



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:51 PM UTC

PDB ID : 2WAQ / pdb_00002waq
Title : The complete structure of the archaeal 13-subunit DNA-directed RNA Polymerase
Authors : Korkhin, Y.; Unligil, U.M.; Littlefield, O.; Nelson, P.J.; Stuart, D.I.; Sigler, P.B.; Bell, S.D.; Abrescia, N.G.A.
Deposited on : 2009-02-11
Resolution : 3.35 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:

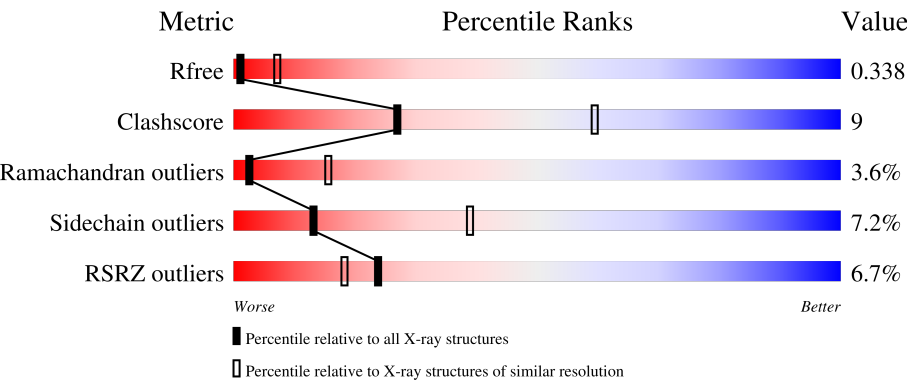
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.35 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	880	6% 67% 25% . .
2	B	1131	5% 66% 26% . .
3	C	395	9% 62% 27% 5% 7%
4	D	265	3% 82% 16% ..
5	E	180	14% 76% 19% . .

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Mol	Chain	Length	Quality of chain
6	F	113	
7	G	132	
8	H	84	
9	K	95	
10	L	92	
11	N	66	
12	P	48	
13	Q	104	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 26471 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 DNA-DIRECTED RNA POLYMERASE RPO1N SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	841	Total	C	N	O	S	0	0	0
			6691	4256	1183	1226	26			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE RPO2 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1090	Total	C	N	O	S	0	0	0
			8652	5484	1534	1605	29			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE RPO1C SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	367	Total	C	N	O	S	0	0	0
			2833	1797	481	547	8			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE RPO3 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	260	Total	C	N	O	S	0	0	0
			2071	1332	334	392	13			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASE RPO7 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	174	Total	C	N	O	S	0	0	0
			1384	893	232	255	4			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASE RPO4 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	90	Total	C	N	O	S	0	0	0
			701	439	114	145	3			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE RPO8 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	113	Total	C	N	O	S	0	0	0
			901	572	152	173	4			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASE RPO5 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	74	Total	C	N	O	S	0	0	0
			609	396	108	105				

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE RPO6 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	82	Total	C	N	O	S	0	0	0
			658	420	121	116	1			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASE RPO11 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	91	Total	C	N	O	S	0	0	0
			707	454	114	137	2			

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE RPO10 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	N	64	Total	C	N	O	S	0	0	0
			514	327	93	87	7			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASE RPO12 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	P	43	Total	C	N	O	S	0	0	0
			346	230	58	53	5			

- Molecule 13 is a protein called DNA-DIRECTED RNA POLYMERASE RPO13 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	Q	45	Total	C	N	O	S	0	0	0
			387	243	68	75	1			

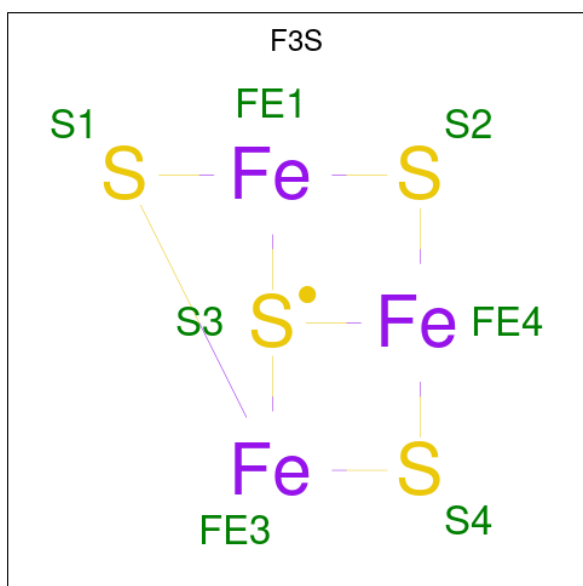
- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	3	Total 3	Zn 3	0	0
14	B	3	Total 3	Zn 3	0	0
14	C	1	Total 1	Zn 1	0	0
14	N	1	Total 1	Zn 1	0	0
14	P	1	Total 1	Zn 1	0	0

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total 1	Mg 1	0	0

- Molecule 16 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe₃S₄).

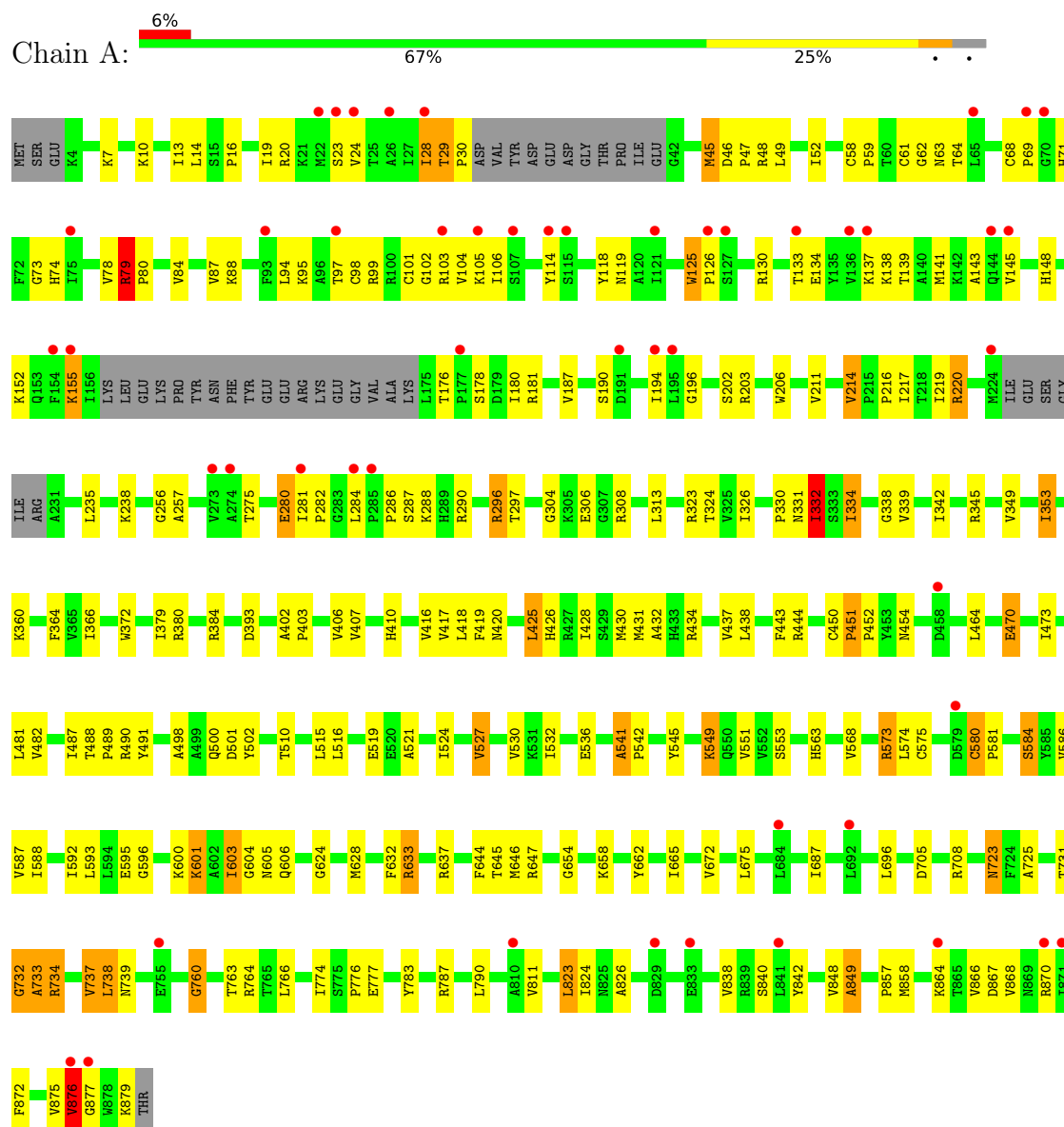


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	D	1	Total 7	Fe 3	S 4	0	0

3 Residue-property plots [i](#)

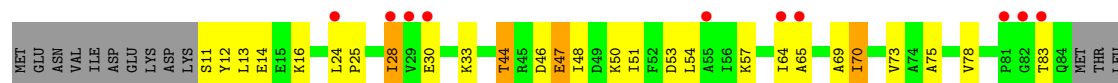
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

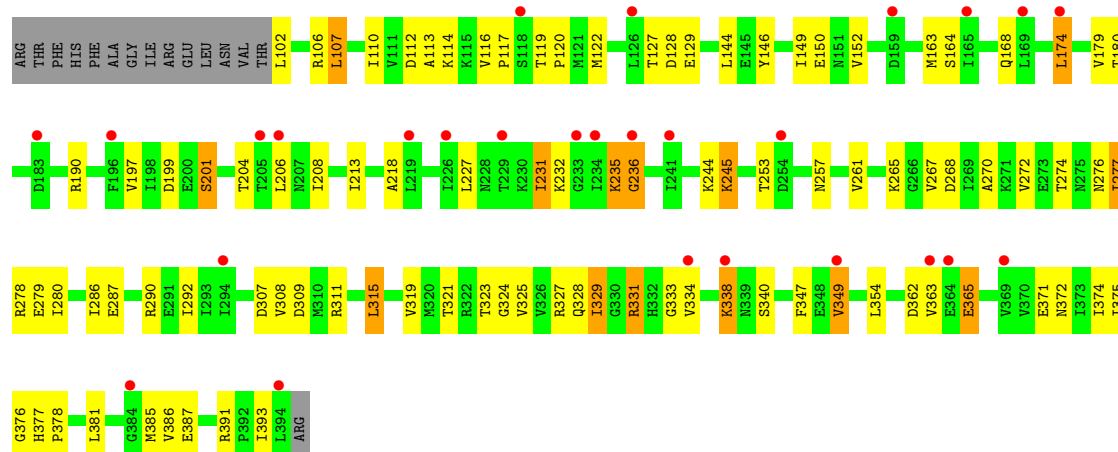
• Molecule 1: DNA-DIRECTED RNA POLYMERASE RPO1N SUBUNIT



