



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:05 PM UTC

PDB ID : 3MQ6 / pdb_00003mq6
Title : Domain swapped SgrAI with DNA and calcium bound
Authors : Dunten, P.W.; Horton, N.C.; Little, E.J.
Deposited on : 2010-04-27
Resolution : 2.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

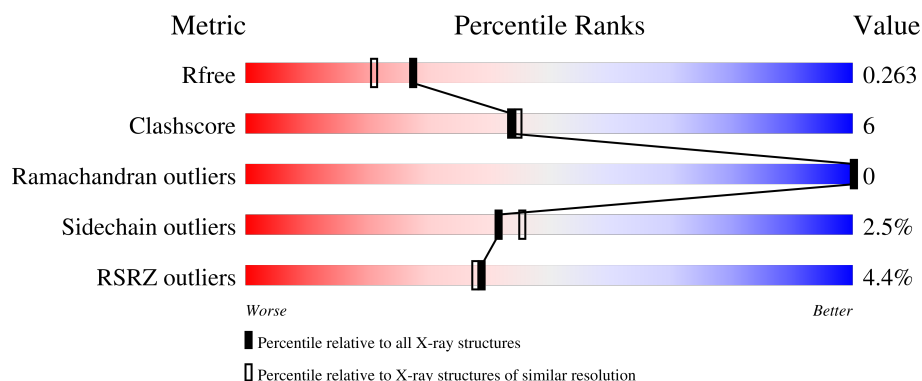
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

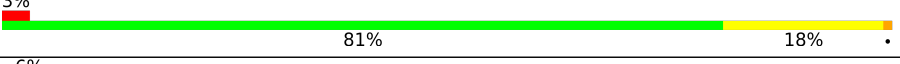
The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



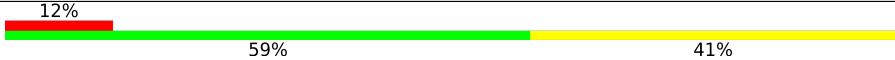
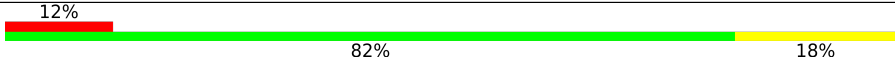
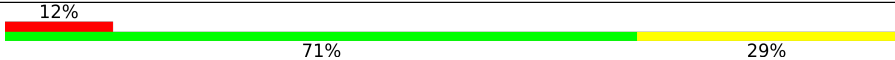
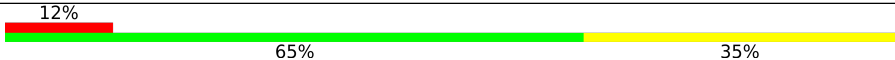
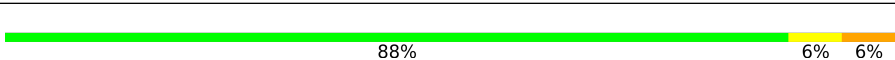
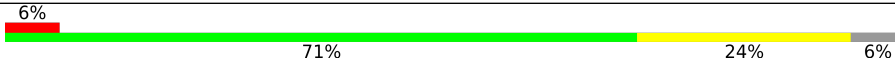
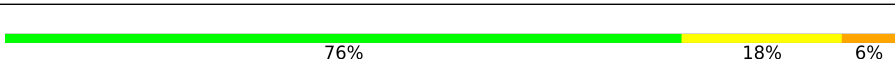
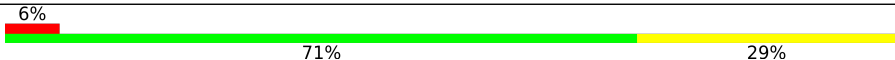
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	338	 4% 83% 15% ..
1	B	338	 3% 81% 18% .
1	C	338	 6% 85% 13% ..
1	D	338	 4% 83% 15% ..
1	E	338	 2% 85% 14% .

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Mol	Chain	Length	Quality of chain
1	F	338	
1	G	338	
1	H	338	
2	K	17	
2	L	17	
2	M	17	
2	N	17	
2	O	17	
2	P	17	
2	Q	17	
2	R	17	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25250 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 SgraIR restriction enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	0	0
			2612	1653	461	489	9			
1	B	338	Total	C	N	O	S	0	0	0
			2658	1681	473	495	9			
1	C	335	Total	C	N	O	S	0	2	0
			2654	1679	476	490	9			
1	D	333	Total	C	N	O	S	0	1	0
			2628	1665	465	489	9			
1	E	333	Total	C	N	O	S	0	1	0
			2645	1673	470	493	9			
1	F	338	Total	C	N	O	S	0	0	0
			2652	1678	470	495	9			
1	G	335	Total	C	N	O	S	0	0	0
			2644	1674	470	491	9			
1	H	336	Total	C	N	O	S	0	1	1
			2653	1681	472	491	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	ASP	ASN	cloning artifact	UNP Q9F6L0
B	63	ASP	ASN	cloning artifact	UNP Q9F6L0
C	63	ASP	ASN	cloning artifact	UNP Q9F6L0
D	63	ASP	ASN	cloning artifact	UNP Q9F6L0
E	63	ASP	ASN	cloning artifact	UNP Q9F6L0
F	63	ASP	ASN	cloning artifact	UNP Q9F6L0
G	63	ASP	ASN	cloning artifact	UNP Q9F6L0
H	63	ASP	ASN	cloning artifact	UNP Q9F6L0

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*AP*GP*TP*CP*CP*AP*CP*CP*GP*GP*TP*GP*GP*AP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	17	Total 346	C 165	N 66	O 99	P 16	0	0	0
2	K	17	Total 346	C 165	N 66	O 99	P 16	0	0	0
2	N	17	Total 346	C 165	N 66	O 99	P 16	0	0	0
2	M	17	Total 346	C 165	N 66	O 99	P 16	0	0	0
2	P	16	Total 325	C 155	N 61	O 94	P 15	0	0	0
2	O	17	Total 346	C 165	N 66	O 99	P 16	0	0	0
2	R	17	Total 346	C 165	N 66	O 99	P 16	0	0	0
2	Q	17	Total 346	C 165	N 66	O 99	P 16	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	Ca 3	0	0
3	B	3	Total 3	Ca 3	0	0
3	C	3	Total 3	Ca 3	0	0
3	D	3	Total 3	Ca 3	0	0
3	E	2	Total 2	Ca 2	0	0
3	F	3	Total 3	Ca 3	0	0
3	G	2	Total 2	Ca 2	0	0
3	H	3	Total 3	Ca 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	135	Total 135	O 135	0	0
4	B	133	Total 133	O 133	0	0

