:E:1174:THR:HG22	5:E:1490:HOH:O	2.20	0.41
1:B:1159:THR:O	1:B:1160:SER:CB	2.62	0.40
1:C:1179:ALA:O	1:C:1220:LYS:HE2	2.21	0.40
1:D:1183:ALA:HB2	1:D:1220:LYS:HB3	2.03	0.40
1:D:1185:LYS:HG3	1:F:1176:TRP:CA	2.42	0.40
1:A:1026:VAL:HG21	1:C:1026:VAL:CG2	2.50	0.40
1:B:1024:ARG:CD	1:B:1024:ARG:C	2.87	0.40
1:C:1016:ARG:O	1:C:1016:ARG:HG3	2.13	0.40
1:D:1147:THR:O	1:D:1148:SER:O	2.39	0.40
1:D:1157:VAL:CG1	1:D:1158:THR:N	2.85	0.40
1:D:1176:TRP:HB2	1:D:1233:ASP:O	2.21	0.40
1:E:999:SER:C	1:E:1000:HIS:O	2.64	0.40
1:B:1174:THR:HB	1:B:1233:ASP:OD2	2.21	0.40
1:A:1017:LEU:O	1:A:1017:LEU:CD2	2.65	0.40
1:B:1166:LYS:HA	1:B:1166:LYS:CE	2.46	0.40
1:C:1023:PRO:HA	1:C:1024:ARG:HH11	1.87	0.40
1:F:1011:VAL:O	1:F:1011:VAL:HG22	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	A	231/242 (96%)	219 (95%)	7 (3%)	5 (2%)	5	1
1	B	240/242 (99%)	231 (96%)	5 (2%)	4 (2%)	7	2
1	C	231/242 (96%)	206 (89%)	13 (6%)	12 (5%)	1	0
1	D	217/242 (90%)	197 (91%)	14 (6%)	6 (3%)	4	1
1	E	222/242 (92%)	208 (94%)	9 (4%)	5 (2%)	5	1
1	F	217/242 (90%)	205 (94%)	6 (3%)	6 (3%)	4	1
All	All	1358/1452 (94%)	1266 (93%)	54 (4%)	38 (3%)	4	1

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1014	ALA
1	A	1159	THR
1	A	1199	THR
1	B	1200	TYR
1	C	1016	ARG
1	C	1196	VAL
1	C	1198	ASP
1	C	1203	SER
1	C	1204	GLU
1	D	1137	GLN
1	D	1148	SER
1	D	1182	THR
1	D	1191	ASP
1	E	1160	SER
1	F	1016	ARG
1	F	1208	ILE
1	A	1013	GLN
1	B	1159	THR
1	C	1028	SER
1	C	1202	GLN

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Mol	Chain	Res	Type
1	F	1204	GLU
1	B	1201	THR
1	C	1160	SER
1	C	1189	ASP
1	B	993	ALA
1	C	1025	ASN
1	C	1026	VAL
1	C	1193	THR
1	D	1187	VAL
1	E	1000	HIS
1	F	1017	LEU
1	E	1178	ALA
1	E	1190	ALA
1	F	1018	ASP
1	D	1181	GLY
1	E	1191	ASP
1	A	1026	VAL
1	F	1168	VAL

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	184/190 (97%)	164 (89%)	20 (11%)	6	1
1	B	190/190 (100%)	179 (94%)	11 (6%)	18	7
1	C	183/190 (96%)	163 (89%)	20 (11%)	6	1
1	D	173/190 (91%)	152 (88%)	21 (12%)	5	1
1	E	176/190 (93%)	161 (92%)	15 (8%)	10	3
1	F	173/190 (91%)	153 (88%)	20 (12%)	5	1
All	All	1079/1140 (95%)	972 (90%)	107 (10%)	7	1