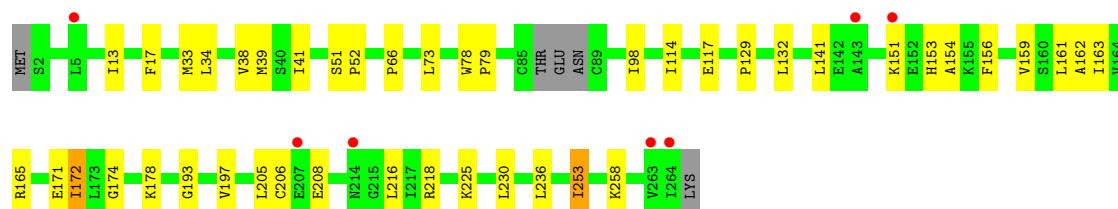
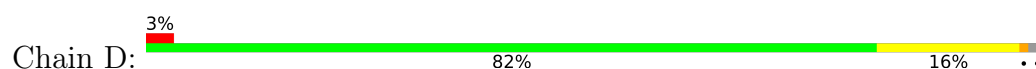
• Molecule 2: DNA-DIRECTED RNA POLYMERASE RPO2 SUBUNIT



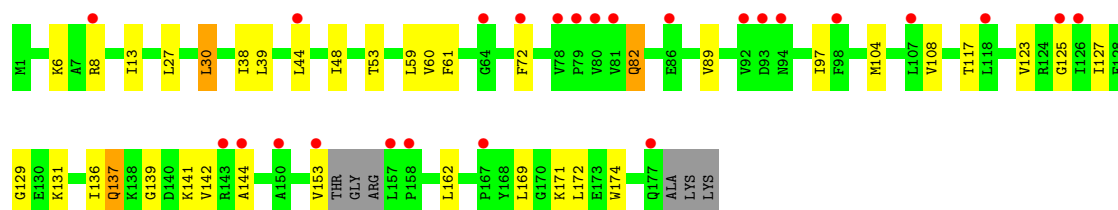
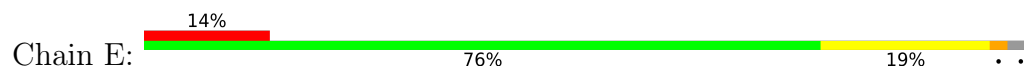




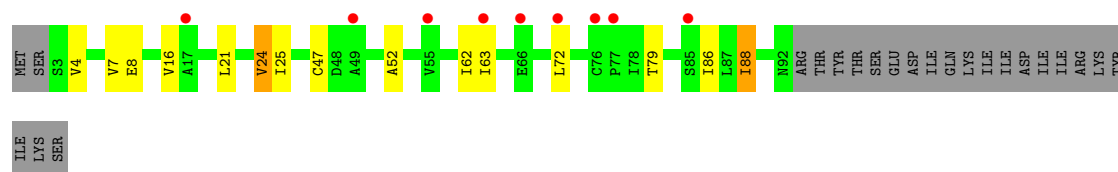
• Molecule 4: DNA-DIRECTED RNA POLYMERASE RPO3 SUBUNIT



• Molecule 5: DNA-DIRECTED RNA POLYMERASE RPO7 SUBUNIT

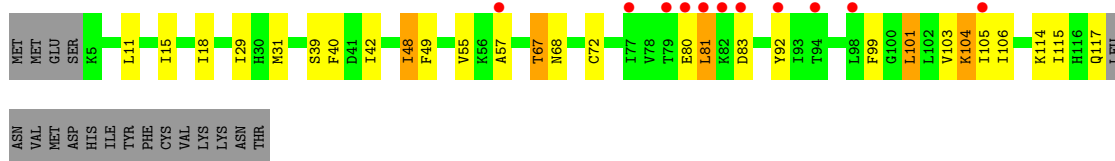


• Molecule 6: DNA-DIRECTED RNA POLYMERASE RPO4 SUBUNIT



• Molecule 7: DNA-DIRECTED RNA POLYMERASE RPO8 SUBUNIT

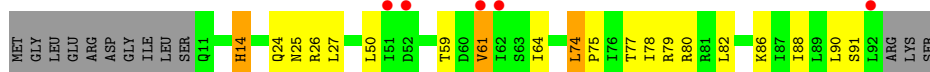




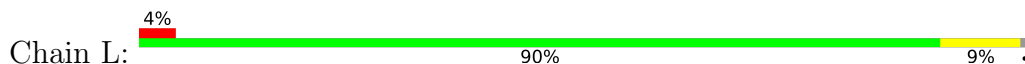
• Molecule 8: DNA-DIRECTED RNA POLYMERASE RPO5 SUBUNIT



• Molecule 9: DNA-DIRECTED RNA POLYMERASE RPO6 SUBUNIT



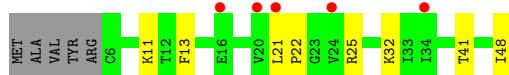
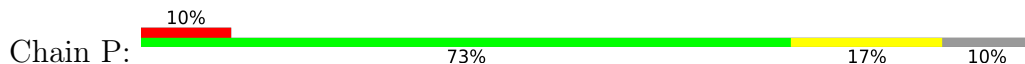
• Molecule 10: DNA-DIRECTED RNA POLYMERASE RPO11 SUBUNIT



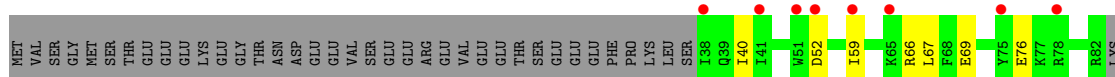
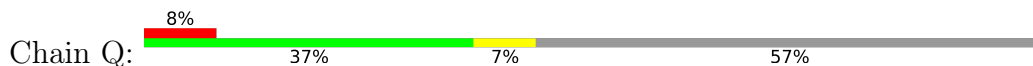
• Molecule 11: DNA-DIRECTED RNA POLYMERASE RPO10 SUBUNIT



• Molecule 12: DNA-DIRECTED RNA POLYMERASE RPO12 SUBUNIT



• Molecule 13: DNA-DIRECTED RNA POLYMERASE RPO13 SUBUNIT



ALA
LYS
LYS
LYS
ALA
ALA
SER
LYS
LYS
VAL
LYS
LYS
LYS
THR
LYS
LYS
LYS
GLU
LYS
SER
VAL
GLU
GLY

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	193.50Å 212.62Å 129.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.78 – 3.35 42.78 – 3.35	Depositor EDS
% Data completeness (in resolution range)	77.0 (42.78-3.35) 77.0 (42.78-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.271 , 0.341 0.270 , 0.338	Depositor DCC
R_{free} test set	3220 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	72.2	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	26471	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: MG, F3S, ZN

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	0/6834	0.83	9/9247 (0.1%)
2	B	0.46	0/8816	0.83	10/11926 (0.1%)
3	C	0.52	0/2857	0.86	1/3847 (0.0%)
4	D	0.43	0/2106	0.77	2/2845 (0.1%)
5	E	0.52	0/1405	0.78	2/1899 (0.1%)
6	F	0.50	0/709	0.76	0/961
7	G	0.47	0/913	0.72	1/1224 (0.1%)
8	H	0.58	1/623 (0.2%)	0.89	2/845 (0.2%)
9	K	0.47	0/667	0.78	0/903
10	L	0.41	0/717	0.78	0/968
11	N	0.48	0/524	0.82	0/706
12	P	0.51	0/354	0.74	0/475
13	Q	0.47	0/391	0.79	0/522
All	All	0.47	1/26916 (0.0%)	0.82	27/36368 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	20	HIS	ND1-CE1	5.17	1.37	1.32

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	20	HIS	CB-CG-CD2	-6.66	122.55	131.20
4	D	78	TRP	CA-C-N	6.55	128.03	119.84
4	D	78	TRP	C-N-CA	6.55	128.03	119.84
1	A	79	ARG	CA-C-N	6.16	126.17	119.89
1	A	79	ARG	C-N-CA	6.16	126.17	119.89
1	A	811	VAL	N-CA-C	5.98	114.96	106.53
1	A	877	GLY	N-CA-C	-5.80	108.29	114.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	20	HIS	CB-CG-ND1	5.78	131.37	122.70
3	C	116	VAL	N-CA-C	5.72	112.76	107.56
1	A	176	THR	CA-C-N	5.51	125.61	119.32
1	A	176	THR	C-N-CA	5.51	125.61	119.32
2	B	1071	GLY	N-CA-C	5.48	118.24	111.93
2	B	599	LYS	CB-CA-C	-5.43	110.29	116.54
2	B	464	GLY	CA-C-N	5.40	125.11	119.82
2	B	464	GLY	C-N-CA	5.40	125.11	119.82
2	B	780	GLU	CA-C-N	5.37	126.55	119.84
2	B	780	GLU	C-N-CA	5.37	126.55	119.84
7	G	81	LEU	N-CA-C	-5.31	107.46	114.31
2	B	778	MET	CA-C-N	5.25	125.54	119.92
2	B	778	MET	C-N-CA	5.25	125.54	119.92
5	E	13	ILE	CA-C-N	5.19	123.39	119.66
5	E	13	ILE	C-N-CA	5.19	123.39	119.66
1	A	451	PRO	N-CA-C	5.16	116.99	110.70
2	B	951	THR	CA-C-N	5.06	125.06	119.90
2	B	951	THR	C-N-CA	5.06	125.06	119.90
1	A	214	VAL	CA-C-N	5.00	123.31	119.66
1	A	214	VAL	C-N-CA	5.00	123.31	119.66

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	6691	0	6758	150	0
2	B	8652	0	8795	203	0
3	C	2833	0	2992	80	0
4	D	2071	0	2116	25	0
5	E	1384	0	1444	16	0
6	F	701	0	708	7	0
7	G	901	0	912	14	0
8	H	609	0	640	13	0
9	K	658	0	692	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	L	707	0	739	3	0
11	N	514	0	528	15	0
12	P	346	0	375	4	0
13	Q	387	0	388	2	0
14	A	3	0	0	0	0
14	B	3	0	0	0	0
14	C	1	0	0	0	0
14	N	1	0	0	0	0
14	P	1	0	0	0	0
15	A	1	0	0	0	0
16	D	7	0	0	0	0
All	All	26471	0	27087	490	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 9.