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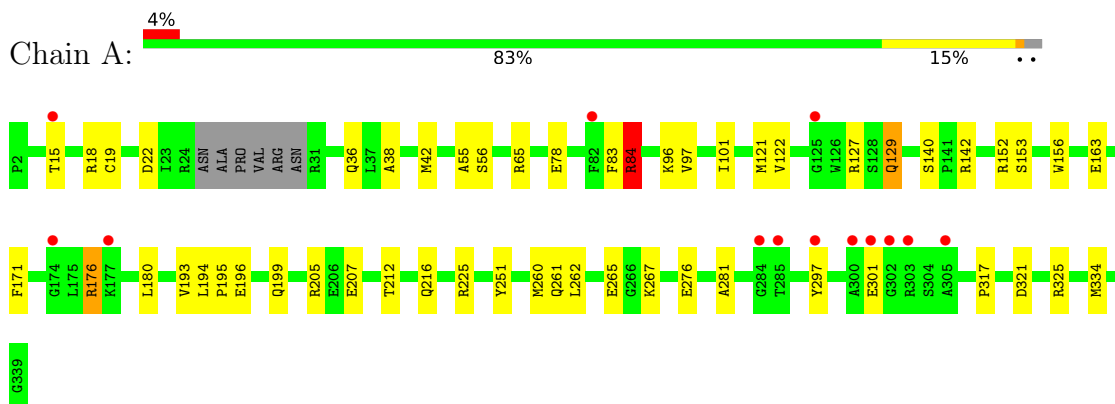
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	132	Total 132	O 132	0	0
4	D	161	Total 161	O 161	0	0
4	E	169	Total 169	O 169	0	0
4	F	151	Total 151	O 151	0	0
4	G	140	Total 140	O 140	0	0
4	H	135	Total 135	O 135	0	0
4	L	25	Total 25	O 25	0	0
4	K	24	Total 24	O 24	0	0
4	N	22	Total 22	O 22	0	0
4	M	19	Total 19	O 19	0	0
4	P	26	Total 26	O 26	0	0
4	O	22	Total 22	O 22	0	0
4	R	20	Total 20	O 20	0	0
4	Q	21	Total 21	O 21	0	0

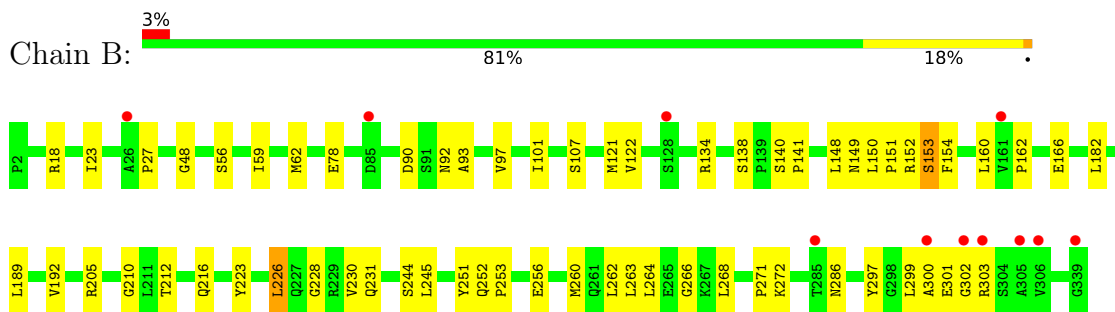
3 Residue-property plots [i](#)

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.

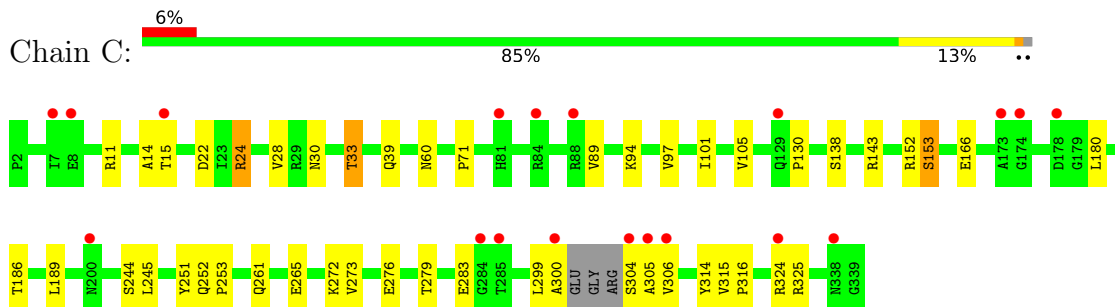
- Molecule 1: SgraIR restriction enzyme



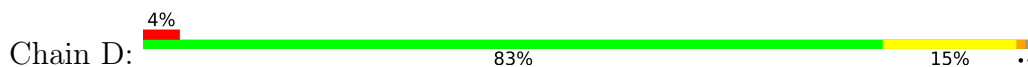
- Molecule 1: SgraIR restriction enzyme

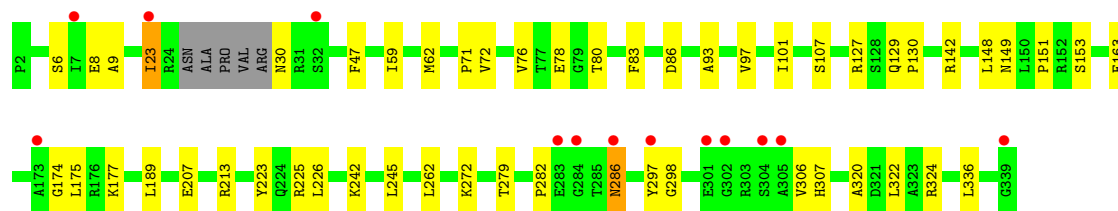


- Molecule 1: SgraIR restriction enzyme

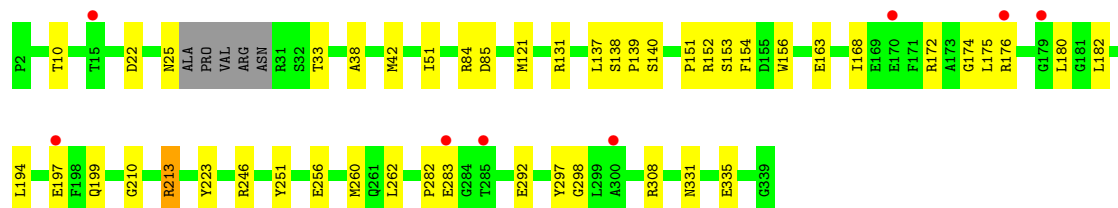
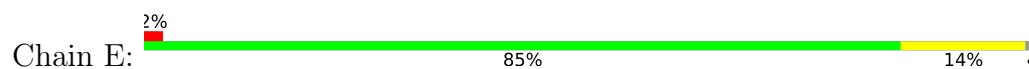


- Molecule 1: SgraIR restriction enzyme

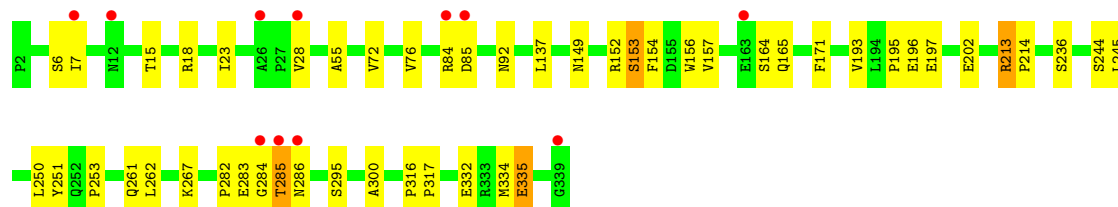
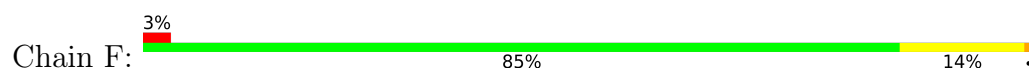