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1010	VAL
1	A	1012	ILE
1	A	1013	GLN
1	A	1015	THR
1	A	1017	LEU
1	A	1024	ARG
1	A	1026	VAL
1	A	1032	LEU
1	A	1054	GLN
1	A	1062	LYS
1	A	1092	THR
1	A	1111	GLU
1	A	1123	ASP
1	A	1144	THR
1	A	1151	LEU
1	A	1155	LEU
1	A	1157	VAL
1	A	1163	VAL
1	A	1168	VAL
1	A	1192	LEU
1	B	1016	ARG
1	B	1026	VAL
1	B	1036	ILE
1	B	1065	GLU
1	B	1155	LEU
1	B	1163	VAL
1	B	1173	GLN
1	B	1182	THR
1	B	1198	ASP
1	B	1202	GLN
1	B	1233	ASP
1	C	1011	VAL
1	C	1016	ARG
1	C	1017	LEU
1	C	1018	ASP
1	C	1024	ARG
1	C	1025	ASN
1	C	1026	VAL
1	C	1033	LEU
1	C	1096	LYS
1	C	1142	SER
1	C	1155	LEU
1	C	1157	VAL

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Mol	Chain	Res	Type
1	C	1163	VAL
1	C	1168	VAL
1	C	1192	LEU
1	C	1202	GLN
1	C	1204	GLU
1	C	1205	ILE
1	C	1210	ASN
1	C	1212	LEU
1	D	1001	MET
1	D	1011	VAL
1	D	1017	LEU
1	D	1026	VAL
1	D	1032	LEU
1	D	1062	LYS
1	D	1079	GLN
1	D	1123	ASP
1	D	1144	THR
1	D	1149	GLN
1	D	1160	SER
1	D	1163	VAL
1	D	1166	LYS
1	D	1169	VAL
1	D	1184	ASN
1	D	1185	LYS
1	D	1194	PHE
1	D	1208	ILE
1	D	1223	GLU
1	D	1224	ASP
1	D	1233	ASP
1	E	1001	MET
1	E	1011	VAL
1	E	1015	THR
1	E	1016	ARG
1	E	1017	LEU
1	E	1024	ARG
1	E	1026	VAL
1	E	1035	VAL
1	E	1122	LEU
1	E	1147	THR
1	E	1155	LEU
1	E	1166	LYS
1	E	1187	VAL

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Mol	Chain	Res	Type
1	E	1193	THR
1	E	1220	LYS
1	F	1011	VAL
1	F	1016	ARG
1	F	1017	LEU
1	F	1018	ASP
1	F	1026	VAL
1	F	1032	LEU
1	F	1062	LYS
1	F	1070	LEU
1	F	1103	VAL
1	F	1115	LEU
1	F	1163	VAL
1	F	1168	VAL
1	F	1172	ARG
1	F	1173	GLN
1	F	1180	THR
1	F	1185	LYS
1	F	1204	GLU
1	F	1205	ILE
1	F	1208	ILE
1	F	1231	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1008	ASN
1	A	1038	GLN
1	A	1054	GLN
1	A	1060	GLN
1	A	1073	HIS
1	A	1116	GLN
1	A	1131	ASN
1	A	1149	GLN
1	A	1173	GLN
1	A	1202	GLN
1	A	1210	ASN
1	B	1008	ASN
1	B	1073	HIS
1	B	1131	ASN
1	B	1137	GLN
1	B	1173	GLN

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Mol	Chain	Res	Type
1	B	1202	GLN
1	B	1206	GLN
1	B	1210	ASN
1	C	1008	ASN
1	C	1038	GLN
1	C	1060	GLN
1	C	1102	ASN
1	C	1131	ASN
1	C	1156	ASN
1	C	1202	GLN
1	C	1210	ASN
1	D	1013	GLN
1	D	1060	GLN
1	D	1073	HIS
1	D	1094	ASN
1	D	1131	ASN
1	D	1156	ASN
1	D	1184	ASN
1	D	1210	ASN
1	E	1008	ASN
1	E	1073	HIS
1	E	1094	ASN
1	E	1131	ASN
1	E	1137	GLN
1	E	1149	GLN
1	E	1173	GLN
1	E	1184	ASN
1	F	1025	ASN
1	F	1050	ASN
1	F	1094	ASN
1	F	1102	ASN
1	F	1118	ASN
1	F	1131	ASN
1	F	1149	GLN
1	F	1173	GLN
1	F	1210	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 18 are 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