All (490) 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:867:ASP:HA	1:A:870:ARG:HH22	1.14	1.12
2:B:110:ILE:HA	2:B:111:GLU:HB2	1.10	1.07
2:B:110:ILE:HA	2:B:111:GLU:CB	1.86	1.03
2:B:110:ILE:CA	2:B:111:GLU:HB2	1.96	0.95
2:B:953:ILE:HD13	2:B:953:ILE:H	1.35	0.92
3:C:64:ILE:HG22	3:C:65:ALA:H	1.37	0.89
2:B:1069:TYR:HA	2:B:1070:ILE:HB	1.56	0.84
3:C:244:LYS:HA	3:C:245:LYS:HB3	1.58	0.84
1:A:867:ASP:HA	1:A:870:ARG:NH2	1.94	0.82
11:N:8:PHE:CD1	11:N:48:MET:HE1	2.15	0.81
8:H:45:ILE:O	8:H:81:VAL:HA	1.82	0.80
1:A:600:LYS:O	1:A:601:LYS:HB2	1.82	0.79
2:B:884:ARG:NH1	2:B:992:TYR:HB3	2.00	0.76
1:A:63:ASN:HB2	1:A:68:CYS:HB2	1.66	0.75
1:A:342:ILE:HD13	1:A:345:ARG:HH12	1.50	0.75
2:B:905:LYS:H	2:B:905:LYS:HE2	1.51	0.75
1:A:875:VAL:HG12	1:A:876:VAL:H	1.52	0.74
2:B:1069:TYR:CA	2:B:1070:ILE:HB	2.16	0.74
1:A:553:SER:OG	1:A:592:ILE:HA	1.88	0.74
2:B:984:SER:O	2:B:985:ARG:HB2	1.86	0.73
3:C:163:MET:CB	3:C:164:SER:HA	2.17	0.73
1:A:524:ILE:HA	1:A:637:ARG:HG2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ARG:HG2	1:A:235:LEU:HD22	1.73	0.71
13:Q:66:ARG:HG2	13:Q:66:ARG:HH11	1.56	0.70
3:C:163:MET:HB2	3:C:164:SER:HA	1.72	0.70
2:B:256:PHE:HB2	2:B:257:PRO:HD3	1.74	0.69
1:A:235:LEU:HA	1:A:238:LYS:HE3	1.75	0.69
1:A:498:ALA:HB1	1:A:502:TYR:HB2	1.74	0.69
1:A:330:PRO:HG3	2:B:734:GLY:HA2	1.75	0.68
1:A:125:TRP:H	1:A:126:PRO:HD2	1.57	0.68
3:C:274:THR:HG22	3:C:276:ASN:H	1.57	0.68
2:B:1082:CYS:HB3	2:B:1091:LEU:HD21	1.74	0.67
3:C:338:LYS:HE2	3:C:338:LYS:H	1.59	0.67
3:C:117:PRO:HG2	3:C:120:PRO:HB3	1.77	0.67
2:B:954:GLU:HA	2:B:957:GLN:HB2	1.77	0.67
4:D:66:PRO:HG2	11:N:13:LEU:HD11	1.77	0.67
2:B:563:THR:HG22	2:B:564:ASP:H	1.58	0.67
3:C:70:ILE:HA	3:C:73:VAL:HG22	1.77	0.66
3:C:30:GLU:O	3:C:33:LYS:HG2	1.98	0.64
1:A:586:VAL:HA	1:A:596:GLY:HA3	1.79	0.64
1:A:78:VAL:O	1:A:79:ARG:HB2	1.99	0.63
1:A:428:ILE:HG22	1:A:452:PRO:HB3	1.79	0.63
2:B:742:ILE:HG23	2:B:912:ILE:HB	1.79	0.63
2:B:166:THR:HG23	2:B:431:ARG:O	1.99	0.63
1:A:603:ILE:HG21	1:A:632:PHE:HE1	1.63	0.63
1:A:49:LEU:HA	1:A:71:HIS:HB2	1.79	0.62
2:B:333:ARG:O	2:B:334:GLU:HB3	1.97	0.62
1:A:360:LYS:HE2	1:A:364:PHE:HE1	1.63	0.62
1:A:430:MET:HE1	2:B:1031:PHE:HE1	1.64	0.62
1:A:7:LYS:HB2	2:B:1119:GLU:HB2	1.82	0.62
1:A:28:ILE:HG22	1:A:30:PRO:HD2	1.81	0.61
4:D:98:ILE:HD11	4:D:114:ILE:HG12	1.83	0.61
2:B:119:ILE:HG22	2:B:393:VAL:HG21	1.82	0.61
9:K:78:ILE:HB	9:K:90:LEU:HD12	1.82	0.61
2:B:873:ARG:HB3	2:B:999:MET:HE1	1.82	0.61
8:H:65:ILE:HD11	8:H:79:ARG:HG2	1.83	0.61
7:G:15:ILE:HG12	7:G:31:MET:HE2	1.82	0.61
2:B:594:ARG:NH1	2:B:615:LYS:HB2	2.15	0.60
1:A:47:PRO:O	1:A:48:ARG:HB2	2.01	0.60
1:A:125:TRP:N	1:A:126:PRO:HD2	2.16	0.60
2:B:432:VAL:HG21	2:B:456:MET:HE3	1.82	0.60
2:B:703:ARG:HD2	2:B:717:THR:HG22	1.82	0.60
2:B:207:ARG:HB2	2:B:216:SER:OG	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:ARG:HG2	2:B:401:LEU:O	2.02	0.60
5:E:6:LYS:HB2	6:F:8:GLU:HB2	1.84	0.60
1:A:603:ILE:HG21	1:A:632:PHE:CE1	2.37	0.59
3:C:244:LYS:HA	3:C:245:LYS:CB	2.27	0.59
2:B:86:MET:HE3	2:B:686:ASN:ND2	2.17	0.59
2:B:682:LEU:HD23	2:B:719:ARG:HG2	1.84	0.59
2:B:733:THR:HG23	2:B:735:TYR:HB2	1.83	0.59
9:K:80:ARG:HB2	9:K:88:ILE:HB	1.83	0.59
2:B:364:PHE:HE1	2:B:388:VAL:HG13	1.66	0.59
2:B:974:TYR:CE2	2:B:981:LYS:HB3	2.37	0.59
2:B:730:ILE:HG12	2:B:986:ILE:HG21	1.85	0.59
2:B:953:ILE:H	2:B:953:ILE:CD1	2.10	0.58
2:B:1046:MET:HE2	2:B:1046:MET:HA	1.84	0.58
1:A:338:GLY:O	1:A:443:PHE:HA	2.02	0.58
8:H:43:PRO:HB2	8:H:79:ARG:HD3	1.85	0.58
3:C:11:SER:HB2	3:C:14:GLU:HB2	1.83	0.58
1:A:20:ARG:HE	1:A:211:VAL:HG21	1.68	0.58
2:B:1104:ILE:HG23	2:B:1114:PRO:HG2	1.84	0.58
1:A:867:ASP:CA	1:A:870:ARG:HH22	2.02	0.58
4:D:34:LEU:HD22	4:D:151:LYS:HB2	1.84	0.58
1:A:130:ARG:HH11	1:A:196:GLY:HA2	1.68	0.58
1:A:573:ARG:CG	1:A:573:ARG:HH11	2.17	0.57
3:C:277:ILE:HG22	3:C:278:ARG:H	1.69	0.57
3:C:25:PRO:HA	3:C:28:ILE:HA	1.85	0.57
2:B:884:ARG:HH11	2:B:884:ARG:HB2	1.68	0.57
3:C:327:ARG:HB2	3:C:333:GLY:HA3	1.87	0.57
2:B:460:GLU:HG2	2:B:673:SER:HB3	1.86	0.57
2:B:702:GLN:HB2	2:B:723:ASN:HA	1.87	0.57
3:C:152:VAL:HG23	3:C:174:LEU:HD12	1.85	0.57
2:B:70:LYS:O	2:B:72:ARG:N	2.37	0.57
2:B:852:LEU:HB3	2:B:868:ARG:HG2	1.87	0.57
3:C:146:TYR:HD1	3:C:235:LYS:H	1.52	0.56
2:B:31:LEU:HA	2:B:125:MET:HE1	1.87	0.56
1:A:134:GLU:HA	1:A:137:LYS:HD2	1.88	0.56
1:A:431:MET:HE2	1:A:482:VAL:HA	1.88	0.56
1:A:600:LYS:HB2	1:A:732:GLY:HA3	1.86	0.56
2:B:898:VAL:HG21	4:D:34:LEU:HD21	1.87	0.56
2:B:974:TYR:HA	2:B:981:LYS:HA	1.86	0.56
2:B:393:VAL:O	2:B:397:ILE:HB	2.06	0.56
3:C:150:GLU:HG3	3:C:227:LEU:HB3	1.88	0.56
2:B:1074:ASP:HB3	2:B:1075:LYS:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:277:ILE:C	3:C:279:GLU:H	2.14	0.55
2:B:605:ILE:HG12	2:B:606:THR:H	1.71	0.55
2:B:1007:ARG:HH21	2:B:1026:GLU:C	2.13	0.55
2:B:86:MET:HE1	2:B:690:ARG:HD3	1.87	0.55
2:B:52:ILE:N	2:B:53:PRO:HD3	2.20	0.55
1:A:510:THR:O	1:A:549:LYS:HD3	2.07	0.55
2:B:694:ARG:HA	2:B:758:PHE:O	2.06	0.55
1:A:97:THR:HG22	1:A:99:ARG:H	1.72	0.55
2:B:701:PRO:HB2	2:B:720:PRO:HG2	1.89	0.55
7:G:72:CYS:HB3	7:G:114:LYS:HG2	1.89	0.55
3:C:47:GLU:HB3	3:C:50:LYS:HB2	1.89	0.55
1:A:864:LYS:HG3	1:A:864:LYS:O	2.06	0.55
3:C:290:ARG:HA	3:C:321:THR:HG21	1.88	0.55
7:G:80:GLU:HG3	7:G:81:LEU:H	1.71	0.55
2:B:400:ALA:HA	2:B:403:THR:HG22	1.88	0.54
2:B:742:ILE:CG2	2:B:912:ILE:HB	2.37	0.54
1:A:488:THR:HG22	1:A:490:ARG:H	1.71	0.54
5:E:123:VAL:HG22	5:E:125:GLY:H	1.72	0.54
2:B:230:MET:HE2	2:B:230:MET:HA	1.88	0.54
3:C:64:ILE:HG22	3:C:65:ALA:N	2.16	0.54
3:C:331:ARG:H	3:C:331:ARG:HD3	1.73	0.54
4:D:51:SER:HB2	4:D:52:PRO:HD2	1.88	0.54
5:E:60:VAL:HG22	5:E:61:PHE:H	1.72	0.54
5:E:89:VAL:HG13	5:E:139:GLY:HA2	1.90	0.54
1:A:16:PRO:HG2	1:A:181:ARG:HH22	1.72	0.54
3:C:102:LEU:HB2	3:C:106:ARG:HB2	1.88	0.54
4:D:171:GLU:HB2	4:D:218:ARG:HB3	1.90	0.54
1:A:125:TRP:H	1:A:126:PRO:CD	2.20	0.54
8:H:39:PRO:HG3	13:Q:67:LEU:HD11	1.89	0.54
1:A:490:ARG:HD2	1:A:491:TYR:HD1	1.73	0.54
11:N:8:PHE:HD1	11:N:48:MET:HE1	1.69	0.54
1:A:777:GLU:HG3	1:A:783:TYR:HE2	1.72	0.53
1:A:330:PRO:HG3	2:B:734:GLY:CA	2.38	0.53
5:E:141:LYS:HB3	5:E:172:LEU:HD13	1.90	0.53
1:A:603:ILE:HG22	1:A:604:GLY:H	1.74	0.53
3:C:340:SER:HB3	3:C:371:GLU:HG2	1.90	0.53
6:F:72:LEU:HD11	6:F:86:ILE:HG12	1.91	0.53
2:B:972:VAL:HG21	4:D:205:LEU:HB3	1.91	0.53
4:D:174:GLY:HA3	4:D:216:LEU:HD22	1.89	0.53
2:B:10:ILE:HA	2:B:13:ARG:HG2	1.90	0.53
2:B:724:ASN:O	11:N:47:ARG:HD2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:270:ALA:HA	8:H:14:HIS:HB3	1.91	0.53
9:K:26:ARG:HG2	9:K:27:LEU:H	1.73	0.53
1:A:662:TYR:HA	1:A:665:ILE:HG12	1.91	0.53
3:C:372:ASN:HA	3:C:375:ILE:HG22	1.89	0.53
5:E:82:GLN:HB3	6:F:88:ILE:HB	1.89	0.53
1:A:848:VAL:O	1:A:849:ALA:HB3	2.07	0.52
2:B:115:GLU:HG2	2:B:384:LEU:HD12	1.92	0.52
2:B:982:ILE:CD1	2:B:985:ARG:H	2.22	0.52
2:B:356:LEU:HA	2:B:407:VAL:HG21	1.91	0.52
3:C:127:THR:H	3:C:268:ASP:HB2	1.74	0.52
1:A:95:LYS:HD3	1:A:138:LYS:HG2	1.91	0.52
1:A:338:GLY:HA3	1:A:444:ARG:HG2	1.92	0.52
1:A:568:VAL:HG22	1:A:731:THR:HG22	1.91	0.52
6:F:88:ILE:HD13	6:F:88:ILE:H	1.74	0.52
3:C:144:LEU:HA	3:C:235:LYS:HG3	1.92	0.51
6:F:16:VAL:HB	6:F:52:ALA:HB3	1.92	0.51
9:K:82:LEU:HD12	9:K:86:LYS:HB3	1.91	0.51
1:A:98:CYS:O	1:A:99:ARG:HB2	2.11	0.51
1:A:879:LYS:NZ	3:C:44:THR:O	2.44	0.51
2:B:648:PRO:HB3	2:B:947:PRO:HG2	1.92	0.51
1:A:553:SER:HG	1:A:592:ILE:HA	1.76	0.51
2:B:560:HIS:HB3	2:B:626:ASN:HD21	1.75	0.51
4:D:154:ALA:C	4:D:156:PHE:H	2.19	0.51
7:G:83:ASP:HB2	7:G:101:LEU:HG	1.92	0.51