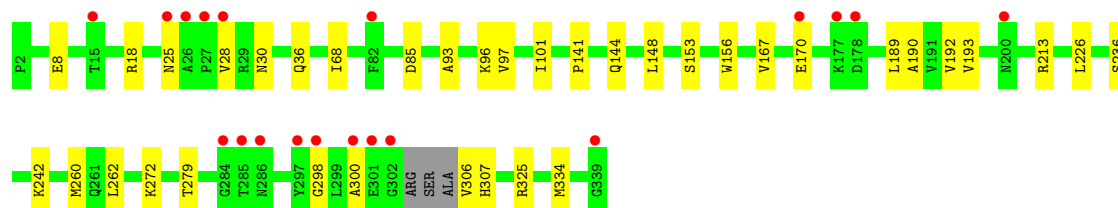
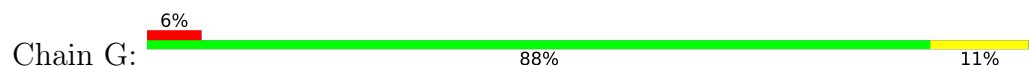
• Molecule 1: SgraIR restriction enzyme



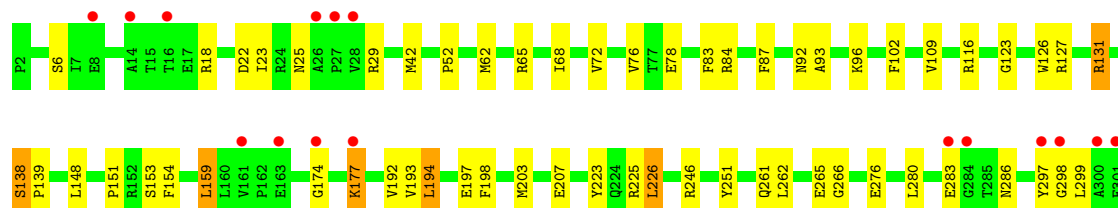
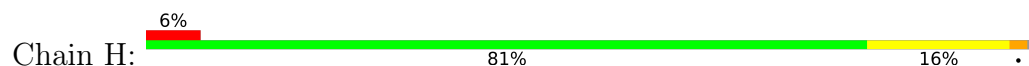
• Molecule 1: SgraIR restriction enzyme

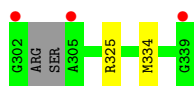


• Molecule 1: SgraIR restriction enzyme

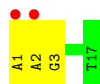
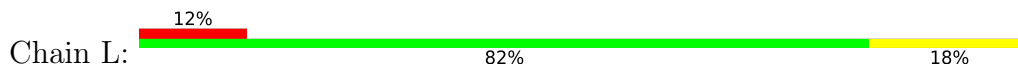


• Molecule 1: SgraIR restriction enzyme

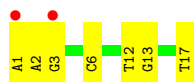




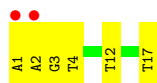
- Molecule 2: DNA (5'-D(*AP*AP*GP*TP*CP*CP*AP*CP*CP*GP*GP*TP*GP*GP*AP*CP*T)-3')



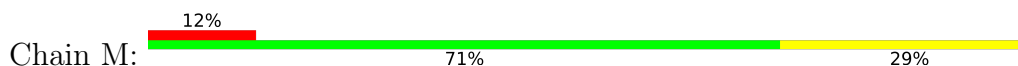
- Molecule 2: DNA (5'-D(*AP*AP*GP*TP*CP*CP*AP*CP*CP*GP*GP*TP*GP*GP*AP*CP*T)-3')



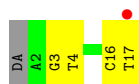
- Molecule 2: DNA (5'-D(*AP*AP*GP*TP*CP*CP*AP*CP*CP*GP*GP*TP*GP*GP*AP*CP*T)-3')



- Molecule 2: DNA (5'-D(*AP*AP*GP*TP*CP*CP*AP*CP*CP*GP*GP*TP*GP*GP*AP*CP*T)-3')

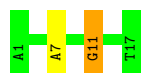


- Molecule 2: DNA (5'-D(*AP*AP*GP*TP*CP*CP*AP*CP*CP*GP*GP*TP*GP*GP*AP*CP*T)-3')



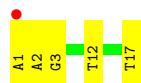
- Molecule 2: DNA (5'-D(*AP*AP*GP*TP*CP*CP*AP*CP*CP*GP*GP*TP*GP*GP*AP*CP*T)-3')

Chain O:  88% 6% 6%



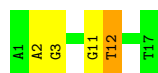
- Molecule 2: DNA (5'-D(*AP*AP*GP*TP*CP*CP*AP*CP*CP*GP*GP*TP*GP*GP*AP*CP*T)-3')

Chain R:  6% 71% 29%



- Molecule 2: DNA (5'-D(*AP*AP*GP*TP*CP*CP*AP*CP*CP*GP*GP*TP*GP*GP*AP*CP*T)-3')

Chain Q:  76% 18% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	130.38Å 134.95Å 237.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.46 – 2.00 25.46 – 2.00	Depositor EDS
% Data completeness (in resolution range)	86.8 (25.46-2.00) 94.9 (25.46-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 1.99Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.211 , 0.261 0.213 , 0.263	Depositor DCC
R_{free} test set	5410 reflections (1.92%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25250	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.48	0/2669	0.82	4/3623 (0.1%)
1	B	0.46	0/2717	0.79	3/3690 (0.1%)
1	C	0.52	0/2713	0.83	3/3684 (0.1%)
1	D	0.50	0/2686	0.81	2/3646 (0.1%)
1	E	0.53	0/2703	0.82	2/3667 (0.1%)
1	F	0.51	0/2711	0.87	2/3683 (0.1%)
1	G	0.48	0/2702	0.81	0/3667
1	H	0.50	0/2712	0.85	6/3683 (0.2%)
2	K	0.36	0/388	1.03	1/597 (0.2%)
2	L	0.36	0/388	1.03	0/597
2	M	0.36	0/388	1.01	1/597 (0.2%)
2	N	0.37	0/388	0.98	0/597
2	O	0.38	0/388	1.18	2/597 (0.3%)
2	P	0.38	0/364	1.18	0/560
2	Q	0.35	0/388	1.05	1/597 (0.2%)
2	R	0.35	0/388	1.03	0/597
All	All	0.48	0/24693	0.86	27/34082 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	134	ARG	CA-C-N	6.47	126.43	119.76
1	B	134	ARG	C-N-CA	6.47	126.43	119.76
1	A	84	ARG	CB-CA-C	-6.42	109.18	116.63
2	K	6	DC	O4'-C1'-N1	-6.42	98.77	108.40
1	H	251	TYR	N-CA-C	6.35	121.10	113.23
2	Q	12	DT	O5'-C5'-C4'	-6.09	101.66	110.80
1	B	251	TYR	N-CA-C	5.97	120.64	113.23
1	C	186	THR	CA-C-N	-5.76	114.81	120.98
1	C	186	THR	C-N-CA	-5.76	114.81	120.98
1	H	138	SER	CA-C-N	5.71	125.64	119.76
1	H	138	SER	C-N-CA	5.71	125.64	119.76
2	O	11	DG	O3'-P-O5'	-5.46	95.81	104.00
1	E	246	ARG	N-CA-C	-5.39	100.87	109.23
1	C	251	TYR	N-CA-C	5.38	119.00	112.23
1	A	281	ALA	CA-C-N	5.37	125.45	119.87
1	A	281	ALA	C-N-CA	5.37	125.45	119.87
1	F	84	ARG	CB-CA-C	-5.33	110.41	116.54
1	H	283	GLU	CB-CA-C	-5.28	110.47	116.54
2	O	11	DG	C4'-C3'-O3'	-5.27	102.10	110.00
1	D	213	ARG	CA-C-N	-5.24	113.64	119.19
1	D	213	ARG	C-N-CA	-5.24	113.64	119.19
1	H	177	LYS	N-CA-C	-5.23	106.85	113.18
1	H	246	ARG	N-CA-C	-5.22	101.36	109.24
1	F	251	TYR	N-CA-C	5.11	118.67	112.23
1	E	251	TYR	N-CA-C	5.10	119.22	112.89
1	A	251	TYR	N-CA-C	5.02	119.45	113.23
2	M	7	DA	C4'-C3'-O3'	-5.00	102.50	110.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	284	GLY	Peptide

