



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:47 PM UTC

PDB ID : 8C4I / pdb_00008c4i
Title : Ligand-free Crystal Structure of the decameric Sulfofructose Transaldolase BmSF-TAL
Authors : Snow, A.J.D.; Sharma, M.; Davies, G.J.
Deposited on : 2023-01-04
Resolution : 3.20 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

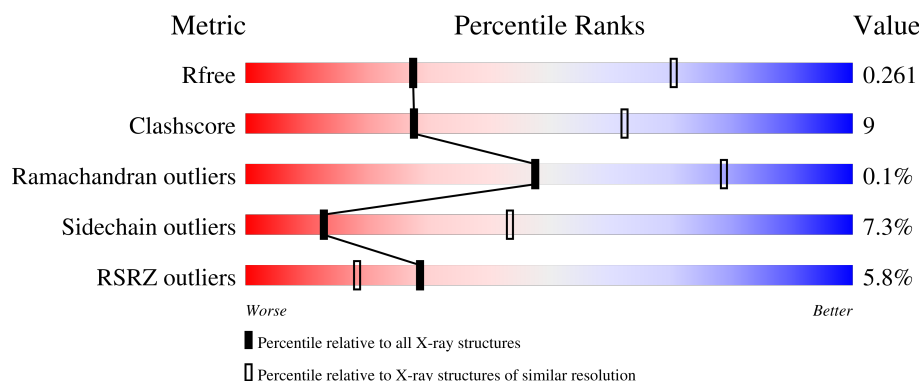
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	226	0% 84% 11% ...
1	B	226	0% 81% 14% ...
1	C	226	2% 82% 15% ...
1	D	226	4% 72% 20% ...
1	E	226	6% 73% 19% ...

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Mol	Chain	Length	Quality of chain
1	F	226	8% 82% 13%
1	G	226	9% 75% 18%
1	H	226	17% 77% 15%
1	J	226	7% 83% 12%
1	K	226	2% 82% 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 32872 atoms, of which 15987 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 BmSF-TAL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	218	Total	C	H	N	O	S	48	0	0
			3359	1094	1652	280	328	5			
1	B	221	Total	C	H	N	O	S	49	0	0
			3418	1112	1688	281	332	5			
1	C	222	Total	C	H	N	O	S	54	0	0
			3376	1101	1660	281	329	5			
1	D	219	Total	C	H	N	O	S	51	0	0
			3372	1094	1666	283	324	5			
1	E	217	Total	C	H	N	O	S	53	0	0
			3306	1079	1621	280	321	5			
1	F	221	Total	C	H	N	O	S	76	0	0
			3145	1037	1514	275	314	5			
1	G	218	Total	C	H	N	O	S	68	0	0
			3170	1039	1538	270	318	5			
1	H	218	Total	C	H	N	O	S	79	0	0
			3049	1009	1463	263	309	5			
1	J	218	Total	C	H	N	O	S	61	0	0
			3202	1051	1554	273	319	5			
1	K	219	Total	C	H	N	O	S	53	0	0
			3331	1087	1631	281	327	5			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	22	Total	O	0	0
			22	22		
2	B	24	Total	O	0	0
			24	24		
2	C	18	Total	O	0	0
			18	18		
2	D	22	Total	O	0	0
			22	22		

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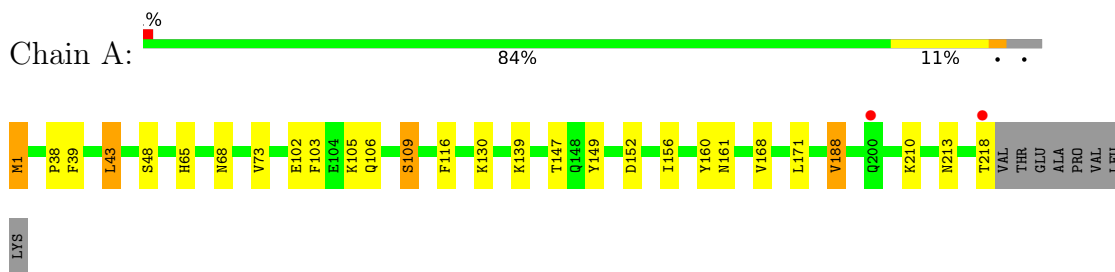
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	11	Total 11	O 11	0	0
2	F	8	Total 8	O 8	0	0
2	G	6	Total 6	O 6	0	0
2	H	7	Total 7	O 7	0	0
2	J	11	Total 11	O 11	0	0
2	K	15	Total 15	O 15	0	0

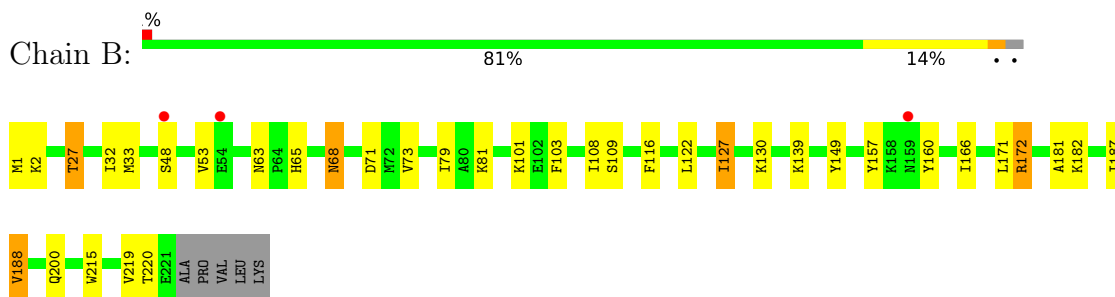
3 Residue-property plots [i](#)

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.