2:B:783:VAL:CG1	2:B:784:ARG:HB2	2.40	0.50
3:C:315:LEU:O	3:C:319:VAL:HG23	2.12	0.50
10:L:46:PRO:HD2	10:L:52:LYS:O	2.11	0.50
5:E:108:VAL:HB	5:E:162:LEU:HB2	1.94	0.50
1:A:353:ILE:HD11	1:A:407:VAL:HG23	1.93	0.50
2:B:192:ILE:HB	2:B:206:GLU:HB2	1.93	0.50
2:B:752:MET:HE1	2:B:910:ASP:HB3	1.93	0.50
2:B:694:ARG:HE	2:B:759:ARG:HH21	1.60	0.50
9:K:50:LEU:HD13	9:K:75:PRO:HD3	1.94	0.50
1:A:654:GLY:HA2	1:A:658:LYS:HE3	1.93	0.50
2:B:483:ILE:HD11	2:B:555:GLU:HB2	1.94	0.50
1:A:870:ARG:HD2	3:C:57:LYS:HB3	1.93	0.50
1:A:281:ILE:N	1:A:282:PRO:CD	2.75	0.49
2:B:59:LEU:HD23	2:B:107:GLU:HG2	1.94	0.49
2:B:774:ASP:HB2	2:B:819:PRO:HD3	1.93	0.49
2:B:1007:ARG:NH2	2:B:1026:GLU:O	2.42	0.49
2:B:1069:TYR:CB	2:B:1070:ILE:HB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1069:TYR:HA	2:B:1070:ILE:CB	2.30	0.49
4:D:159:VAL:HG22	4:D:161:LEU:H	1.76	0.49
2:B:897:GLN:HG3	2:B:908:VAL:HG21	1.95	0.49
2:B:680:LEU:HD21	2:B:997:HIS:HB3	1.95	0.49
2:B:741:ILE:HG22	2:B:891:ILE:HA	1.94	0.49
3:C:122:MET:HG2	3:C:274:THR:HG23	1.93	0.49
2:B:406:TRP:CG	2:B:407:VAL:N	2.78	0.49
2:B:520:TRP:O	2:B:521:SER:CB	2.60	0.49
2:B:591:LEU:HD23	2:B:615:LYS:HB3	1.93	0.49
3:C:274:THR:HB	3:C:280:ILE:HD11	1.95	0.49
2:B:961:LEU:HA	2:B:965:TYR:O	2.13	0.49
1:A:733:ALA:O	1:A:734:ARG:C	2.56	0.48
2:B:31:LEU:HA	2:B:125:MET:CE	2.43	0.48
2:B:448:LEU:HD11	2:B:458:PRO:HB3	1.94	0.48
1:A:541:ALA:HB2	7:G:72:CYS:HB2	1.95	0.48
2:B:1112:ILE:O	2:B:1114:PRO:HD3	2.12	0.48
1:A:624:GLY:O	1:A:628:MET:HG2	2.13	0.48
1:A:646:MET:HE3	1:A:647:ARG:H	1.79	0.48
2:B:734:GLY:HA3	2:B:735:TYR:CG	2.49	0.48
7:G:11:LEU:HB2	7:G:57:ALA:HB3	1.95	0.48
7:G:29:ILE:O	7:G:39:SER:HA	2.14	0.48
3:C:261:VAL:HG12	3:C:267:VAL:HG11	1.96	0.48
5:E:144:ALA:HA	5:E:169:LEU:HD23	1.94	0.48
2:B:55:GLU:HG3	2:B:373:GLU:HG3	1.96	0.48
3:C:112:ASP:HA	3:C:328:GLN:HG3	1.95	0.48
4:D:73:LEU:HD11	4:D:236:LEU:HD21	1.95	0.48
2:B:893:MET:HE3	2:B:894:LEU:H	1.79	0.48
2:B:1051:ARG:NE	2:B:1051:ARG:HA	2.28	0.48
4:D:33:MET:HE3	4:D:162:ALA:HB3	1.96	0.48
7:G:42:ILE:HG21	7:G:48:ILE:HG23	1.96	0.48
1:A:737:VAL:HG23	1:A:738:LEU:H	1.77	0.48
2:B:209:LYS:C	2:B:211:GLY:H	2.22	0.48
2:B:873:ARG:HH22	2:B:1002:ASP:CG	2.22	0.48
1:A:125:TRP:N	1:A:126:PRO:CD	2.77	0.47
1:A:141:MET:HE3	1:A:148:HIS:HB3	1.96	0.47
1:A:402:ALA:HB1	1:A:403:PRO:HD2	1.95	0.47
2:B:816:LYS:H	2:B:839:SER:HB3	1.79	0.47
7:G:55:VAL:HG23	7:G:117:GLN:HA	1.94	0.47
4:D:253:ILE:HG13	10:L:73:ILE:HG23	1.95	0.47
5:E:171:LYS:HB2	5:E:174:TRP:HB2	1.96	0.47
4:D:153:HIS:HE2	12:P:48:ILE:HG23	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:476:MET:HE1	2:B:645:ILE:HB	1.96	0.47
2:B:856:THR:HG22	2:B:857:GLU:H	1.80	0.47
1:A:216:PRO:HD2	1:A:219:ILE:HD12	1.97	0.47
1:A:428:ILE:CG2	1:A:452:PRO:HB3	2.45	0.47
1:A:734:ARG:HH12	2:B:917:ALA:HA	1.79	0.47
2:B:653:ILE:H	2:B:653:ILE:HD12	1.78	0.47
2:B:745:ARG:HD2	2:B:896:PRO:HG3	1.96	0.47
3:C:78:VAL:HG23	3:C:308:VAL:HG11	1.95	0.47
3:C:287:GLU:HG2	8:H:79:ARG:HH21	1.80	0.47
2:B:659:PRO:HG3	2:B:884:ARG:NH2	2.30	0.47
1:A:432:ALA:O	1:A:482:VAL:HG23	2.15	0.47
1:A:488:THR:HG22	1:A:490:ARG:N	2.29	0.47
2:B:406:TRP:CG	2:B:407:VAL:H	2.33	0.47
2:B:975:ASP:HB3	2:B:978:THR:HG22	1.97	0.47
5:E:44:LEU:HD13	5:E:104:MET:HE2	1.97	0.47
2:B:200:ARG:HH12	2:B:298:LYS:HD2	1.80	0.47
1:A:541:ALA:HB3	1:A:542:PRO:HD3	1.96	0.46
2:B:175:VAL:HG22	2:B:192:ILE:HG12	1.97	0.46
2:B:742:ILE:HD11	2:B:895:ILE:HB	1.97	0.46
2:B:1074:ASP:HB3	2:B:1075:LYS:CA	2.45	0.46
1:A:28:ILE:HG22	1:A:29:THR:H	1.80	0.46
1:A:326:ILE:HG22	1:A:443:PHE:HB2	1.98	0.46
4:D:66:PRO:HG3	11:N:6:ARG:HH21	1.81	0.46
1:A:80:PRO:HD2	1:A:178:SER:HB3	1.97	0.46
1:A:280:GLU:H	1:A:282:PRO:HD2	1.81	0.46
1:A:420:ASN:HB2	1:A:430:MET:HE3	1.97	0.46
7:G:40:PHE:HA	7:G:92:TYR:HD1	1.79	0.46
1:A:286:PRO:HG2	1:A:288:LYS:HE3	1.96	0.46
2:B:536:GLY:HA3	2:B:560:HIS:CE1	2.51	0.46
1:A:380:ARG:HH11	1:A:384:ARG:HH21	1.63	0.46
1:A:848:VAL:O	1:A:849:ALA:CB	2.63	0.46
2:B:675:MET:HG3	2:B:996:LEU:HD21	1.97	0.46
2:B:877:ILE:HD12	2:B:877:ILE:H	1.81	0.46
1:A:491:TYR:OH	1:A:606:GLN:HG2	2.16	0.46
1:A:600:LYS:O	1:A:601:LYS:CB	2.57	0.46
2:B:459:PHE:O	2:B:461:THR:N	2.49	0.46
7:G:48:ILE:HG22	7:G:49:PHE:H	1.81	0.46
1:A:296:ARG:H	1:A:296:ARG:HD2	1.80	0.46
1:A:323:ARG:HB2	2:B:1029:LEU:HD21	1.96	0.46
2:B:973:THR:HG21	2:B:988:PHE:CE1	2.50	0.46
3:C:28:ILE:HD13	9:K:14:HIS:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:98:ILE:HD13	4:D:141:LEU:HD11	1.97	0.46
1:A:94:LEU:HD21	1:A:180:ILE:HG23	1.97	0.46
1:A:334:ILE:HD12	1:A:628:MET:HB3	1.98	0.46
3:C:168:GLN:HG2	3:C:204:THR:HG23	1.98	0.46
8:H:39:PRO:HB2	8:H:80:TYR:CD2	2.50	0.46
1:A:489:PRO:HA	1:A:858:MET:HB2	1.98	0.46
2:B:874:ILE:HD12	2:B:874:ILE:H	1.81	0.46
3:C:122:MET:HB2	3:C:253:THR:OG1	2.16	0.46
4:D:129:PRO:HD2	11:N:15:ALA:HB1	1.97	0.46
1:A:777:GLU:HG3	1:A:783:TYR:CE2	2.50	0.45
4:D:161:LEU:O	4:D:230:LEU:HA	2.16	0.45
9:K:61:VAL:H	9:K:64:ILE:HD12	1.81	0.45
1:A:541:ALA:HB3	1:A:542:PRO:CD	2.47	0.45
1:A:501:ASP:H	2:B:737:MET:HE3	1.82	0.45
3:C:70:ILE:HD13	3:C:70:ILE:H	1.82	0.45
1:A:519:GLU:HG2	10:L:33:ARG:HD2	1.99	0.45
1:A:530:VAL:HB	1:A:532:ILE:HG13	1.98	0.45
2:B:86:MET:O	2:B:90:LEU:HG	2.16	0.45
2:B:417:LEU:HD21	2:B:425:MET:HG3	1.98	0.45
2:B:500:VAL:O	2:B:504:ILE:HG12	2.16	0.45
2:B:1005:HIS:NE2	2:B:1023:ARG:HA	2.30	0.45
2:B:598:GLU:HB3	2:B:599:LYS:H	1.66	0.45
4:D:38:VAL:HG12	4:D:39:MET:N	2.31	0.45
2:B:51:GLU:HB2	2:B:53:PRO:HD3	1.98	0.45
3:C:199:ASP:HB2	3:C:206:LEU:HB2	1.98	0.45
1:A:238:LYS:NZ	1:A:297:THR:HA	2.32	0.45
1:A:516:LEU:HD23	1:A:521:ALA:HA	1.99	0.45
1:A:732:GLY:O	1:A:733:ALA:C	2.60	0.45
2:B:420:THR:O	2:B:421:ASN:CG	2.59	0.45
3:C:28:ILE:H	3:C:28:ILE:HG13	1.57	0.45
3:C:340:SER:CB	3:C:371:GLU:HG2	2.47	0.45
1:A:275:THR:O	1:A:297:THR:HG21	2.17	0.44
2:B:86:MET:HE3	2:B:686:ASN:HD21	1.82	0.44
2:B:438:ARG:C	2:B:440:GLN:H	2.24	0.44
2:B:1050:ASP:HA	2:B:1054:ASP:HB2	1.99	0.44
1:A:331:ASN:O	1:A:332:ILE:HG12	2.17	0.44
2:B:235:ILE:HA	2:B:312:ARG:HH21	1.83	0.44
2:B:689:LEU:HD13	11:N:62:TYR:HB3	1.99	0.44
3:C:347:PHE:C	3:C:349:VAL:H	2.24	0.44
1:A:190:SER:O	1:A:194:ILE:HG13	2.18	0.44
2:B:341:TYR:CE1	2:B:452:GLN:HG2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:21:LEU:O	6:F:24:VAL:HG12	2.17	0.44
1:A:102:GLY:HA3	1:A:187:VAL:HG12	1.99	0.44
1:A:296:ARG:HD2	1:A:296:ARG:N	2.32	0.44
1:A:434:ARG:HD3	1:A:481:LEU:HD21	2.00	0.44
1:A:857:PRO:HB3	3:C:309:ASP:OD1	2.18	0.44
2:B:430:ARG:HH11	2:B:653:ILE:HG13	1.82	0.44
1:A:644:PHE:HB3	2:B:731:SER:OG	2.18	0.44
3:C:13:LEU:HD23	3:C:16:LYS:HD3	1.99	0.44
5:E:97:ILE:HB	5:E:108:VAL:HG13	1.98	0.44
2:B:110:ILE:CA	2:B:111:GLU:CB	2.71	0.44
2:B:786:TYR:CE2	2:B:788:GLY:HA2	2.53	0.44
2:B:970:THR:HA	2:B:987:TYR:HA	1.99	0.44
3:C:13:LEU:HD13	3:C:48:ILE:HG12	1.99	0.44
3:C:179:VAL:HG21	3:C:232:LYS:HZ2	1.83	0.44
3:C:391:ARG:NH2	9:K:77:THR:OG1	2.51	0.44
12:P:25:ARG:HG2	12:P:32:LYS:HG2	2.00	0.44
1:A:527:VAL:HG12	1:A:633:ARG:HG2	1.99	0.44
2:B:937:ALA:O	11:N:46:ARG:HD2	2.18	0.44
1:A:646:MET:HE1	1:A:725:ALA:HB2	1.99	0.44
2:B:597:ILE:HD13	2:B:597:ILE:H	1.82	0.44
2:B:742:ILE:HG12	2:B:893:MET:O	2.17	0.44
3:C:231:ILE:HG22	3:C:232:LYS:H	1.83	0.44
3:C:286:ILE:HG12	8:H:49:ASP:CG	2.43	0.44
11:N:7:CYS:HB3	11:N:10:CYS:SG	2.58	0.44
1:A:573:ARG:HG3	1:A:573:ARG:NH1	2.33	0.44
2:B:583:ILE:HD12	2:B:591:LEU:HD21	1.99	0.44
2:B:737:MET:H	2:B:740:SER:HB3	1.82	0.44
2:B:985:ARG:HH12	4:D:208:GLU:HG2	1.83	0.44
2:B:242:VAL:HG22	2:B:256:PHE:HB3	2.00	0.43
2:B:744:ASN:HA	2:B:900:MET:HE3	2.00	0.43