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	2612	0	2560	33	0
1	B	2658	0	2614	37	0
1	C	2654	0	2607	30	0
1	D	2628	0	2577	43	0
1	E	2645	0	2598	37	0
1	F	2652	0	2603	31	0
1	G	2644	0	2605	25	0
1	H	2653	0	2608	41	0
2	K	346	0	192	6	0
2	L	346	0	192	6	0
2	M	346	0	192	6	0
2	N	346	0	192	8	0
2	O	346	0	192	2	0
2	P	325	0	181	3	0
2	Q	346	0	192	6	0
2	R	346	0	192	7	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	2	0	0	0	0
3	F	3	0	0	0	0
3	G	2	0	0	0	0
3	H	3	0	0	0	0
4	A	135	0	0	6	0
4	B	133	0	0	0	0
4	C	132	0	0	1	0
4	D	161	0	0	4	0
4	E	169	0	0	2	0
4	F	151	0	0	3	0
4	G	140	0	0	1	0
4	H	135	0	0	1	0
4	K	24	0	0	0	0
4	L	25	0	0	0	0
4	M	19	0	0	0	0
4	N	22	0	0	0	0
4	O	22	0	0	0	0
4	P	26	0	0	0	0
4	Q	21	0	0	0	0
4	R	20	0	0	0	0
All	All	25250	0	22297	282	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 6.