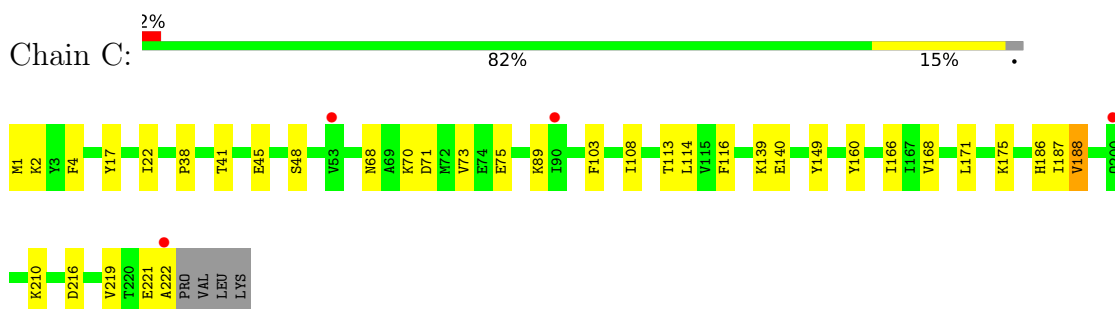
- Molecule 1: BmSF-TAL



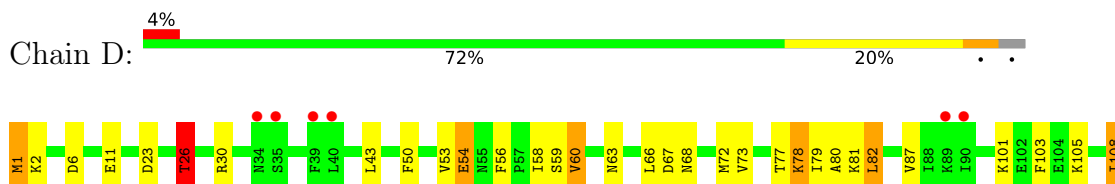
- Molecule 1: BmSF-TAL



- Molecule 1: BmSF-TAL

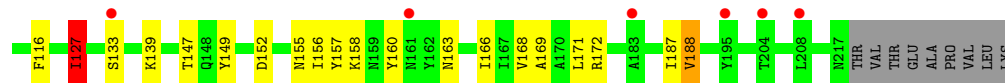
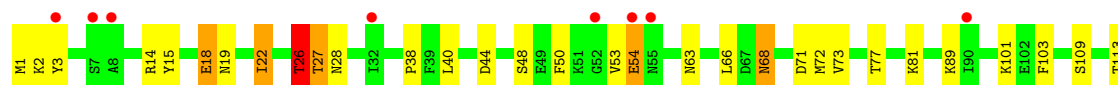


- Molecule 1: BmSF-TAL

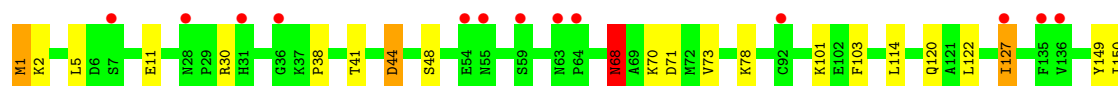
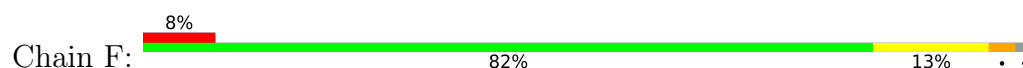




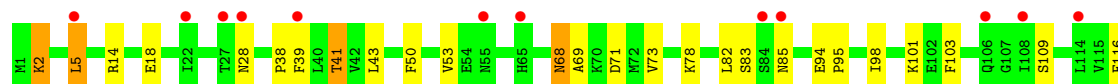
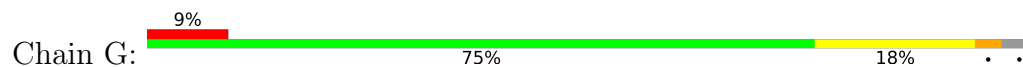
• Molecule 1: BmSF-TAL



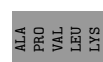
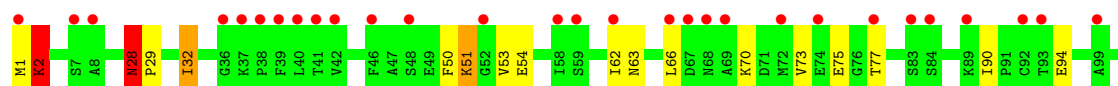
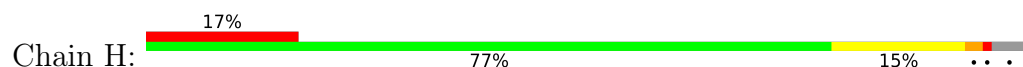
• Molecule 1: BmSF-TAL