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	233/242 (96%)	0.58	20 (8%)	16 19	15, 33, 63, 99	0
1	B	242/242 (100%)	0.58	20 (8%)	17 20	10, 34, 60, 88	0
1	C	233/242 (96%)	0.83	41 (17%)	4 4	13, 33, 86, 112	0
1	D	221/242 (91%)	1.10	46 (20%)	2 2	18, 38, 80, 97	0
1	E	226/242 (93%)	0.81	30 (13%)	7 8	10, 37, 78, 98	0
1	F	221/242 (91%)	0.87	34 (15%)	5 5	18, 35, 73, 91	0
All	All	1376/1452 (94%)	0.79	191 (13%)	6 7	10, 35, 75, 112	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1193	THR	7.4
1	C	1201	THR	6.7
1	E	1208	ILE	6.1
1	D	1211	ALA	6.0
1	C	1192	LEU	5.9
1	D	1185	LYS	5.5
1	E	998	GLY	5.4
1	D	1190	ALA	5.3
1	D	1176	TRP	5.1
1	B	1200	TYR	4.9
1	D	1194	PHE	4.8
1	F	1205	ILE	4.8
1	E	1159	THR	4.7
1	C	1113	ALA	4.6
1	C	1015	THR	4.6
1	F	1213	ILE	4.6
1	C	1017	LEU	4.6
1	D	1192	LEU	4.6
1	E	1190	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	1202	GLN	4.3
1	F	1206	GLN	4.3
1	F	1176	TRP	4.3
1	C	1199	THR	4.3
1	A	1014	ALA	4.3
1	D	1178	ALA	4.3
1	E	1163	VAL	4.0
1	E	1209	ALA	4.0
1	C	1014	ALA	3.9
1	E	1194	PHE	3.9
1	C	1027	PHE	3.9
1	D	1191	ASP	3.9
1	D	1233	ASP	3.8
1	A	1016	ARG	3.8
1	A	1013	GLN	3.8
1	C	1205	ILE	3.8
1	F	1208	ILE	3.8
1	F	1174	THR	3.7
1	E	1188	PHE	3.7
1	E	1000	HIS	3.7
1	C	1233	ASP	3.7
1	D	1186	GLY	3.7
1	D	1179	ALA	3.6
1	A	1158	THR	3.6
1	E	997	ARG	3.6
1	C	1033	LEU	3.6
1	F	1159	THR	3.5
1	D	1011	VAL	3.5
1	B	1206	GLN	3.5
1	C	1203	SER	3.5
1	D	1169	VAL	3.4
1	F	1209	ALA	3.4
1	C	1197	SER	3.4
1	A	1012	ILE	3.3
1	D	1182	THR	3.3
1	F	1186	GLY	3.3
1	C	1159	THR	3.3
1	F	1018	ASP	3.3
1	A	1011	VAL	3.2
1	F	1214	THR	3.2
1	D	1189	ASP	3.2
1	E	1189	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	1183	ALA	3.2
1	D	1209	ALA	3.2
1	E	1193	THR	3.2
1	F	1204	GLU	3.2
1	B	1178	ALA	3.1
1	D	1207	ALA	3.1
1	F	1178	ALA	3.1
1	D	1130	GLU	3.1
1	F	1135	ALA	3.1
1	E	1192	LEU	3.0
1	C	1195	ALA	3.0
1	F	1221	ALA	3.0
1	A	1032	LEU	3.0
1	D	1225	ALA	3.0
1	C	1207	ALA	3.0
1	F	1233	ASP	2.9
1	E	1001	MET	2.9
1	E	1195	ALA	2.9
1	A	1197	SER	2.9
1	C	1012	ILE	2.9
1	E	1018	ASP	2.9
1	C	1206	GLN	2.8
1	F	1207	ALA	2.8
1	C	1204	GLU	2.8
1	A	1025	ASN	2.8
1	C	1032	LEU	2.8
1	E	1103	VAL	2.8
1	C	1190	ALA	2.8
1	C	1193	THR	2.8
1	E	1158	THR	2.8
1	D	1168	VAL	2.8
1	F	1227	ARG	2.8
1	D	1148	SER	2.7
1	C	1026	VAL	2.7
1	F	1181	GLY	2.7
1	C	1041	ASP	2.7
1	A	1021	ILE	2.7
1	F	1225	ALA	2.7
1	D	1208	ILE	2.7
1	B	1196	VAL	2.7
1	A	1017	LEU	2.6
1	B	1201	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	1200	TYR	2.6