All (282) 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:174:GLY:O	1:D:177:LYS:HG2	1.83	0.77
1:H:148:LEU:HD21	1:H:226:LEU:HD13	1.66	0.76
1:E:297[B]:TYR:CG	1:E:298:GLY:N	2.57	0.73
1:B:301:GLU:HG3	1:B:302:GLY:H	1.53	0.72
1:F:193:VAL:HG22	1:F:334:MET:HE1	1.74	0.70
1:D:59:ILE:HA	1:D:62:MET:HE3	1.74	0.69
1:D:76:VAL:O	1:D:80:THR:HG23	1.95	0.67
1:G:167:VAL:O	1:G:170:GLU:HG3	1.94	0.67
1:G:298:GLY:O	1:G:306:VAL:HG22	1.94	0.67
2:M:2:DA:H2''	2:M:3:DG:OP2	1.96	0.66
1:D:93:ALA:HA	2:N:12:DT:H4'	1.78	0.66
1:C:300:ALA:HB2	1:D:297[A]:TYR:CE1	2.30	0.65
1:E:262:LEU:HD23	1:E:262:LEU:C	2.22	0.65
1:F:285:THR:HG23	1:F:285:THR:O	1.97	0.65
1:H:154:PHE:HZ	1:H:159:LEU:HD13	1.62	0.64
1:G:189:LEU:HD23	1:G:190:ALA:N	2.12	0.63
1:G:189:LEU:HD23	1:G:189:LEU:C	2.26	0.61
1:E:121:MET:HB3	1:E:140:SER:O	2.01	0.60
1:B:301:GLU:HG3	1:B:302:GLY:N	2.14	0.59
2:R:17:DT:H3	2:Q:2:DA:H61	1.49	0.59
1:C:252:GLN:HB3	1:C:253:PRO:HD3	1.85	0.59
1:E:297[B]:TYR:CD2	1:E:298:GLY:N	2.71	0.58
1:E:137:LEU:HD13	1:E:335:GLU:HG2	1.86	0.58
1:B:266:GLY:HA2	1:B:297:TYR:OH	2.03	0.58
1:B:23:ILE:HD13	1:G:36:GLN:HG3	1.85	0.58
1:B:122:VAL:HG21	1:B:205:ARG:HD3	1.86	0.58
2:L:2:DA:H61	2:K:17:DT:H3	1.52	0.58
1:F:332:GLU:O	1:F:335:GLU:HB2	2.03	0.57
1:D:97:VAL:HG12	1:D:101:ILE:HD12	1.86	0.57
1:E:151:PRO:HG3	1:E:223:TYR:CZ	2.39	0.57
1:H:52:PRO:O	1:H:109:VAL:HG22	2.04	0.57
1:B:48:GLY:O	1:B:210:GLY:HA3	2.05	0.56
1:D:272:LYS:HG3	1:D:307:HIS:CD2	2.40	0.56
1:G:272:LYS:HG3	1:G:307:HIS:CD2	2.40	0.56
1:A:83:PHE:C	1:A:84:ARG:HG2	2.30	0.56
1:B:262:LEU:C	1:B:262:LEU:HD23	2.31	0.56
2:R:17:DT:H3	2:Q:2:DA:N6	2.03	0.56
1:E:137:LEU:CD1	1:E:335:GLU:HG2	2.36	0.55
1:E:163:GLU:CD	1:E:163:GLU:H	2.13	0.55
1:F:282:PRO:HD2	1:F:283:GLU:OE2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:261:GLN:OE1	1:F:295:SER:HB2	2.07	0.55
1:D:286:ASN:HB2	4:D:874:HOH:O	2.05	0.55
1:E:151:PRO:HD2	1:E:154:PHE:HB2	1.89	0.55
2:Q:2:DA:H1'	2:Q:3:DG:C8	2.41	0.55
1:D:93:ALA:HB2	2:N:12:DT:H5''	1.90	0.54
2:K:1:DA:H2''	2:K:2:DA:N7	2.23	0.54
1:G:93:ALA:HA	2:R:12:DT:H4'	1.90	0.54
1:H:154:PHE:CZ	1:H:159:LEU:HD13	2.41	0.53
1:A:317:PRO:HD2	1:A:321:ASP:HB3	1.90	0.53
1:A:129:GLN:HG3	1:A:129:GLN:O	2.08	0.53
2:N:17:DT:O2	2:M:2:DA:N1	2.41	0.53
1:B:182:LEU:HD23	1:B:263:LEU:HD21	1.90	0.53
1:H:203:MET:HE1	1:H:225:ARG:CD	2.39	0.53
1:D:245:LEU:HD12	1:D:282:PRO:HA	1.91	0.53
2:N:17:DT:H3	2:M:2:DA:H61	1.55	0.53
2:R:2:DA:H2''	2:R:3:DG:OP2	2.08	0.53
1:B:97:VAL:HG12	1:B:101:ILE:HD12	1.91	0.53
1:G:148:LEU:HD21	1:G:226:LEU:HD13	1.90	0.53
1:A:261:GLN:HG2	1:A:265:GLU:OE2	2.08	0.53
1:F:7:ILE:HG22	4:F:1222:HOH:O	2.09	0.52
1:C:324[B]:ARG:HG2	1:C:324[B]:ARG:HH11	1.73	0.52
1:H:262:LEU:HD23	1:H:262:LEU:C	2.35	0.52
1:D:23:ILE:HG23	1:D:23:ILE:O	2.08	0.52
1:E:297[A]:TYR:CD1	1:F:300:ALA:HB2	2.45	0.52
1:B:148:LEU:HD21	1:B:226:LEU:HD13	1.92	0.52
1:A:65:ARG:HG3	4:A:441:HOH:O	2.10	0.52
1:B:244:SER:C	1:B:245:LEU:HD23	2.35	0.52
1:D:83:PHE:CZ	1:E:22:ASP:HB2	2.45	0.52
1:E:131:ARG:HG3	4:E:369:HOH:O	2.10	0.52
1:F:15:THR:HA	1:F:18:ARG:HG3	1.92	0.51
1:B:56:SER:OG	1:B:59:ILE:HG13	2.11	0.51
1:G:193:VAL:HG22	1:G:334:MET:HE1	1.91	0.51
1:D:148:LEU:HD21	1:D:226:LEU:HD22	1.93	0.51
1:C:71:PRO:HB2	1:C:101:ILE:HD13	1.93	0.51
1:D:322:LEU:HD12	4:D:907:HOH:O	2.11	0.51
2:L:2:DA:N1	2:K:17:DT:O2	2.43	0.51
1:H:151:PRO:HG3	1:H:223:TYR:CZ	2.46	0.50
1:H:193:VAL:HG22	1:H:334:MET:HE1	1.94	0.50
2:L:1:DA:H2'	2:L:1:DA:N3	2.26	0.50
1:B:264:LEU:HD23	1:B:268:LEU:HD12	1.93	0.50
1:G:192:VAL:HG21	1:G:226:LEU:HD22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:GLU:O	1:B:260:MET:HG3	2.11	0.50
1:F:157:VAL:HG12	1:F:165:GLN:HG2	1.93	0.50
1:A:78:GLU:OE2	1:H:18:ARG:HB3	2.11	0.50
1:H:276:GLU:CD	1:H:325:ARG:HH12	2.20	0.50
1:H:192:VAL:HG21	1:H:226:LEU:HD22	1.93	0.50
1:A:38:ALA:O	1:A:42:MET:HG3	2.12	0.49
1:B:212:THR:O	1:B:216:GLN:HG3	2.12	0.49
1:H:93:ALA:HB2	2:Q:12:DT:H4'	1.94	0.49
1:E:151:PRO:HG3	1:E:223:TYR:CE1	2.48	0.49
1:E:194:LEU:HD23	1:E:199:GLN:HA	1.95	0.49
1:A:83:PHE:CZ	1:H:22:ASP:HB2	2.47	0.49
1:C:39:GLN:HB3	1:C:97:VAL:HG13	1.94	0.49
1:D:262:LEU:C	1:D:262:LEU:HD23	2.38	0.49
1:E:176:ARG:HA	1:E:180:LEU:O	2.13	0.49
1:G:97:VAL:O	1:G:101:ILE:HG12	2.12	0.49
1:A:127:ARG:NH1	1:A:207:GLU:HG3	2.28	0.49
1:B:160:LEU:O	1:B:228:GLY:HA2	2.12	0.49
1:C:283:GLU:HA	1:C:283:GLU:OE1	2.13	0.49
1:E:154:PHE:CE2	1:E:156:TRP:HA	2.48	0.49
1:D:151:PRO:HG3	1:D:223:TYR:CZ	2.48	0.48
2:N:2:DA:H2''	2:N:3:DG:OP2	2.13	0.48
1:B:121:MET:HB3	1:B:140:SER:O	2.13	0.48
1:D:297[B]:TYR:HB3	4:D:381:HOH:O	2.14	0.48
1:H:83:PHE:C	1:H:84:ARG:HG2	2.38	0.48
1:E:197:GLU:CD	1:E:197:GLU:H	2.21	0.48
1:H:197:GLU:CD	1:H:197:GLU:H	2.22	0.48
1:A:176:ARG:HA	1:A:180:LEU:O	2.13	0.48
1:F:171:PHE:CE1	1:F:267:LYS:HE3	2.48	0.48
1:D:72:VAL:HG23	4:D:354:HOH:O	2.13	0.48
1:C:314:TYR:CE2	1:C:316:PRO:HB3	2.49	0.47
1:F:250:LEU:O	1:F:253:PRO:HD2	2.14	0.47
1:A:97:VAL:HG12	1:A:101:ILE:HD12	1.95	0.47
1:C:261:GLN:HG2	1:C:273:VAL:HB	1.96	0.47
1:F:92:ASN:HB3	2:O:11:DG:N3	2.30	0.47
2:R:1:DA:H3'	2:R:2:DA:C8	2.49	0.47
1:A:18:ARG:HB3	1:H:78:GLU:OE2	2.15	0.47
1:E:84:ARG:HB3	1:E:85:ASP:H	1.59	0.47
1:G:262:LEU:C	1:G:262:LEU:HD23	2.40	0.47
1:G:325:ARG:HG2	1:G:325:ARG:HH11	1.80	0.47
1:A:18:ARG:HD3	4:A:372:HOH:O	2.15	0.47
1:B:152:ARG:O	1:B:153:SER:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:154:PHE:CE2	1:F:156:TRP:HA	2.49	0.47
1:H:116:ARG:HG2	1:H:126:TRP:CZ3	2.50	0.47
1:H:194:LEU:HD22	1:H:198:PHE:HB2	1.96	0.47
2:M:17:DT:H3'	2:M:17:DT:H6	1.79	0.46
1:C:60:ASN:HD21	1:C:130:PRO:HG3	1.80	0.46
1:C:244:SER:C	1:C:245:LEU:HD23	2.40	0.46
1:E:38:ALA:O	1:E:42:MET:HG3	2.15	0.46
1:B:149:ASN:OD1	1:B:149:ASN:C	2.58	0.46
1:F:149:ASN:C	1:F:149:ASN:OD1	2.59	0.46
1:E:25:ASN:C	1:E:25:ASN:HD22	2.24	0.46
1:E:138:SER:HA	1:E:139:PRO:HD3	1.79	0.46
1:H:138:SER:HA	1:H:139:PRO:HD3	1.78	0.46
1:B:151:PRO:HG2	1:B:154:PHE:HB2	1.97	0.46
1:H:92:ASN:HB3	2:Q:11:DG:N3	2.31	0.46
1:F:72:VAL:O	1:F:76:VAL:HG23	2.15	0.46
2:K:2:DA:H2''	2:K:3:DG:OP2	2.16	0.46
1:C:28:VAL:O	1:C:28:VAL:HG13	2.16	0.46
1:D:97:VAL:CG1	1:D:101:ILE:HD12	2.46	0.46
1:E:262:LEU:HD23	1:E:262:LEU:O	2.16	0.46
1:A:205:ARG:NH1	4:A:1235:HOH:O	2.48	0.45
1:A:262:LEU:C	1:A:262:LEU:HD23	2.40	0.45
2:P:3:DG:H2'	2:P:4:DT:H72	1.97	0.45
1:C:180:LEU:CD1	1:D:306:VAL:HG12	2.46	0.45
2:L:2:DA:H1'	2:L:3:DG:C5'	2.46	0.45
1:A:276:GLU:CD	1:A:325:ARG:HH12	2.24	0.45
1:D:127:ARG:HD2	1:D:207:GLU:OE2	2.16	0.45
2:L:2:DA:H2''	2:L:3:DG:OP2	2.16	0.45
1:B:90:ASP:OD2	1:B:92:ASN:HB2	2.17	0.45
1:D:320:ALA:O	1:D:324:ARG:HG3	2.16	0.45