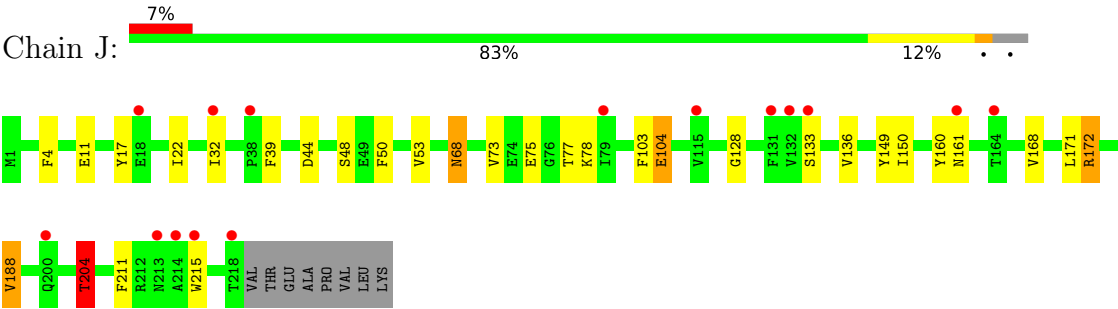
• Molecule 1: BmSF-TAL



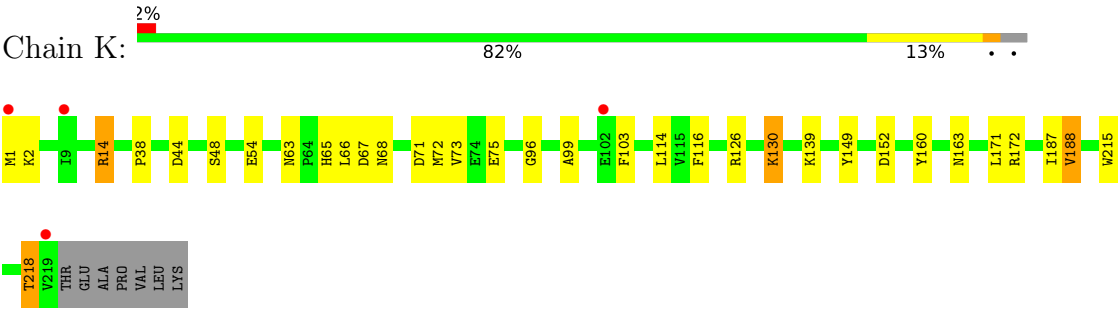
• Molecule 1: BmSF-TAL



• Molecule 1: BmSF-TAL



• Molecule 1: BmSF-TAL



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.89Å 120.84Å 152.64Å 90.00° 93.40° 90.00°	Depositor
Resolution (Å)	68.08 – 3.20 68.08 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (68.08-3.20) 99.2 (68.08-3.20)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0403, REFMAC 5.8.0403	Depositor
R, R_{free}	0.235 , 0.268 0.234 , 0.261	Depositor DCC
R_{free} test set	2102 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	48.3	Xtriage
Anisotropy	0.744	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	32872	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/1748	1.03	1/2378 (0.0%)
1	B	0.53	0/1771	1.04	1/2407 (0.0%)
1	C	0.52	0/1757	1.02	0/2393
1	D	0.52	0/1746	1.03	1/2374 (0.0%)
1	E	0.52	0/1726	1.05	3/2346 (0.1%)
1	F	0.54	0/1670	1.04	3/2281 (0.1%)
1	G	0.52	0/1669	1.03	3/2274 (0.1%)
1	H	0.54	0/1624	1.06	4/2224 (0.2%)
1	J	0.53	0/1688	1.03	3/2304 (0.1%)
1	K	0.53	0/1741	1.03	1/2369 (0.0%)
All	All	0.53	0/17140	1.03	20/23350 (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	B	0	1
1	D	0	2
1	F	0	1
1	H	0	2
1	K	0	1
All	All	0	7

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	67	ASP	CA-CB-CG	7.94	120.54	112.60
1	E	26	THR	CA-CB-OG1	-7.53	98.31	109.60
1	J	161	ASN	CA-CB-CG	7.18	119.78	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	204	THR	CA-CB-OG1	6.78	119.77	109.60
1	A	161	ASN	CA-CB-CG	6.72	119.32	112.60
1	J	204	THR	CA-CB-OG1	6.62	119.54	109.60
1	F	188	VAL	CA-CB-CG1	6.33	121.16	110.40
1	D	26	THR	CA-CB-OG1	-6.16	100.35	109.60
1	F	44	ASP	CA-CB-CG	5.62	118.22	112.60
1	J	68	ASN	CA-CB-CG	5.51	118.11	112.60
1	B	65	HIS	CB-CG-CD2	-5.50	124.06	131.20
1	G	2	LYS	CB-CG-CD	5.45	123.83	111.30
1	H	2	LYS	CB-CA-C	-5.45	99.58	110.42
1	H	28	ASN	CB-CA-C	-5.34	99.64	110.17
1	E	127	ILE	N-CA-CB	-5.31	103.17	112.08
1	E	26	THR	CA-CB-CG2	5.29	119.49	110.50
1	G	127	ILE	N-CA-CB	-5.20	103.35	112.08
1	G	28	ASN	CA-CB-CG	5.11	117.71	112.60
1	F	68	ASN	CA-CB-CG	5.08	117.69	112.60
1	H	32	ILE	CB-CA-C	5.08	118.47	111.97

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	172	ARG	Sidechain
1	D	212	ARG	Sidechain
1	D	30	ARG	Sidechain
1	F	30	ARG	Sidechain
1	H	126	ARG	Sidechain
1	H	212	ARG	Sidechain
1	K	14	ARG	Sidechain