2:B:936:ALA:HA	2:B:941:ASN:O	2.17	0.43
1:A:450:CYS:HB2	1:A:451:PRO:HD3	2.00	0.43
1:A:672:VAL:HG11	1:A:776:PRO:HD3	2.00	0.43
2:B:46:ILE:HG13	2:B:66:ILE:HG12	2.00	0.43
2:B:582:LEU:HD12	2:B:619:LEU:HD12	2.00	0.43
3:C:201:SER:HB2	3:C:204:THR:HB	2.00	0.43
1:A:23:SER:HB2	1:A:74:HIS:NE2	2.33	0.43
1:A:645:THR:OG1	1:A:646:MET:N	2.45	0.43
4:D:159:VAL:HG21	4:D:230:LEU:HD22	1.99	0.43
2:B:733:THR:HG23	2:B:734:GLY:N	2.34	0.43
8:H:62:ILE:HG22	8:H:80:TYR:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:LEU:HD23	3:C:83:THR:HG21	2.00	0.43
1:A:823:LEU:HA	1:A:826:ALA:HB3	2.01	0.43
2:B:400:ALA:O	2:B:405:ASN:HA	2.17	0.43
3:C:197:VAL:HB	3:C:208:ILE:HB	2.00	0.43
3:C:268:ASP:O	3:C:272:VAL:HG23	2.19	0.43
12:P:21:LEU:HD22	12:P:22:PRO:HA	2.01	0.43
2:B:532:TYR:O	2:B:533:TYR:HB3	2.17	0.43
3:C:107:LEU:HA	3:C:110:ILE:HG22	2.00	0.43
2:B:594:ARG:HH12	2:B:615:LYS:HB2	1.82	0.43
2:B:961:LEU:HD12	2:B:967:PRO:HD3	2.01	0.43
2:B:594:ARG:HH11	2:B:610:LEU:HD23	1.84	0.43
3:C:385:MET:HE2	3:C:385:MET:HB3	1.92	0.43
5:E:30:LEU:HD22	5:E:72:PHE:CE1	2.54	0.43
12:P:21:LEU:HA	12:P:22:PRO:HA	1.87	0.43
1:A:10:LYS:HG2	3:C:363:VAL:HG13	2.01	0.43
1:A:372:TRP:O	1:A:410:HIS:ND1	2.51	0.43
1:A:587:VAL:HB	1:A:595:GLU:HB2	2.01	0.43
2:B:345:ARG:HG3	2:B:576:GLY:HA3	2.01	0.43
3:C:127:THR:HB	3:C:128:ASP:H	1.66	0.43
1:A:739:ASN:HB2	2:B:922:MET:SD	2.59	0.43
2:B:84:SER:HB2	2:B:144:ILE:HD12	2.01	0.43
2:B:147:ASP:HB3	2:B:685:ALA:HB3	2.01	0.43
2:B:454:GLY:HA3	2:B:580:ARG:HE	1.83	0.43
4:D:17:PHE:O	4:D:225:LYS:HA	2.19	0.43
3:C:127:THR:N	3:C:268:ASP:HB2	2.34	0.42
1:A:104:VAL:HG13	1:A:143:ALA:HB2	2.00	0.42
2:B:190:ALA:HB3	2:B:208:LEU:HD12	2.02	0.42
1:A:13:ILE:HD12	1:A:202:SER:HB2	2.01	0.42
1:A:16:PRO:HA	1:A:19:ILE:HD12	2.00	0.42
2:B:262:ALA:HB1	2:B:265:ILE:HB	2.00	0.42
2:B:406:TRP:O	2:B:408:GLY:N	2.52	0.42
2:B:816:LYS:N	2:B:839:SER:HB3	2.35	0.42
4:D:38:VAL:CG1	4:D:39:MET:N	2.82	0.42
3:C:50:LYS:O	3:C:54:LEU:HG	2.19	0.42
1:A:313:LEU:HD22	3:C:374:ILE:HG23	2.01	0.42
1:A:575:CYS:SG	1:A:584:SER:HB3	2.60	0.42
2:B:720:PRO:HG3	11:N:53:ILE:HD12	2.01	0.42
2:B:884:ARG:HH12	2:B:992:TYR:HB3	1.80	0.42
2:B:1061:ILE:HD13	2:B:1096:VAL:HB	2.00	0.42
3:C:47:GLU:CB	3:C:50:LYS:HB2	2.50	0.42
5:E:129:GLY:H	5:E:137:GLN:HB3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:MET:HG3	1:A:148:HIS:HA	2.02	0.42
1:A:760:GLY:HA2	2:B:450:GLY:HA3	2.02	0.42
2:B:174:ARG:HB3	2:B:527:GLY:HA3	2.01	0.42
2:B:430:ARG:HD3	2:B:653:ILE:CG1	2.50	0.42
2:B:1040:ILE:HG23	3:C:381:LEU:HD11	2.02	0.42
1:A:58:CYS:HA	1:A:59:PRO:HD3	1.91	0.42
1:A:705:ASP:O	1:A:708:ARG:HG3	2.20	0.42
2:B:41:LYS:O	2:B:43:GLN:N	2.52	0.42
2:B:646:TRP:CD2	2:B:648:PRO:HD2	2.55	0.42
2:B:651:LEU:HB3	2:B:655:ALA:HB3	2.01	0.42
2:B:938:LEU:HD23	11:N:43:TYR:HB3	2.01	0.42
2:B:953:ILE:HD13	2:B:953:ILE:N	2.18	0.42
3:C:257:ASN:O	3:C:261:VAL:HG23	2.20	0.42
2:B:918:LEU:H	2:B:919:PRO:HD2	1.85	0.42
7:G:18:ILE:HD12	7:G:29:ILE:HG12	2.02	0.42
1:A:450:CYS:O	1:A:454:ASN:N	2.53	0.42
2:B:430:ARG:HD3	2:B:653:ILE:HG12	2.02	0.42
2:B:1107:LEU:HD21	3:C:354:LEU:HD13	2.01	0.42
1:A:515:LEU:HB3	1:A:545:TYR:CD1	2.55	0.41
2:B:285:ARG:HD3	2:B:289:ILE:HD11	2.02	0.41
2:B:705:LEU:O	2:B:706:VAL:HB	2.20	0.41
2:B:783:VAL:HG13	2:B:784:ARG:HB2	2.02	0.41
2:B:1111:ILE:O	2:B:1111:ILE:HG22	2.20	0.41
7:G:103:VAL:HG13	7:G:104:LYS:HG2	2.02	0.41
1:A:426:HIS:NE2	1:A:489:PRO:HD2	2.35	0.41
1:A:502:TYR:CD1	1:A:632:PHE:HB3	2.55	0.41
1:A:646:MET:HG2	2:B:918:LEU:HD13	2.01	0.41
1:A:723:ASN:HD22	1:A:723:ASN:C	2.28	0.41
2:B:589:ASN:HA	2:B:590:PRO:HD3	1.90	0.41
1:A:580:CYS:HA	1:A:581:PRO:HD3	1.88	0.41
2:B:914:ASN:HA	2:B:915:PRO:HD2	1.88	0.41
1:A:69:PRO:HG2	2:B:1101:LYS:HE3	2.02	0.41
2:B:99:LEU:HD11	2:B:122:LEU:HB2	2.02	0.41
2:B:1081:VAL:HG22	2:B:1085:HIS:HA	2.01	0.41
3:C:387:GLU:HG3	9:K:79:ARG:HB2	2.02	0.41
5:E:8:ARG:HH12	6:F:7:VAL:HG11	1.85	0.41
8:H:44:TRP:O	8:H:79:ARG:HD2	2.20	0.41
11:N:24:ARG:HD2	11:N:34:VAL:HG13	2.03	0.41
1:A:339:VAL:O	1:A:437:VAL:HA	2.20	0.41
3:C:323:THR:O	3:C:325:VAL:N	2.53	0.41
3:C:377:HIS:HA	3:C:378:PRO:HD2	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:172:ILE:HD11	4:D:197:VAL:HG23	2.03	0.41
9:K:74:LEU:HA	9:K:75:PRO:HD3	1.91	0.41
1:A:379:ILE:HB	1:A:406:VAL:HB	2.03	0.41
1:A:416:VAL:HB	1:A:473:ILE:HG23	2.03	0.41
1:A:866:VAL:O	1:A:870:ARG:NH1	2.35	0.41
2:B:974:TYR:CD2	2:B:981:LYS:HB3	2.56	0.41
1:A:52:ILE:HG23	1:A:217:ILE:HG23	2.02	0.41
1:A:114:TYR:HA	1:A:118:TYR:HD2	1.85	0.41
1:A:304:GLY:C	1:A:306:GLU:H	2.28	0.41
1:A:823:LEU:HD13	3:C:75:ALA:HB1	2.03	0.41
2:B:174:ARG:HH21	2:B:526:ASN:HA	1.86	0.41
2:B:818:SER:HB2	2:B:836:ARG:HB2	2.03	0.41
11:N:5:ILE:O	11:N:6:ARG:HB2	2.21	0.41
1:A:500:GLN:HB2	2:B:916:HIS:CD2	2.56	0.41
2:B:497:VAL:HA	2:B:533:TYR:HB2	2.02	0.41
1:A:73:GLY:O	1:A:214:VAL:N	2.53	0.41
1:A:203:ARG:HB2	1:A:206:TRP:CD2	2.56	0.41
1:A:840:SER:C	1:A:842:TYR:H	2.29	0.41
2:B:658:ILE:HG12	2:B:672:GLN:HG2	2.01	0.41
2:B:946:THR:HA	2:B:947:PRO:HD2	1.91	0.41
2:B:1057:ASP:OD2	2:B:1057:ASP:N	2.54	0.41
3:C:235:LYS:HB3	3:C:235:LYS:HE3	1.95	0.41
8:H:20:HIS:CG	8:H:51:VAL:HG11	2.55	0.41
8:H:23:LEU:HB3	8:H:28:ALA:HB2	2.03	0.41
1:A:418:LEU:HB3	1:A:430:MET:HE2	2.03	0.41
2:B:884:ARG:NH1	2:B:884:ARG:HB2	2.34	0.41
2:B:1053:LEU:HD13	3:C:376:GLY:HA3	2.03	0.41
3:C:69:ALA:HB2	3:C:381:LEU:HD13	2.03	0.41
1:A:470:GLU:H	1:A:470:GLU:HG2	1.63	0.40
1:A:563:HIS:HB2	1:A:872:PHE:HE2	1.86	0.40
2:B:579:ARG:HD3	2:B:618:TYR:HB3	2.03	0.40
2:B:1005:HIS:CE1	2:B:1007:ARG:CZ	3.04	0.40
2:B:1077:LYS:HA	2:B:1078:ASN:HA	1.78	0.40
8:H:49:ASP:OD2	8:H:50:PRO:HD2	2.21	0.40
1:A:10:LYS:HG3	2:B:1117:ILE:HD11	2.03	0.40
2:B:605:ILE:HG23	2:B:606:THR:N	2.36	0.40
2:B:1054:ASP:HA	2:B:1058:ARG:HD2	2.02	0.40
3:C:51:ILE:C	3:C:53:ASP:H	2.29	0.40
3:C:235:LYS:HB3	3:C:236:GLY:H	1.66	0.40
4:D:41:ILE:H	4:D:41:ILE:HG12	1.72	0.40
1:A:14:LEU:HB3	2:B:1111:ILE:HG23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:LEU:HG	1:A:238:LYS:HE3	2.03	0.40
1:A:838:VAL:HG13	3:C:70:ILE:HD11	2.03	0.40
2:B:81:ARG:HA	2:B:81:ARG:HD3	1.89	0.40
2:B:720:PRO:HG3	11:N:53:ILE:CD1	2.51	0.40
2:B:814:ILE:HB	2:B:840:ILE:HB	2.03	0.40
3:C:11:SER:O	3:C:13:LEU:N	2.54	0.40
3:C:329:ILE:HA	3:C:334:VAL:HB	2.04	0.40
5:E:131:LYS:HD2	5:E:136:ILE:HD13	2.02	0.40
7:G:67:THR:HG22	7:G:68:ASN:H	1.86	0.40
2:B:585:VAL:HG21	2:B:636:LEU:HD11	2.04	0.40
2:B:783:VAL:HG12	2:B:784:ARG:HB2	2.02	0.40
2:B:913:LEU:HD12	2:B:926:GLN:HE21	1.86	0.40
5:E:39:LEU:HA	5:E:153:VAL:HG23	2.04	0.40
1:A:29:THR:HB	1:A:30:PRO:HD3	2.03	0.40
2:B:84:SER:OG	2:B:144:ILE:HG23	2.21	0.40
3:C:265:LYS:H	3:C:265:LYS:HD2	1.86	0.40
11:N:19:GLN:N	11:N:20:PRO:HD2	2.37	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	833/880 (95%)	692 (83%)	112 (13%)	29 (4%)	3	16
2	B	1082/1131 (96%)	908 (84%)	127 (12%)	47 (4%)	2	13
3	C	363/395 (92%)	288 (79%)	61 (17%)	14 (4%)	2	14
4	D	256/265 (97%)	227 (89%)	25 (10%)	4 (2%)	7	28
5	E	170/180 (94%)	152 (89%)	16 (9%)	2 (1%)	10	33
6	F	88/113 (78%)	74 (84%)	11 (12%)	3 (3%)	3	16
7	G	111/132 (84%)	96 (86%)	13 (12%)	2 (2%)	6	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	72/84 (86%)	59 (82%)	8 (11%)	5 (7%)	1	6
9	K	80/95 (84%)	69 (86%)	7 (9%)	4 (5%)	1	10
10	L	89/92 (97%)	79 (89%)	8 (9%)	2 (2%)	5	23
11	N	62/66 (94%)	50 (81%)	10 (16%)	2 (3%)	3	17
12	P	41/48 (85%)	32 (78%)	7 (17%)	2 (5%)	1	10
13	Q	43/104 (41%)	36 (84%)	6 (14%)	1 (2%)	5	22
All	All	3290/3585 (92%)	2762 (84%)	411 (12%)	117 (4%)	2	15