1:A:194:LEU:HD12	1:A:195:PRO:HD2	1.98	0.45
1:C:138:SER:O	1:C:143:ARG:NH1	2.48	0.45
1:G:141:PRO:O	1:G:144:GLN:HG3	2.17	0.45
1:H:83:PHE:HB2	1:H:87:PHE:HB2	1.98	0.45
1:C:60:ASN:ND2	1:C:130:PRO:HG3	2.32	0.45
1:C:152:ARG:O	1:C:153:SER:CB	2.64	0.45
1:H:65:ARG:HA	1:H:280:LEU:HD13	1.99	0.45
1:A:193:VAL:HG22	1:A:334:MET:HE1	1.99	0.45
1:D:297[B]:TYR:CD2	1:D:298:GLY:N	2.85	0.45
1:F:283:GLU:H	1:F:283:GLU:CD	2.25	0.45
1:D:72:VAL:O	1:D:76:VAL:HG23	2.17	0.45
1:A:56:SER:HB2	4:A:892:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:131:ARG:H	1:H:131:ARG:HG2	1.58	0.44
1:H:151:PRO:HG2	1:H:154:PHE:HB2	1.99	0.44
1:B:303:ARG:HA	1:B:303:ARG:HD3	1.74	0.44
1:A:55:ALA:HB1	4:A:1285:HOH:O	2.16	0.44
1:B:244:SER:O	1:B:245:LEU:HD23	2.17	0.44
1:D:6:SER:HB3	1:D:9:ALA:HB3	1.99	0.44
1:D:107:SER:OG	1:D:189:LEU:HD12	2.17	0.44
1:C:189:LEU:HD23	1:C:189:LEU:C	2.43	0.44
1:G:96:LYS:HD3	1:G:96:LYS:C	2.43	0.44
1:H:96:LYS:HG3	2:Q:12:DT:O2	2.18	0.44
1:E:168:ILE:HG22	1:E:172:ARG:HD2	2.00	0.44
2:P:16:DC:H2''	2:P:17:DT:OP2	2.17	0.44
1:B:78:GLU:OE2	1:G:18:ARG:HB3	2.18	0.44
1:A:22:ASP:HB2	1:H:83:PHE:CZ	2.52	0.44
1:D:226:LEU:N	1:D:226:LEU:HD12	2.33	0.44
1:H:194:LEU:HD23	1:H:194:LEU:HA	1.84	0.44
1:D:83:PHE:O	1:D:86:ASP:HB2	2.18	0.43
1:C:324[B]:ARG:HG2	1:C:324[B]:ARG:NH1	2.33	0.43
1:A:36:GLN:HB2	1:H:23:ILE:HD13	2.00	0.43
1:B:162:PRO:O	1:B:166:GLU:HG3	2.19	0.43
1:D:23:ILE:HG22	1:E:33:THR:O	2.18	0.43
1:C:89:VAL:HG23	1:C:94:LYS:HE3	2.00	0.43
1:F:152:ARG:O	1:F:153:SER:CB	2.66	0.43
1:D:242:LYS:O	1:D:279:THR:HA	2.19	0.43
2:M:2:DA:C2'	2:M:3:DG:OP2	2.65	0.43
1:B:93:ALA:HA	2:K:12:DT:H4'	2.01	0.43
2:M:16:DC:H2''	2:M:17:DT:H5'	2.00	0.43
2:N:1:DA:H4'	2:N:2:DA:O5'	2.19	0.43
1:E:292:GLU:HG2	1:E:308:ARG:NH2	2.34	0.43
1:H:148:LEU:CD2	1:H:226:LEU:HD13	2.41	0.43
2:K:12:DT:H2'	2:K:13:DG:N7	2.34	0.43
1:A:163:GLU:CD	1:A:163:GLU:H	2.27	0.42
1:A:171:PHE:CE1	1:A:267:LYS:HE3	2.54	0.42
1:D:225:ARG:C	1:D:226:LEU:HD12	2.44	0.42
1:H:262:LEU:O	1:H:266:GLY:HA3	2.19	0.42
2:L:2:DA:H1'	2:L:3:DG:H5'	2.01	0.42
1:F:55:ALA:HB1	4:F:1317:HOH:O	2.18	0.42
1:C:299:LEU:HD21	1:D:175:LEU:HD21	2.01	0.42
1:H:174:GLY:O	1:H:177:LYS:HG2	2.18	0.42
1:A:152:ARG:O	1:A:153:SER:CB	2.68	0.42
1:C:180:LEU:HD13	1:D:306:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:213:ARG:HD2	1:E:213:ARG:HA	1.68	0.42
1:E:297[A]:TYR:CE1	1:F:300:ALA:HA	2.55	0.42
1:F:137:LEU:HD13	1:F:335:GLU:HG2	2.01	0.42
1:F:285:THR:O	1:F:285:THR:CG2	2.67	0.42
1:G:93:ALA:HB2	2:R:12:DT:C5'	2.48	0.42
1:H:261:GLN:HG2	1:H:265:GLU:OE2	2.19	0.42
1:E:174:GLY:O	1:E:175:LEU:C	2.63	0.42
1:E:331:ASN:HB3	4:E:348:HOH:O	2.19	0.42
1:F:195:PRO:O	1:F:196:GLU:C	2.63	0.42
1:F:244:SER:C	1:F:245:LEU:HD23	2.45	0.42
1:G:68:ILE:HD13	1:G:68:ILE:HA	1.84	0.42
1:B:271:PRO:O	1:B:272:LYS:C	2.63	0.42
1:C:304:SER:OG	1:C:305:ALA:N	2.52	0.42
1:G:213:ARG:HD3	4:G:927:HOH:O	2.19	0.42
1:E:262:LEU:C	1:E:262:LEU:CD2	2.93	0.42
1:A:96:LYS:HD3	1:A:96:LYS:C	2.45	0.42
1:D:47:PHE:HE2	1:D:71:PRO:CG	2.33	0.42
1:D:149:ASN:OD1	1:D:149:ASN:C	2.62	0.42
1:G:242:LYS:O	1:G:279:THR:HA	2.20	0.42
1:B:27:PRO:HG2	1:G:25:ASN:HB2	2.02	0.42
1:B:299:LEU:O	1:B:300:ALA:C	2.63	0.42
1:B:150:LEU:HD22	1:B:154:PHE:CE2	2.55	0.42
1:F:152:ARG:O	1:F:153:SER:HB2	2.20	0.42
1:F:213:ARG:N	1:F:214:PRO:CD	2.83	0.42
1:B:59:ILE:HA	1:B:62:MET:HE3	2.01	0.41
1:E:256:GLU:O	1:E:260:MET:HG3	2.19	0.41
1:F:28:VAL:O	1:F:28:VAL:HG13	2.18	0.41
1:H:127:ARG:HH21	1:H:207:GLU:HG3	1.84	0.41
1:C:101:ILE:O	1:C:105:VAL:HG23	2.20	0.41
1:C:276:GLU:CD	1:C:325:ARG:HH12	2.24	0.41
1:D:78:GLU:HG3	1:E:10:THR:HG21	2.01	0.41
1:F:6:SER:HB2	4:F:618:HOH:O	2.19	0.41
1:A:212:THR:O	1:A:216:GLN:HG3	2.19	0.41
1:D:297[B]:TYR:CG	1:D:298:GLY:N	2.86	0.41
1:E:51:ILE:CD1	1:E:210:GLY:HA2	2.51	0.41
1:G:156:TRP:CE2	1:G:260:MET:HG2	2.55	0.41
1:B:151:PRO:HG3	1:B:223:TYR:CZ	2.55	0.41
1:D:71:PRO:HB2	1:D:101:ILE:HD13	2.02	0.41
1:E:282:PRO:O	1:E:283:GLU:C	2.64	0.41
1:A:19:CYS:HB3	1:H:42:MET:HG2	2.03	0.41
1:B:192:VAL:HG21	1:B:226:LEU:HD22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:72:VAL:O	1:H:76:VAL:HG23	2.20	0.41
1:C:272:LYS:CE	4:C:379:HOH:O	2.67	0.41
1:D:47:PHE:CE2	1:D:71:PRO:HG3	2.55	0.41
1:A:156:TRP:CE2	1:A:260:MET:HG2	2.55	0.41
1:A:194:LEU:HA	1:A:195:PRO:HD3	1.87	0.41
1:C:261:GLN:O	1:C:265:GLU:HB2	2.21	0.41
1:F:262:LEU:C	1:F:262:LEU:HD23	2.46	0.41
1:F:282:PRO:O	1:F:283:GLU:C	2.62	0.41
1:G:96:LYS:HG3	2:R:12:DT:O2	2.20	0.41
1:B:107:SER:OG	1:B:189:LEU:HD12	2.20	0.41
1:C:22:ASP:OD2	1:C:24:ARG:HG2	2.21	0.41
1:C:33:THR:HB	1:F:23:ILE:HD11	2.02	0.41
1:D:93:ALA:CA	2:N:12:DT:H4'	2.46	0.41
1:D:129:GLN:HA	1:D:130:PRO:C	2.46	0.41
1:B:140:SER:HA	1:B:141:PRO:HD3	1.89	0.41
1:B:230:VAL:HG12	1:B:231:GLN:O	2.21	0.41
1:D:189:LEU:C	1:D:189:LEU:HD23	2.45	0.41
1:F:316:PRO:HA	1:F:317:PRO:HD3	1.87	0.41
1:G:300:ALA:HB2	1:H:297[A]:TYR:CD1	2.56	0.41
1:H:62:MET:HE3	1:H:62:MET:HB2	1.92	0.41
1:H:68:ILE:HD12	1:H:102:PHE:HA	2.02	0.41
1:H:297[B]:TYR:CG	1:H:298:GLY:N	2.85	0.41
1:A:225:ARG:HD3	4:A:1196:HOH:O	2.21	0.41
1:H:123:GLY:HA2	4:H:1280:HOH:O	2.21	0.41
2:N:3:DG:H2''	2:N:4:DT:OP2	2.20	0.41
1:A:121:MET:HB3	1:A:140:SER:O	2.20	0.40
1:C:279:THR:O	1:C:315:VAL:HA	2.21	0.40
1:D:23:ILE:CG2	1:E:33:THR:O	2.69	0.40
1:E:182:LEU:HD12	1:E:182:LEU:HA	1.84	0.40
2:P:17:DT:OP2	2:P:17:DT:H2'	2.21	0.40
1:A:196:GLU:HA	1:A:199:GLN:NE2	2.36	0.40
1:B:252:GLN:N	1:B:253:PRO:CD	2.84	0.40
1:E:152:ARG:HG2	2:O:7:DA:H5'	2.03	0.40
1:G:325:ARG:HG2	1:G:325:ARG:NH1	2.36	0.40
1:C:22:ASP:CG	1:C:24:ARG:HH21	2.29	0.40
1:C:14:ALA:O	1:C:15:THR:C	2.64	0.40
1:H:299:LEU:HD23	1:H:299:LEU:HA	1.85	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	328/338 (97%)	316 (96%)	12 (4%)	0	100	100
1	B	336/338 (99%)	324 (96%)	12 (4%)	0	100	100
1	C	333/338 (98%)	324 (97%)	9 (3%)	0	100	100
1	D	330/338 (98%)	321 (97%)	9 (3%)	0	100	100
1	E	330/338 (98%)	317 (96%)	13 (4%)	0	100	100
1	F	336/338 (99%)	327 (97%)	9 (3%)	0	100	100
1	G	331/338 (98%)	321 (97%)	10 (3%)	0	100	100
1	H	333/338 (98%)	318 (96%)	15 (4%)	0	100	100
All	All	2657/2704 (98%)	2568 (97%)	89 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	274/282 (97%)	266 (97%)	8 (3%)	37	40
1	B	279/282 (99%)	274 (98%)	5 (2%)	51	58
1	C	278/282 (99%)	271 (98%)	7 (2%)	42	45
1	D	275/282 (98%)	267 (97%)	8 (3%)	37	40
1	E	278/282 (99%)	276 (99%)	2 (1%)	76	82
1	F	278/282 (99%)	268 (96%)	10 (4%)	31	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	278/282 (99%)	272 (98%)	6 (2%)	45	50
1	H	278/282 (99%)	269 (97%)	9 (3%)	34	35
All	All	2218/2256 (98%)	2163 (98%)	55 (2%)	42	45