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	1707	1652	1638	14	0
1	B	1730	1688	1674	27	0
1	C	1716	1660	1637	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1706	1666	1646	64	0
1	E	1685	1621	1599	46	0
1	F	1631	1514	1446	24	0
1	G	1632	1538	1486	39	0
1	H	1586	1463	1388	41	0
1	J	1648	1554	1514	21	0
1	K	1700	1631	1611	26	0
2	A	22	0	0	2	0
2	B	24	0	0	1	0
2	C	18	0	0	5	0
2	D	22	0	0	2	0
2	E	11	0	0	2	0
2	F	8	0	0	0	0
2	G	6	0	0	1	0
2	H	7	0	0	1	0
2	J	11	0	0	0	0
2	K	15	0	0	1	0
All	All	16885	15987	15639	290	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 (290) 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:136:VAL:HG11	1:D:171:LEU:HD23	1.31	1.06
1:B:219:VAL:HG13	1:E:38:PRO:HB3	1.37	1.05
1:D:136:VAL:HG11	1:D:171:LEU:CD2	1.86	1.03
1:D:79:ILE:HA	1:D:82:LEU:HD22	1.41	1.00
1:D:103:PHE:HD1	1:D:108:ILE:HG21	1.25	0.98
1:D:101:LYS:NZ	1:G:18:GLU:O	1.99	0.96
1:D:79:ILE:HA	1:D:82:LEU:CD2	1.95	0.95
1:F:166:ILE:HG12	1:F:186:HIS:HD2	1.31	0.91
1:K:72:MET:HE1	1:K:96:GLY:HA2	1.50	0.90
1:D:136:VAL:CG1	1:D:171:LEU:HD23	2.02	0.90
1:C:140:GLU:CB	2:C:318:HOH:O	2.17	0.90
1:D:103:PHE:CD1	1:D:108:ILE:HG21	2.08	0.88
1:C:221:GLU:O	1:C:222:ALA:O	1.90	0.88
1:D:67:ASP:CB	2:D:314:HOH:O	2.22	0.86
1:C:160:TYR:CD2	1:F:1:MET:HB2	2.14	0.82
1:D:175:LYS:O	1:D:178:VAL:HG22	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:LYS:O	1:D:178:VAL:CG2	2.28	0.80
1:D:103:PHE:HD1	1:D:108:ILE:CG2	1.95	0.80
1:D:79:ILE:CA	1:D:82:LEU:HD22	2.12	0.79
1:H:157:TYR:CD2	1:H:166:ILE:HD11	2.17	0.79
1:B:157:TYR:CD2	1:B:166:ILE:HD11	2.18	0.78
1:K:72:MET:HE2	1:K:99:ALA:CB	2.14	0.77
1:E:157:TYR:CD2	1:E:166:ILE:HD11	2.20	0.77
1:D:157:TYR:CD2	1:D:166:ILE:HD11	2.19	0.77
1:D:157:TYR:CE2	1:D:166:ILE:HD11	2.20	0.77
1:E:157:TYR:CE2	1:E:166:ILE:HD11	2.20	0.76
1:D:103:PHE:CD1	1:D:108:ILE:CG2	2.68	0.76
1:B:157:TYR:CE2	1:B:166:ILE:HD11	2.21	0.76
1:F:166:ILE:HG12	1:F:186:HIS:CD2	2.19	0.75
1:F:120:GLN:HE22	1:H:204:THR:HG21	1.49	0.75
1:H:66:LEU:CB	2:H:305:HOH:O	2.34	0.75
1:E:54:GLU:N	1:E:54:GLU:OE1	2.19	0.75
1:D:54:GLU:OE1	1:D:54:GLU:N	2.18	0.74
1:H:157:TYR:CE2	1:H:166:ILE:HD11	2.22	0.73
1:E:89:LYS:NZ	2:E:301:HOH:O	2.20	0.73
1:B:181:ALA:HB1	1:E:156:ILE:HD12	1.69	0.73
1:G:95:PRO:HA	1:G:98:ILE:CG2	2.19	0.73
1:E:1:MET:HB2	1:G:160:TYR:CD1	2.24	0.73
1:G:39:PHE:O	1:G:43:LEU:HD13	1.88	0.72
1:H:1:MET:O	1:H:2:LYS:CB	2.37	0.70
1:F:114:LEU:O	1:H:204:THR:HG22	1.92	0.70
1:D:59:SER:HA	1:D:87:VAL:HG13	1.75	0.69
1:C:113:THR:HG22	1:C:114:LEU:N	2.07	0.69
1:E:14:ARG:O	1:E:18:GLU:HG3	1.91	0.69
1:H:104:GLU:OE2	1:H:110:THR:HG22	1.93	0.68
1:A:1:MET:N	2:A:302:HOH:O	2.26	0.68
1:B:1:MET:HB2	1:E:160:TYR:CD1	2.29	0.67
1:J:50:PHE:HD1	1:J:53:VAL:HG21	1.61	0.66
1:D:136:VAL:HG12	1:D:169:ALA:O	1.96	0.65
1:H:50:PHE:O	1:H:51:LYS:C	2.38	0.65
1:C:70:LYS:O	1:C:73:VAL:HG22	1.95	0.65
1:E:14:ARG:O	1:E:18:GLU:CG	2.45	0.65
1:A:38:PRO:HB3	1:C:219:VAL:HB	1.78	0.65
1:H:50:PHE:O	1:H:51:LYS:O	2.15	0.64
1:D:219:VAL:HB	1:K:38:PRO:HB3	1.80	0.64
1:D:103:PHE:HB3	1:D:108:ILE:HG22	1.80	0.64
1:H:29:PRO:HA	1:H:32:ILE:HG12	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:136:VAL:HG22	1:J:150:ILE:HD11	1.80	0.63
1:B:73:VAL:HA	1:B:103:PHE:CZ	2.34	0.63
1:G:78:LYS:O	1:G:82:LEU:HD23	1.99	0.63
1:E:3:TYR:O	1:E:22:ILE:HD13	1.99	0.62
1:E:73:VAL:HA	1:E:103:PHE:CZ	2.34	0.62
1:A:73:VAL:HA	1:A:103:PHE:CZ	2.34	0.62
1:F:73:VAL:HA	1:F:103:PHE:CZ	2.35	0.62
1:G:73:VAL:HA	1:G:103:PHE:CZ	2.34	0.62
1:K:171:LEU:HD12	1:K:188:VAL:HG22	1.82	0.62
1:D:175:LYS:O	1:D:178:VAL:HG23	2.00	0.62
1:H:73:VAL:HA	1:H:103:PHE:CZ	2.34	0.62
1:C:73:VAL:HA	1:C:103:PHE:CZ	2.34	0.62
1:G:94:GLU:O	1:G:98:ILE:HG22	1.99	0.62
1:K:73:VAL:HA	1:K:103:PHE:CZ	2.34	0.62
1:D:171:LEU:HD12	1:D:188:VAL:HG22	1.82	0.62
1:H:28:ASN:OD1	1:J:211:PHE:CZ	2.53	0.62
1:D:73:VAL:HA	1:D:103:PHE:CZ	2.34	0.61
1:F:171:LEU:HD12	1:F:190:CYS:SG	2.40	0.61
1:H:109:SER:HB3	1:H:130:LYS:HD2	1.82	0.61
1:J:73:VAL:HA	1:J:103:PHE:CZ	2.34	0.61
1:K:171:LEU:CD1	1:K:188:VAL:HG22	2.30	0.61
1:B:171:LEU:HD12	1:B:188:VAL:HG22	1.83	0.61
1:B:171:LEU:CD1	1:B:188:VAL:HG22	2.31	0.61
1:D:171:LEU:CD1	1:D:188:VAL:HG22	2.30	0.61
1:G:175:LYS:HE3	1:H:145:ASP:OD1	1.99	0.61
1:D:23:ASP:OD1	1:K:126:ARG:NH2	2.34	0.60
1:G:213:ASN:O	1:G:217:ASN:OD1	2.18	0.60
1:J:50:PHE:CD1	1:J:53:VAL:HG21	2.36	0.60
1:K:72:MET:HE2	1:K:99:ALA:HB3	1.83	0.60
1:H:120:GLN:HE22	1:J:204:THR:HG21	1.66	0.60
1:B:181:ALA:CB	1:E:156:ILE:HD12	2.31	0.60
1:C:171:LEU:CD1	1:C:188:VAL:HG22	2.31	0.60
1:D:175:LYS:C	1:D:178:VAL:HG22	2.26	0.60
1:C:171:LEU:HD12	1:C:188:VAL:HG22	1.83	0.60
1:H:171:LEU:CD1	1:H:188:VAL:HG22	2.32	0.59