All (117) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	ARG
1	A	734	ARG
1	A	737	VAL
2	B	28	ARG
2	B	111	GLU
2	B	460	GLU
2	B	521	SER
2	B	590	PRO
2	B	735	TYR
2	B	950	LYS
2	B	1070	ILE
8	H	13	ILE
9	K	61	VAL
1	A	256	GLY
1	A	280	GLU
1	A	332	ILE
1	A	732	GLY
1	A	876	VAL
2	B	605	ILE
2	B	739	ASP
2	B	797	ASP
2	B	809	GLY
2	B	877	ILE
2	B	1072	TRP
3	C	12	TYR
3	C	245	LYS
3	C	324	GLY
3	C	365	GLU
3	C	393	ILE

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Mol	Chain	Res	Type
4	D	117	GLU
4	D	206	CYS
1	A	45	MET
1	A	290	ARG
1	A	536	GLU
1	A	733	ALA
1	A	849	ALA
2	B	26	LEU
2	B	49	GLN
2	B	250	GLU
2	B	256	PHE
2	B	734	GLY
2	B	918	LEU
2	B	943	VAL
2	B	985	ARG
2	B	1026	GLU
2	B	1029	LEU
3	C	113	ALA
3	C	114	LYS
7	G	99	PHE
9	K	25	ASN
9	K	91	SER
11	N	41	LYS
12	P	13	PHE
1	A	46	ASP
1	A	79	ARG
1	A	155	LYS
1	A	287	SER
1	A	393	ASP
1	A	601	LYS
2	B	71	PRO
2	B	202	PRO
2	B	375	SER
2	B	407	VAL
2	B	606	THR
2	B	706	VAL
2	B	773	GLU
2	B	949	TYR
2	B	951	THR
3	C	201	SER
4	D	79	PRO
4	D	193	GLY