1	D	1213	ILE	2.6
1	E	1185	LYS	2.6
1	D	1228	ALA	2.6
1	C	1040	THR	2.6
1	F	1182	THR	2.6
1	D	1008	ASN	2.5
1	C	1011	VAL	2.5
1	B	1024	ARG	2.5
1	D	1224	ASP	2.5
1	D	1210	ASN	2.5
1	D	1135	ALA	2.5
1	D	1159	THR	2.5
1	D	1187	VAL	2.5
1	F	1173	GLN	2.5
1	C	1034	TYR	2.5
1	E	1221	ALA	2.5
1	A	1200	TYR	2.4
1	C	1210	ASN	2.4
1	D	1188	PHE	2.4
1	B	1205	ILE	2.4
1	E	1164	GLY	2.4
1	A	1040	THR	2.4
1	D	1144	THR	2.4
1	E	1145	ALA	2.4
1	F	1171	ALA	2.4
1	C	1013	GLN	2.4
1	F	1184	ASN	2.4
1	A	1175	GLY	2.4
1	F	1177	THR	2.3
1	E	1016	ARG	2.3
1	B	1199	THR	2.3
1	C	1024	ARG	2.3
1	E	1024	ARG	2.3
1	F	1232	ILE	2.3
1	A	1193	THR	2.3
1	C	1029	LYS	2.3
1	E	1214	THR	2.3
1	F	1219	THR	2.3
1	B	1183	ALA	2.2
1	F	1179	ALA	2.2
1	B	1233	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	1123	ASP	2.2
1	A	1199	THR	2.2
1	D	1122	LEU	2.2
1	B	1209	ALA	2.2
1	C	1194	PHE	2.2
1	D	1217	ARG	2.2
1	F	1168	VAL	2.2
1	A	1198	ASP	2.2
1	F	1145	ALA	2.2
1	E	1232	ILE	2.2
1	F	1185	LYS	2.2
1	D	1180	THR	2.2
1	D	1214	THR	2.2
1	C	1198	ASP	2.2
1	C	1020	SER	2.2
1	C	1134	SER	2.2
1	A	1019	ALA	2.2
1	F	1138	ALA	2.2
1	F	1190	ALA	2.2
1	B	1168	VAL	2.1
1	B	1182	THR	2.1
1	D	1139	ASP	2.1
1	C	1035	VAL	2.1
1	D	1136	LEU	2.1
1	E	1154	PRO	2.1
1	B	992	GLY	2.1
1	D	1118	ASN	2.1
1	D	1152	ALA	2.1
1	B	1016	ARG	2.1
1	C	1028	SER	2.1
1	A	1001	MET	2.1
1	B	1026	VAL	2.1
1	B	1179	ALA	2.1
1	B	1144	THR	2.0
1	E	1177	THR	2.0
1	B	1186	GLY	2.0
1	D	1068	VAL	2.0
1	B	1195	ALA	2.0
1	C	1019	ALA	2.0
1	E	1211	ALA	2.0
1	D	1175	GLY	2.0
1	D	1181	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	1144	THR	2.0
1	F	1180	THR	2.0
1	A	1026	VAL	2.0
1	C	1196	VAL	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
2	XE	D	11	1/1	0.89	0.20	121,121,121,121	0
2	XE	D	14	1/1	0.89	0.20	122,122,122,122	0
2	XE	A	7	1/1	0.90	0.13	96,96,96,96	0
2	XE	F	10	1/1	0.95	0.09	65,65,65,65	0
4	CL	D	4	1/1	0.95	0.05	33,33,33,33	0
3	CA	A	1	1/1	0.98	0.03	21,21,21,21	0
4	CL	A	2	1/1	0.98	0.03	28,28,28,28	0
2	XE	C	4	1/1	0.98	0.17	73,73,73,73	0
2	XE	A	1234	1/1	0.99	0.09	59,59,59,59	0
2	XE	D	12	1/1	0.99	0.04	35,35,35,35	0
3	CA	D	3	1/1	0.99	0.05	23,23,23,23	0
2	XE	D	13	1/1	0.99	0.02	35,35,35,35	0
2	XE	D	8	1/1	0.99	0.05	33,33,33,33	0
2	XE	D	9	1/1	1.00	0.01	32,32,32,32	0
2	XE	A	6	1/1	1.00	0.01	31,31,31,31	0
2	XE	A	1235	1/1	1.00	0.01	34,34,34,34	0
2	XE	A	3	1/1	1.00	0.04	39,39,39,39	0
2	XE	A	5	1/1	1.00	0.01	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.