1:C:113:THR:HG22	1:C:114:LEU:H	1.67	0.59
1:E:171:LEU:CD2	1:E:188:VAL:HG22	2.31	0.59
1:B:27:THR:HG21	1:B:32:ILE:HD11	1.84	0.59
1:C:17:TYR:HA	1:C:22:ILE:HG22	1.85	0.59
1:B:215:TRP:CZ2	1:E:63:ASN:HB2	2.38	0.58
1:E:68:ASN:HA	2:E:304:HOH:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:TYR:CE2	1:B:166:ILE:CD1	2.86	0.58
1:G:171:LEU:HD12	1:G:188:VAL:HG22	1.85	0.58
1:J:104:GLU:HG2	1:J:128:GLY:O	2.04	0.58
1:J:171:LEU:CD1	1:J:188:VAL:HG22	2.34	0.58
1:D:157:TYR:CE2	1:D:166:ILE:CD1	2.87	0.57
1:E:18:GLU:O	1:G:101:LYS:NZ	2.34	0.57
1:G:171:LEU:CD1	1:G:188:VAL:HG22	2.34	0.57
1:J:171:LEU:HD12	1:J:188:VAL:HG22	1.86	0.57
1:H:90:ILE:HD12	1:H:110:THR:OG1	2.04	0.57
1:E:157:TYR:CE2	1:E:166:ILE:CD1	2.87	0.57
1:H:171:LEU:HD12	1:H:188:VAL:HG22	1.85	0.57
1:H:113:THR:HG23	1:H:114:LEU:HD13	1.87	0.57
1:D:136:VAL:HG11	1:D:171:LEU:HD21	1.80	0.57
1:B:219:VAL:HG13	1:E:38:PRO:CB	2.25	0.57
1:H:157:TYR:CE2	1:H:166:ILE:CD1	2.87	0.56
1:E:77:THR:HG22	1:E:81:LYS:HE3	1.87	0.56
1:E:113:THR:HA	1:E:133:SER:OG	2.04	0.56
1:E:77:THR:O	1:E:81:LYS:HG2	2.05	0.56
1:E:171:LEU:N	1:E:171:LEU:CD1	2.69	0.56
1:G:136:VAL:CG2	1:G:137:GLY:N	2.69	0.56
1:D:68:ASN:HB2	2:D:317:HOH:O	2.05	0.56
1:A:171:LEU:HD13	1:A:188:VAL:HG22	1.88	0.56
1:H:109:SER:HB3	1:H:130:LYS:CD	2.36	0.55
1:H:114:LEU:O	1:J:204:THR:HG22	2.06	0.55
1:G:50:PHE:HB3	1:G:53:VAL:CG2	2.35	0.55
1:E:66:LEU:HD23	1:E:72:MET:HA	1.89	0.55
1:G:95:PRO:O	1:G:98:ILE:HG23	2.07	0.55
1:E:152:ASP:O	1:E:156:ILE:HG12	2.07	0.54
1:C:113:THR:CG2	1:C:114:LEU:H	2.21	0.54
1:D:78:LYS:HE2	1:D:82:LEU:HD11	1.89	0.54
1:J:4:PHE:C	1:J:22:ILE:HD11	2.33	0.54
1:C:4:PHE:C	1:C:22:ILE:HD11	2.33	0.54
1:C:113:THR:CG2	1:C:114:LEU:N	2.70	0.54
1:J:32:ILE:HD13	1:J:39:PHE:CE1	2.43	0.54
1:D:136:VAL:CG1	1:D:171:LEU:CD2	2.71	0.54
1:B:1:MET:HB2	1:E:160:TYR:CE1	2.43	0.54
1:E:50:PHE:HB3	1:E:53:VAL:CG2	2.39	0.53
1:D:77:THR:O	1:D:81:LYS:HG3	2.08	0.53
1:D:103:PHE:CB	1:D:108:ILE:HG22	2.38	0.53
1:F:120:GLN:HE22	1:H:204:THR:CG2	2.20	0.53
1:G:5:LEU:HD23	1:G:190:CYS:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:ILE:C	1:D:82:LEU:HD22	2.34	0.52
1:H:70:LYS:O	1:H:73:VAL:HG12	2.10	0.52
1:G:38:PRO:HG2	1:G:41:THR:CG2	2.40	0.52
1:G:38:PRO:HG2	1:G:41:THR:HG23	1.91	0.52
1:H:171:LEU:C	1:H:172:ARG:HG2	2.35	0.52
1:J:17:TYR:HA	1:J:22:ILE:HG22	1.92	0.52
1:K:66:LEU:HD23	1:K:72:MET:HA	1.91	0.52
1:F:101:LYS:HA	1:F:127:ILE:HG23	1.91	0.51
1:F:152:ASP:O	1:F:156:ILE:HG12	2.10	0.51
1:A:116:PHE:HB3	1:A:139:LYS:HE3	1.91	0.51
1:D:50:PHE:HD1	1:D:53:VAL:HG21	1.75	0.51
1:K:72:MET:CE	1:K:99:ALA:HB3	2.41	0.51
1:B:63:ASN:HB2	1:K:215:TRP:CZ2	2.46	0.51
1:D:116:PHE:O	1:D:139:LYS:HE3	2.10	0.51
1:G:136:VAL:HG22	1:G:170:ALA:O	2.10	0.51
1:F:70:LYS:O	1:F:73:VAL:HG12	2.11	0.51
1:C:45:GLU:HB2	2:C:304:HOH:O	2.10	0.50
1:D:66:LEU:HD23	1:D:72:MET:HA	1.91	0.50
1:D:175:LYS:HA	1:D:178:VAL:HG22	1.92	0.50
1:J:171:LEU:C	1:J:172:ARG:HG2	2.36	0.50
1:B:33:MET:HA	1:K:218:THR:HG23	1.92	0.50
1:C:160:TYR:CE2	1:F:1:MET:HB2	2.44	0.50
1:B:160:TYR:CD1	1:K:1:MET:HB2	2.46	0.50
1:E:169:ALA:C	1:E:171:LEU:HD13	2.37	0.50
1:E:116:PHE:O	1:E:139:LYS:HE3	2.11	0.50
1:G:95:PRO:HA	1:G:98:ILE:HG22	1.94	0.50
1:D:59:SER:HA	1:D:87:VAL:CG1	2.41	0.49
1:H:168:VAL:HG12	1:H:171:LEU:HD21	1.95	0.49
1:B:219:VAL:O	1:E:38:PRO:HB3	2.12	0.49
1:D:1:MET:HB2	1:K:160:TYR:CD1	2.47	0.49
1:G:101:LYS:HA	1:G:127:ILE:HG23	1.95	0.49
1:F:168:VAL:HG12	1:F:188:VAL:HG12	1.94	0.49
1:D:78:LYS:HE3	1:D:78:LYS:O	2.12	0.49
1:C:113:THR:HG21	2:C:310:HOH:O	2.12	0.49
1:D:2:LYS:HB2	1:D:187:ILE:HG12	1.94	0.49
1:E:101:LYS:HA	1:E:127:ILE:HG23	1.95	0.49
1:H:62:ILE:HD11	1:H:75:GLU:CB	2.43	0.49
1:F:156:ILE:HD12	1:H:181:ALA:HB1	1.94	0.48
1:G:153:ILE:HG22	1:G:166:ILE:HD13	1.95	0.48
1:G:171:LEU:C	1:G:172:ARG:HG2	2.37	0.48
1:D:136:VAL:HG13	1:D:170:ALA:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:GLU:HG2	1:D:200:GLN:NE2	2.29	0.48
1:E:2:LYS:HB2	1:E:187:ILE:HG12	1.96	0.48
1:B:101:LYS:HA	1:B:127:ILE:HG23	1.96	0.48
1:B:171:LEU:C	1:B:172:ARG:HG2	2.37	0.48
1:G:175:LYS:CE	1:H:145:ASP:OD1	2.61	0.48
1:C:2:LYS:HB2	1:C:187:ILE:HG12	1.96	0.48
1:C:221:GLU:O	1:C:222:ALA:C	2.57	0.48
1:D:175:LYS:CA	1:D:178:VAL:HG22	2.44	0.48
1:D:200:GLN:O	1:D:200:GLN:HG2	2.14	0.47
1:E:1:MET:HB2	1:G:160:TYR:CE1	2.49	0.47
1:A:109:SER:HB3	1:A:130:LYS:HG3	1.97	0.47
1:D:80:ALA:CB	1:D:108:ILE:HD11	2.45	0.47
1:G:14:ARG:O	1:G:18:GLU:HG2	2.14	0.47
1:H:50:PHE:HB3	1:H:53:VAL:CG2	2.44	0.47
1:E:15:TYR:CE1	1:E:19:ASN:ND2	2.82	0.47
1:E:155:ASN:O	1:E:158:LYS:HG2	2.13	0.47
1:J:50:PHE:HB3	1:J:53:VAL:CG2	2.45	0.47
1:B:2:LYS:HB2	1:B:187:ILE:HG12	1.96	0.47