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Mol	Chain	Res	Type
5	E	82	GLN
8	H	15	TYR
8	H	81	VAL
10	L	19	GLY
11	N	6	ARG
1	A	106	ILE
1	A	125	TRP
1	A	257	ALA
1	A	308	ARG
1	A	541	ALA
1	A	738	LEU
2	B	56	ILE
2	B	334	GLU
2	B	437	ALA
2	B	453	TRP
2	B	533	TYR
2	B	771	GLY
2	B	781	PRO
2	B	907	VAL
3	C	44	THR
3	C	218	ALA
3	C	349	VAL
9	K	14	HIS
10	L	10	SER
12	P	11	LYS
1	A	62	GLY
2	B	183	GLY
2	B	948	PHE
2	B	1073	TYR
3	C	190	ARG
3	C	235	LYS
3	C	236	GLY
5	E	127	ILE
6	F	47	CYS
7	G	105	ILE
8	H	10	ASP
8	H	60	GLY
1	A	145	VAL
1	A	29	THR
1	A	760	GLY
2	B	113	GLU
2	B	588	GLY

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Mol	Chain	Res	Type
2	B	1114	PRO
13	Q	59	ILE
6	F	25	ILE
6	F	4	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	729/766 (95%)	672 (92%)	57 (8%)	11	37
2	B	941/975 (96%)	859 (91%)	82 (9%)	9	32
3	C	315/341 (92%)	291 (92%)	24 (8%)	12	38
4	D	233/238 (98%)	225 (97%)	8 (3%)	32	58
5	E	154/158 (98%)	145 (94%)	9 (6%)	18	45
6	F	84/107 (78%)	79 (94%)	5 (6%)	17	44
7	G	106/125 (85%)	100 (94%)	6 (6%)	18	46
8	H	67/75 (89%)	63 (94%)	4 (6%)	17	44
9	K	72/83 (87%)	69 (96%)	3 (4%)	26	52
10	L	79/80 (99%)	77 (98%)	2 (2%)	42	61
11	N	58/60 (97%)	52 (90%)	6 (10%)	7	25
12	P	39/43 (91%)	38 (97%)	1 (3%)	40	61
13	Q	43/96 (45%)	39 (91%)	4 (9%)	8	30
All	All	2920/3147 (93%)	2709 (93%)	211 (7%)	13	39

All (211) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	28	ILE
1	A	45	MET
1	A	61	CYS

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Mol	Chain	Res	Type
1	A	64	THR
1	A	84	VAL
1	A	87	VAL
1	A	88	LYS
1	A	101	CYS
1	A	105	LYS
1	A	119	ASN
1	A	133	THR
1	A	139	THR
1	A	152	LYS
1	A	155	LYS
1	A	220	ARG
1	A	284	LEU
1	A	296	ARG
1	A	324	THR
1	A	332	ILE
1	A	334	ILE
1	A	349	VAL
1	A	353	ILE
1	A	366	ILE
1	A	417	VAL
1	A	419	PHE
1	A	425	LEU
1	A	438	LEU
1	A	464	LEU
1	A	470	GLU
1	A	487	ILE
1	A	527	VAL
1	A	549	LYS
1	A	551	VAL
1	A	573	ARG
1	A	574	LEU
1	A	580	CYS
1	A	584	SER
1	A	588	ILE
1	A	593	LEU
1	A	603	ILE
1	A	605	ASN
1	A	633	ARG
1	A	675	LEU
1	A	687	ILE
1	A	696	LEU

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Mol	Chain	Res	Type
1	A	723	ASN
1	A	763	THR
1	A	764	ARG
1	A	766	LEU
1	A	774	ILE
1	A	787	ARG
1	A	790	LEU
1	A	823	LEU
1	A	824	ILE
1	A	868	VAL
1	A	876	VAL
2	B	17	ILE
2	B	41	LYS
2	B	52	ILE
2	B	54	THR
2	B	66	ILE
2	B	68	ILE
2	B	84	SER
2	B	93	LEU
2	B	101	LEU
2	B	104	ILE
2	B	111	GLU
2	B	138	LEU
2	B	166	THR
2	B	177	VAL
2	B	186	ILE
2	B	230	MET
2	B	237	THR
2	B	252	GLN
2	B	259	LEU
2	B	318	LEU
2	B	330	LEU
2	B	336	ASP
2	B	345	ARG
2	B	397	ILE
2	B	426	LEU
2	B	436	LEU
2	B	444	GLU
2	B	448	LEU
2	B	456	MET
2	B	460	GLU
2	B	470	VAL

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Mol	Chain	Res	Type
2	B	471	LYS
2	B	478	GLN
2	B	481	VAL
2	B	505	ARG
2	B	525	LEU
2	B	529	LEU
2	B	539	LEU
2	B	563	THR
2	B	579	ARG
2	B	591	LEU
2	B	597	ILE
2	B	610	LEU
2	B	639	GLU
2	B	653	ILE
2	B	657	ILE
2	B	662	GLU
2	B	675	MET
2	B	688	GLN
2	B	711	LEU
2	B	717	THR
2	B	726	ILE
2	B	730	ILE
2	B	731	SER
2	B	735	TYR
2	B	741	ILE
2	B	742	ILE
2	B	760	LEU
2	B	763	THR
2	B	777	VAL
2	B	802	SER
2	B	840	ILE
2	B	843	ARG
2	B	854	LEU
2	B	856	THR
2	B	874	ILE
2	B	884	ARG
2	B	898	VAL
2	B	903	THR
2	B	905	LYS
2	B	913	LEU
2	B	924	LEU
2	B	943	VAL

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Mol	Chain	Res	Type
2	B	953	ILE
2	B	977	ARG
2	B	994	GLN
2	B	1017	ARG
2	B	1026	GLU
2	B	1059	THR
2	B	1070	ILE
2	B	1081	VAL
2	B	1122	VAL
3	C	24	LEU
3	C	28	ILE
3	C	46	ASP
3	C	47	GLU
3	C	70	ILE
3	C	107	LEU
3	C	119	THR
3	C	129	GLU
3	C	149	ILE
3	C	174	LEU
3	C	180	THR
3	C	213	ILE
3	C	231	ILE
3	C	277	ILE
3	C	292	ILE
3	C	307	ASP
3	C	311	ARG
3	C	315	LEU
3	C	329	ILE
3	C	331	ARG
3	C	338	LYS
3	C	362	ASP
3	C	365	GLU
3	C	386	VAL
4	D	13	ILE
4	D	132	LEU
4	D	163	ILE
4	D	165	ARG
4	D	172	ILE
4	D	178	LYS
4	D	253	ILE
4	D	258	LYS
5	E	27	LEU

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Mol	Chain	Res	Type
5	E	30	LEU
5	E	38	ILE
5	E	48	ILE
5	E	53	THR
5	E	59	LEU
5	E	117	THR
5	E	137	GLN
5	E	142	VAL
6	F	24	VAL
6	F	62	ILE
6	F	63	ILE
6	F	79	THR
6	F	88	ILE
7	G	48	ILE
7	G	67	THR
7	G	101	LEU
7	G	104	LYS
7	G	106	ILE
7	G	115	ILE
8	H	16	LEU
8	H	34	GLU
8	H	45	ILE
8	H	63	ILE
9	K	24	GLN
9	K	59	THR
9	K	74	LEU
10	L	24	LEU
10	L	31	THR
11	N	1	MET
11	N	3	ILE
11	N	5	ILE
11	N	45	CYS
11	N	61	HIS
11	N	63	THR
12	P	41	THR
13	Q	40	ILE
13	Q	52	ASP
13	Q	69	GLU
13	Q	76	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	A	312	ASN
1	A	367	ASN
1	A	565	GLN
1	A	742	GLN
2	B	261	GLN
2	B	343	ASN
2	B	415	GLN
2	B	442	ASN
2	B	664	ASN
2	B	665	GLN
2	B	736	ASN
2	B	1090	ASN
3	C	19	GLN
3	C	312	HIS
3	C	377	HIS
4	D	60	HIS
5	E	137	GLN
5	E	177	GLN
7	G	30	HIS
7	G	117	GLN
8	H	14	HIS
9	K	14	HIS
10	L	11	ASN
13	Q	47	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
16	F3S	D	1001	4	0,9,9	-	-	-		