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	THR
1	A	84	ARG
1	A	122	VAL
1	A	129	GLN
1	A	142	ARG
1	A	176	ARG
1	A	297	TYR
1	A	301	GLU
1	B	18	ARG
1	B	138	SER
1	B	153	SER
1	B	226	LEU
1	B	286	ASN
1	C	11	ARG
1	C	24	ARG
1	C	30	ASN
1	C	33	THR
1	C	153	SER
1	C	166	GLU
1	C	306	VAL
1	D	8	GLU
1	D	23	ILE
1	D	30	ASN
1	D	142	ARG
1	D	153	SER
1	D	163	GLU
1	D	286	ASN
1	D	336	LEU
1	E	153	SER
1	E	213	ARG
1	F	85	ASP
1	F	153	SER
1	F	164	SER
1	F	197	GLU

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Mol	Chain	Res	Type
1	F	202	GLU
1	F	213	ARG
1	F	236	SER
1	F	285	THR
1	F	286	ASN
1	F	335	GLU
1	G	8	GLU
1	G	28	VAL
1	G	30	ASN
1	G	85	ASP
1	G	153	SER
1	G	236	SER
1	H	6	SER
1	H	25	ASN
1	H	29	ARG
1	H	131	ARG
1	H	153	SER
1	H	159	LEU
1	H	194	LEU
1	H	226	LEU
1	H	286	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	216	GLN
1	A	231	GLN
1	B	41	ASN
1	B	200	ASN
1	B	338	ASN
1	C	25	ASN
1	C	74	ASN
1	C	216	GLN
1	D	30	ASN
1	D	200	ASN
1	D	286	ASN
1	E	12	ASN
1	E	25	ASN
1	E	74	ASN
1	E	199	GLN
1	E	200	ASN