1:D:1:MET:HG3	1:D:2:LYS:N	2.30	0.47
1:K:171:LEU:C	1:K:172:ARG:HG2	2.39	0.47
1:D:43:LEU:HD21	1:D:60:VAL:HG21	1.96	0.46
1:F:162:TYR:CE1	1:H:1:MET:HE2	2.50	0.46
1:C:166:ILE:H	1:C:186:HIS:HD2	1.63	0.46
1:D:6:ASP:OD1	1:D:26:THR:HG22	2.14	0.46
1:F:68:ASN:ND2	1:F:71:ASP:H	2.13	0.46
1:C:168:VAL:HG12	1:C:171:LEU:HD21	1.97	0.46
1:C:175:LYS:CB	2:C:315:HOH:O	2.62	0.46
1:E:171:LEU:N	1:E:171:LEU:HD12	2.31	0.46
1:D:80:ALA:HB1	1:D:108:ILE:HD11	1.98	0.46
1:A:160:TYR:CD1	1:C:1:MET:HB2	2.51	0.46
1:C:221:GLU:C	1:C:222:ALA:O	2.59	0.46
1:A:102:GLU:OE1	1:A:106:GLN:NE2	2.48	0.46
1:C:38:PRO:HB3	1:F:219:VAL:HB	1.98	0.45
1:D:215:TRP:CZ2	1:K:63:ASN:HB2	2.51	0.45
1:G:68:ASN:ND2	1:G:71:ASP:H	2.13	0.45
1:B:68:ASN:ND2	1:B:71:ASP:H	2.13	0.45
1:C:68:ASN:ND2	1:C:71:ASP:H	2.14	0.45
1:F:38:PRO:HD2	1:F:41:THR:OG1	2.15	0.45
1:B:27:THR:CG2	1:B:32:ILE:HD11	2.47	0.45
1:H:122:LEU:HD12	1:H:122:LEU:HA	1.86	0.45
1:E:15:TYR:CD1	1:E:19:ASN:ND2	2.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:ASN:ND2	1:E:71:ASP:H	2.13	0.45
1:C:75:GLU:OE1	1:C:75:GLU:HA	2.16	0.45
1:D:56:PHE:CE2	1:D:58:ILE:HD11	2.52	0.45
1:D:141:ASN:HD21	1:D:172:ARG:NH2	2.15	0.45
1:K:68:ASN:ND2	1:K:71:ASP:H	2.14	0.45
1:K:130:LYS:HD3	1:K:130:LYS:HA	1.83	0.45
1:E:26:THR:HG23	1:E:89:LYS:NZ	2.32	0.44
1:A:152:ASP:O	1:A:156:ILE:HG13	2.17	0.44
1:E:27:THR:CG2	1:E:28:ASN:N	2.80	0.44
1:G:69:ALA:HB2	1:G:98:ILE:HG23	1.99	0.44
1:E:14:ARG:O	1:E:18:GLU:HG2	2.16	0.44
1:C:41:THR:HG21	2:C:311:HOH:O	2.17	0.44
1:H:114:LEU:HD11	1:J:211:PHE:CE2	2.54	0.43
1:B:130:LYS:HB2	2:B:310:HOH:O	2.17	0.43
1:D:63:ASN:HB2	1:G:215:TRP:CZ2	2.53	0.43
1:D:79:ILE:O	1:D:82:LEU:HD22	2.18	0.43
1:E:171:LEU:C	1:E:172:ARG:HG2	2.43	0.43
1:H:70:LYS:O	1:H:73:VAL:CG1	2.66	0.43
1:F:166:ILE:HG12	1:F:166:ILE:H	1.69	0.43
1:G:14:ARG:HD2	2:G:304:HOH:O	2.19	0.43
1:D:82:LEU:HD13	1:D:82:LEU:N	2.33	0.43
1:F:70:LYS:O	1:F:73:VAL:CG1	2.66	0.43
1:H:50:PHE:HB3	1:H:53:VAL:HG22	2.00	0.43
1:A:1:MET:HB2	1:J:160:TYR:CD1	2.54	0.43
1:F:1:MET:HG3	1:F:2:LYS:N	2.32	0.43
1:E:63:ASN:HB3	1:E:66:LEU:HD13	2.01	0.43
1:H:29:PRO:HA	1:H:32:ILE:CG1	2.46	0.43
1:F:171:LEU:C	1:F:172:ARG:HG2	2.44	0.42
1:G:50:PHE:HB3	1:G:53:VAL:HG22	2.01	0.42
1:E:19:ASN:OD1	1:G:98:ILE:HD12	2.18	0.42
1:C:89:LYS:HG2	1:C:113:THR:OG1	2.20	0.42
1:H:63:ASN:HB2	1:J:215:TRP:CZ2	2.54	0.42
1:K:187:ILE:HG22	1:K:188:VAL:N	2.35	0.42
1:B:182:LYS:HD2	1:E:152:ASP:CG	2.45	0.42
1:C:116:PHE:HB3	1:C:139:LYS:HE2	2.01	0.42
1:H:116:PHE:HB3	1:H:139:LYS:HE3	2.02	0.42
1:H:62:ILE:HG13	1:H:63:ASN:N	2.34	0.42
1:C:187:ILE:HG22	1:C:188:VAL:N	2.34	0.41
1:A:213:ASN:C	2:A:307:HOH:O	2.63	0.41
1:A:168:VAL:O	1:A:171:LEU:HD11	2.20	0.41
1:B:116:PHE:HB3	1:B:139:LYS:HE3	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:168:VAL:HG12	1:J:171:LEU:HD21	2.03	0.41
1:D:187:ILE:HG22	1:D:188:VAL:N	2.35	0.41
1:G:2:LYS:HB2	1:G:187:ILE:HG12	2.02	0.41
1:H:62:ILE:HD12	1:H:63:ASN:H	1.86	0.41
1:A:39:PHE:O	1:A:43:LEU:HD22	2.20	0.41
1:G:78:LYS:O	1:G:82:LEU:CD2	2.67	0.41
1:F:187:ILE:HG22	1:F:188:VAL:N	2.35	0.41
1:G:50:PHE:CD1	1:G:53:VAL:HG21	2.56	0.41
1:K:72:MET:CE	1:K:99:ALA:CB	2.94	0.41
1:D:216:ASP:OD1	1:K:65:HIS:HE1	2.04	0.41
1:G:136:VAL:CG2	1:G:171:LEU:HD23	2.50	0.41
1:G:136:VAL:HG21	1:G:171:LEU:HD23	2.02	0.41
1:K:1:MET:N	2:K:304:HOH:O	2.53	0.41
1:K:116:PHE:HB3	1:K:139:LYS:HE3	2.02	0.41
1:D:182:LYS:HE3	1:K:152:ASP:OD1	2.21	0.41
1:C:166:ILE:H	1:C:186:HIS:CD2	2.38	0.40
1:D:43:LEU:HD21	1:D:60:VAL:CG2	2.51	0.40
1:D:103:PHE:HB3	1:D:108:ILE:CG2	2.50	0.40
1:E:168:VAL:HG12	1:E:171:LEU:HD11	2.02	0.40
1:G:116:PHE:HB3	1:G:139:LYS:HE3	2.03	0.40
1:K:2:LYS:HB2	1:K:187:ILE:HG12	2.03	0.40
1:A:65:HIS:HE1	1:C:216:ASP:OD1	2.05	0.40
1:F:150:ILE:HD12	1:F:168:VAL:HG23	2.03	0.40
1:H:120:GLN:HE22	1:J:204:THR:CG2	2.31	0.40
1:J:32:ILE:HD13	1:J:39:PHE:CD1	2.56	0.40
1:B:187:ILE:HG22	1:B:188:VAL:N	2.36	0.40
1:D:204:THR:HG23	1:K:114:LEU:HB3	2.03	0.40
1:G:136:VAL:HG23	1:G:137:GLY:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	216/226 (96%)	213 (99%)	3 (1%)	0	100	100
1	B	219/226 (97%)	215 (98%)	4 (2%)	0	100	100
1	C	220/226 (97%)	216 (98%)	4 (2%)	0	100	100
1	D	217/226 (96%)	214 (99%)	3 (1%)	0	100	100
1	E	215/226 (95%)	211 (98%)	4 (2%)	0	100	100
1	F	219/226 (97%)	216 (99%)	3 (1%)	0	100	100
1	G	216/226 (96%)	213 (99%)	3 (1%)	0	100	100
1	H	216/226 (96%)	207 (96%)	7 (3%)	2 (1%)	14	47
1	J	216/226 (96%)	212 (98%)	4 (2%)	0	100	100
1	K	217/226 (96%)	214 (99%)	3 (1%)	0	100	100
All	All	2171/2260 (96%)	2131 (98%)	38 (2%)	2 (0%)	48	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	2	LYS
1	H	51	LYS