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
16	F3S	D	1001	4	-	-	0/3/3/3

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	841/880 (95%)	0.51	50 (5%) 28 20	40, 69, 119, 184	0
2	B	1090/1131 (96%)	0.60	58 (5%) 32 23	43, 71, 136, 201	0
3	C	367/395 (92%)	0.81	37 (10%) 12 12	48, 81, 151, 202	0
4	D	260/265 (98%)	0.51	7 (2%) 56 41	66, 93, 131, 200	0
5	E	174/180 (96%)	1.09	25 (14%) 6 7	58, 144, 188, 210	0
6	F	90/113 (79%)	0.97	9 (10%) 12 12	95, 175, 222, 230	0
7	G	113/132 (85%)	0.95	11 (9%) 13 12	66, 105, 147, 156	0
8	H	74/84 (88%)	0.70	4 (5%) 31 23	60, 84, 103, 108	0
9	K	82/95 (86%)	0.47	5 (6%) 27 20	50, 67, 90, 99	0
10	L	91/92 (98%)	0.42	4 (4%) 39 28	51, 90, 121, 140	0
11	N	64/66 (96%)	0.26	0 100 100	60, 71, 113, 140	0
12	P	43/48 (89%)	0.87	5 (11%) 9 9	72, 93, 135, 146	0
13	Q	45/104 (43%)	1.27	8 (17%) 4 4	83, 121, 150, 169	0
All	All	3334/3585 (92%)	0.64	223 (6%) 24 18	40, 81, 156, 230	0

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	144	GLN	4.9
1	A	115	SER	4.7
2	B	1106	GLU	4.5
7	G	83	ASP	4.3
2	B	113	GLU	4.1
5	E	81	VAL	4.1
7	G	80	GLU	4.0
3	C	82	GLY	4.0
2	B	1072	TRP	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	519	LYS	3.9
5	E	86	GLU	3.7
3	C	183	ASP	3.7
2	B	110	ILE	3.6
6	F	77	PRO	3.6
3	C	65	ALA	3.5
2	B	196	THR	3.5
5	E	72	PHE	3.5
2	B	377	VAL	3.5
1	A	684	LEU	3.4
3	C	24	LEU	3.4
2	B	227	VAL	3.4
1	A	274	ALA	3.4
5	E	93	ASP	3.4
3	C	83	THR	3.4
1	A	121	ILE	3.4
1	A	177	PRO	3.4
2	B	52	ILE	3.3
2	B	558	VAL	3.3
2	B	476	MET	3.3
7	G	81	LEU	3.3
2	B	108	ASN	3.2
8	H	13	ILE	3.2
2	B	1089	SER	3.2
5	E	118	LEU	3.2
9	K	51	ILE	3.2
2	B	1027	GLY	3.1
7	G	94	THR	3.1
5	E	79	PRO	3.1
1	A	28	ILE	3.1
2	B	252	GLN	3.1
2	B	437	ALA	3.0
5	E	150	ALA	3.0
2	B	251	ILE	3.0
4	D	143	ALA	3.0
3	C	29	VAL	3.0
5	E	98	PHE	3.0
6	F	55	VAL	3.0
13	Q	78	ARG	3.0
9	K	52	ASP	2.9
7	G	105	ILE	2.9
8	H	27	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
3	C	169	LEU	2.9
2	B	405	ASN	2.9
5	E	92	VAL	2.9
1	A	810	ALA	2.9
1	A	833	GLU	2.9
3	C	334	VAL	2.9
1	A	93	PHE	2.9
2	B	715	GLY	2.8
2	B	1116	LEU	2.8
1	A	876	VAL	2.8
1	A	191	ASP	2.8
2	B	111	GLU	2.8
2	B	193	ILE	2.8
10	L	83	TYR	2.8
1	A	864	LYS	2.7
1	A	154	PHE	2.7
1	A	755	GLU	2.7
2	B	436	LEU	2.7
5	E	153	VAL	2.7
1	A	281	ILE	2.7
2	B	261	GLN	2.7
2	B	306	THR	2.7
3	C	118	SER	2.7
2	B	178	ASP	2.7
2	B	171	ALA	2.6
3	C	294	ILE	2.6
10	L	89	GLY	2.6
3	C	363	VAL	2.6
1	A	107	SER	2.6
1	A	103	ARG	2.6
2	B	806	GLU	2.6
5	E	107	LEU	2.6
1	A	133	THR	2.6
3	C	206	LEU	2.6
2	B	605	ILE	2.5
6	F	76	CYS	2.5
3	C	126	LEU	2.5
6	F	72	LEU	2.5
3	C	364	GLU	2.5
2	B	296	ILE	2.5
3	C	394	LEU	2.5
3	C	28	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
8	H	62	ILE	2.5
12	P	34	ILE	2.5
5	E	158	PRO	2.5
2	B	234	GLY	2.5
1	A	145	VAL	2.5
6	F	66	GLU	2.5
3	C	81	PRO	2.5
2	B	87	GLU	2.5
3	C	254	ASP	2.5
4	D	151	LYS	2.5
1	A	114	TYR	2.5
5	E	64	GLY	2.5
1	A	26	ALA	2.4
1	A	70	GLY	2.4
1	A	127	SER	2.4
5	E	8	ARG	2.4
1	A	458	ASP	2.4
8	H	82	ILE	2.4
3	C	159	ASP	2.4
9	K	62	ILE	2.4
2	B	380	ARG	2.4
1	A	24	VAL	2.4
5	E	125	GLY	2.4
3	C	64	ILE	2.4
3	C	30	GLU	2.4
4	D	207	GLU	2.4
5	E	167	PRO	2.4
1	A	75	ILE	2.3
7	G	92	TYR	2.3
1	A	285	PRO	2.3
2	B	403	THR	2.3
3	C	55	ALA	2.3
5	E	144	ALA	2.3
6	F	17	ALA	2.3
1	A	224	MET	2.3
1	A	65	LEU	2.3
5	E	157	LEU	2.3
1	A	97	THR	2.3
2	B	84	SER	2.3
1	A	579	ASP	2.3
1	A	829	ASP	2.3
2	B	498	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
12	P	20	VAL	2.3
1	A	23	SER	2.3
2	B	54	THR	2.3
1	A	692	LEU	2.3
7	G	82	LYS	2.3
1	A	136	VAL	2.3
2	B	595	GLU	2.3
5	E	80	VAL	2.3
10	L	1	MET	2.3
2	B	267	ASN	2.3
2	B	507	VAL	2.3
6	F	49	ALA	2.2
5	E	44	LEU	2.2
1	A	137	LYS	2.2
3	C	234	ILE	2.2
1	A	22	MET	2.2
1	A	877	GLY	2.2
1	A	871	ILE	2.2
2	B	224	ILE	2.2
2	B	1038	CYS	2.2
4	D	264	ILE	2.2
7	G	77	ILE	2.2
1	A	841	LEU	2.2
9	K	92	LEU	2.2
7	G	79	THR	2.2
2	B	136	TYR	2.2
3	C	165	ILE	2.2
5	E	126	ILE	2.2
12	P	21	LEU	2.2
3	C	196	PHE	2.2
5	E	143	ARG	2.2
5	E	78	VAL	2.2
3	C	226	ILE	2.2
2	B	860	GLU	2.2
1	A	155	LYS	2.2
3	C	236	GLY	2.2
3	C	384	GLY	2.2
2	B	256	PHE	2.2
13	Q	51	TRP	2.2
3	C	205	THR	2.1
13	Q	59	ILE	2.1
3	C	174	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	105	LYS	2.1
12	P	16	GLU	2.1
3	C	349	VAL	2.1
3	C	369	VAL	2.1
2	B	237	THR	2.1
13	Q	41	ILE	2.1
3	C	338	LYS	2.1
2	B	415	GLN	2.1
5	E	177	GLN	2.1
2	B	71	PRO	2.1
2	B	376	LYS	2.1
6	F	63	ILE	2.1
13	Q	65	LYS	2.1
1	A	126	PRO	2.1
3	C	233	GLY	2.1
2	B	213	PHE	2.1
4	D	214	ASN	2.1
4	D	263	VAL	2.1
1	A	195	LEU	2.1
1	A	870	ARG	2.1
7	G	57	ALA	2.1
1	A	69	PRO	2.1
6	F	85	SER	2.1
9	K	61	VAL	2.1
5	E	94	ASN	2.1
2	B	56	ILE	2.1
13	Q	75	TYR	2.1
2	B	146	GLU	2.1
1	A	273	VAL	2.0
1	A	194	ILE	2.0
4	D	5	LEU	2.0
13	Q	52	ASP	2.0
12	P	24	VAL	2.0
1	A	284	LEU	2.0
2	B	241	ILE	2.0
2	B	204	THR	2.0
2	B	315	ALA	2.0
3	C	229	THR	2.0
2	B	379	GLY	2.0
2	B	948	PHE	2.0
10	L	18	GLU	2.0
2	B	233	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
3	C	219	LEU	2.0
7	G	98	LEU	2.0
3	C	241	ILE	2.0
13	Q	38	ILE	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(Å ²)	Q<0.9
15	MG	A	1400	1/1	0.83	0.36	58,58,58,58	0
14	ZN	A	1360	1/1	0.95	0.15	58,58,58,58	0
14	ZN	B	1500	1/1	0.97	0.04	62,62,62,62	0
16	F3S	D	1001	7/7	0.97	0.08	67,67,67,67	0
14	ZN	P	50	1/1	0.98	0.04	71,71,71,71	0
14	ZN	B	1400	1/1	0.98	0.09	62,62,62,62	0
14	ZN	A	1350	1/1	0.98	0.03	58,58,58,58	0
14	ZN	N	100	1/1	0.99	0.03	63,63,63,63	0
14	ZN	B	1300	1/1	0.99	0.03	62,62,62,62	0
14	ZN	A	1300	1/1	1.00	0.02	58,58,58,58	0
14	ZN	C	1000	1/1	1.00	0.03	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.