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Mol	Chain	Res	Type
1	E	216	GLN
1	F	12	ASN
1	F	25	ASN
1	F	307	HIS
1	F	338	ASN
1	G	74	ASN
1	G	81	HIS
1	G	129	GLN
1	G	200	ASN
1	H	25	ASN
1	H	227	GLN
1	H	286	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 22 ligands modelled in this entry, 22 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	332/338 (98%)	0.38	13 (3%)	43	42	29, 41, 60, 82	0
1	B	338/338 (100%)	0.46	11 (3%)	49	48	29, 44, 65, 78	0
1	C	335/338 (99%)	0.34	19 (5%)	29	28	17, 38, 60, 80	2 (0%)
1	D	333/338 (98%)	0.31	13 (3%)	43	42	25, 38, 58, 81	1 (0%)
1	E	333/338 (98%)	0.18	8 (2%)	59	59	22, 36, 56, 74	1 (0%)
1	F	338/338 (100%)	0.30	11 (3%)	49	48	26, 40, 59, 68	0
1	G	335/338 (99%)	0.30	19 (5%)	29	28	28, 42, 63, 79	0
1	H	336/338 (99%)	0.45	19 (5%)	29	28	27, 41, 64, 80	1 (0%)
2	K	17/17 (100%)	0.21	2 (11%)	9	8	30, 37, 89, 96	0
2	L	17/17 (100%)	0.41	2 (11%)	9	8	31, 38, 99, 103	0
2	M	17/17 (100%)	0.13	2 (11%)	9	8	29, 36, 86, 87	0
2	N	17/17 (100%)	0.15	2 (11%)	9	8	30, 36, 95, 95	0
2	O	17/17 (100%)	-0.15	0	100	100	29, 34, 93, 96	0
2	P	16/17 (94%)	0.03	1 (6%)	26	24	28, 37, 61, 78	0
2	Q	17/17 (100%)	0.15	0	100	100	30, 38, 79, 82	0
2	R	17/17 (100%)	0.06	1 (5%)	28	27	29, 36, 89, 90	0
All	All	2815/2840 (99%)	0.33	123 (4%)	39	38	17, 40, 62, 103	5 (0%)

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	302	GLY	6.9
1	H	297[A]	TYR	5.7
1	B	300	ALA	4.5
1	C	305	ALA	4.4
1	F	28	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	285	THR	4.1
1	F	285	THR	4.1
1	E	300	ALA	4.1
1	G	284	GLY	4.0
1	G	301	GLU	4.0
2	L	1	DA	3.9
1	D	302	GLY	3.9
1	B	305	ALA	3.9
1	C	81[A]	HIS	3.8
1	G	339	GLY	3.8
1	G	298	GLY	3.8
2	L	2	DA	3.7
1	E	15	THR	3.5
1	H	339	GLY	3.4
1	F	26	ALA	3.4
1	B	303	ARG	3.4
1	E	283	GLU	3.3
1	H	177	LYS	3.3
1	A	300	ALA	3.2
1	H	28	VAL	3.2
1	C	300	ALA	3.2
1	H	300	ALA	3.2
1	D	32	SER	3.2
1	G	178	ASP	3.1
1	C	304	SER	3.1
1	D	283	GLU	3.1
1	G	27	PRO	3.0
1	A	177	LYS	3.0
1	G	15	THR	3.0
1	B	306	VAL	3.0
1	F	7	ILE	3.0
1	C	284	GLY	2.9
1	A	285	THR	2.9
1	B	85	ASP	2.9
1	C	285	THR	2.9
2	N	1	DA	2.9
1	H	298	GLY	2.9
1	B	26	ALA	2.8
1	D	297[A]	TYR	2.8
1	F	12	ASN	2.8
1	A	301	GLU	2.8
2	R	1	DA	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	84	ARG	2.7
1	D	173	ALA	2.7
1	A	174	GLY	2.7
1	F	284	GLY	2.7
1	C	8	GLU	2.6
1	A	125	GLY	2.6
1	G	286	ASN	2.6
2	K	1	DA	2.6
1	D	304	SER	2.6
1	E	197	GLU	2.6
1	C	200	ASN	2.6
1	G	302	GLY	2.6
1	A	82	PHE	2.5
1	D	286	ASN	2.5
2	N	2	DA	2.5
1	C	88	ARG	2.5
1	D	305	ALA	2.5
1	G	170	GLU	2.5
1	B	339	GLY	2.5
1	E	179	GLY	2.5
1	A	303	ARG	2.5
1	C	178	ASP	2.5
1	G	300	ALA	2.5
1	G	28	VAL	2.4
1	E	285	THR	2.4
1	H	161	VAL	2.4
1	C	324[A]	ARG	2.4
1	E	176	ARG	2.4
1	H	27	PRO	2.4
1	F	286	ASN	2.4
1	D	23	ILE	2.4
1	D	284	GLY	2.3
1	F	339	GLY	2.3
1	B	161	VAL	2.3
1	B	302	GLY	2.3
2	K	3	DG	2.3
2	P	17	DT	2.3
1	B	128	SER	2.3
1	A	305	ALA	2.3
1	F	85	ASP	2.3
1	G	177	LYS	2.3
1	H	174	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	163	GLU	2.2
1	A	302	GLY	2.2
1	G	26	ALA	2.2
1	H	284	GLY	2.2
1	D	301	GLU	2.2
1	A	284	GLY	2.2
1	C	173	ALA	2.2
1	H	8	GLU	2.2
1	H	301	GLU	2.2
1	H	26	ALA	2.2
1	H	305	ALA	2.2
1	G	285	THR	2.2
1	H	16	THR	2.1
2	M	1	DA	2.1
1	C	7	ILE	2.1
1	C	84	ARG	2.1
1	C	338	ASN	2.1
1	G	200	ASN	2.1
1	A	15	THR	2.1
1	C	15	THR	2.1
1	D	7	ILE	2.1
1	C	306	VAL	2.1
1	H	163	GLU	2.1
1	H	283	GLU	2.1
1	G	25	ASN	2.1
1	C	129	GLN	2.1
1	C	174	GLY	2.1
1	D	339	GLY	2.1
1	G	82	PHE	2.1
1	E	170	GLU	2.0
1	H	14	ALA	2.1
1	A	297	TYR	2.0
2	M	17	DT	2.0
1	G	297	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
3	CA	F	342	1/1	0.79	0.12	68,68,68,68	0
3	CA	A	341	1/1	0.81	0.11	77,77,77,77	0
3	CA	C	342	1/1	0.85	0.11	65,65,65,65	0
3	CA	D	342	1/1	0.88	0.08	66,66,66,66	0
3	CA	H	342	1/1	0.91	0.13	74,74,74,74	0
3	CA	B	342	1/1	0.93	0.09	68,68,68,68	0
3	CA	C	341	1/1	0.94	0.06	43,43,43,43	0
3	CA	G	341	1/1	0.95	0.07	48,48,48,48	0
3	CA	B	341	1/1	0.96	0.09	48,48,48,48	0
3	CA	D	341	1/1	0.97	0.06	42,42,42,42	0
3	CA	E	341	1/1	0.97	0.05	41,41,41,41	0
3	CA	H	341	1/1	0.97	0.04	43,43,43,43	0
3	CA	F	341	1/1	0.97	0.04	43,43,43,43	0
3	CA	B	340	1/1	0.99	0.04	33,33,33,33	0
3	CA	F	340	1/1	0.99	0.04	30,30,30,30	0
3	CA	A	340	1/1	0.99	0.04	45,45,45,45	0
3	CA	D	340	1/1	0.99	0.04	29,29,29,29	0
3	CA	G	340	1/1	0.99	0.04	34,34,34,34	0
3	CA	A	1	1/1	0.99	0.04	31,31,31,31	0
3	CA	H	340	1/1	0.99	0.04	33,33,33,33	0
3	CA	C	340	1/1	0.99	0.05	31,31,31,31	0
3	CA	E	340	1/1	0.99	0.08	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.