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	181/193 (94%)	170 (94%)	11 (6%)	17	49
1	B	184/193 (95%)	170 (92%)	14 (8%)	12	42
1	C	179/193 (93%)	174 (97%)	5 (3%)	38	68
1	D	179/193 (93%)	164 (92%)	15 (8%)	10	38
1	E	174/193 (90%)	159 (91%)	15 (9%)	10	36
1	F	152/193 (79%)	138 (91%)	14 (9%)	8	33
1	G	158/193 (82%)	143 (90%)	15 (10%)	8	32
1	H	147/193 (76%)	136 (92%)	11 (8%)	12	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	165/193 (86%)	152 (92%)	13 (8%)	11	40
1	K	177/193 (92%)	167 (94%)	10 (6%)	19	52
All	All	1696/1930 (88%)	1573 (93%)	123 (7%)	13	43

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	43	LEU
1	A	48	SER
1	A	68	ASN
1	A	105	LYS
1	A	109	SER
1	A	147	THR
1	A	149	TYR
1	A	188	VAL
1	A	210	LYS
1	A	218	THR
1	B	27	THR
1	B	48	SER
1	B	53	VAL
1	B	68	ASN
1	B	79	ILE
1	B	81	LYS
1	B	108	ILE
1	B	109	SER
1	B	122	LEU
1	B	127	ILE
1	B	149	TYR
1	B	188	VAL
1	B	200	GLN
1	B	220	THR
1	C	48	SER
1	C	108	ILE
1	C	149	TYR
1	C	188	VAL
1	C	210	LYS
1	D	1	MET
1	D	11	GLU
1	D	26	THR
1	D	54	GLU

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Mol	Chain	Res	Type
1	D	60	VAL
1	D	78	LYS
1	D	82	LEU
1	D	105	LYS
1	D	108	ILE
1	D	130	LYS
1	D	136	VAL
1	D	139	LYS
1	D	149	TYR
1	D	188	VAL
1	D	219	VAL
1	E	18	GLU
1	E	22	ILE
1	E	26	THR
1	E	27	THR
1	E	40	LEU
1	E	44	ASP
1	E	48	SER
1	E	54	GLU
1	E	68	ASN
1	E	109	SER
1	E	127	ILE
1	E	147	THR
1	E	149	TYR
1	E	163	ASN
1	E	188	VAL
1	F	1	MET
1	F	5	LEU
1	F	11	GLU
1	F	44	ASP
1	F	48	SER
1	F	68	ASN
1	F	78	LYS
1	F	122	LEU
1	F	127	ILE
1	F	149	TYR
1	F	166	ILE
1	F	175	LYS
1	F	219	VAL
1	F	221	GLU
1	G	5	LEU
1	G	41	THR

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Mol	Chain	Res	Type
1	G	68	ASN
1	G	83	SER
1	G	85	ASN
1	G	109	SER
1	G	127	ILE
1	G	136	VAL
1	G	147	THR
1	G	149	TYR
1	G	188	VAL
1	G	197	GLU
1	G	210	LYS
1	G	217	ASN
1	G	218	THR
1	H	28	ASN
1	H	54	GLU
1	H	77	THR
1	H	94	GLU
1	H	109	SER
1	H	147	THR
1	H	149	TYR
1	H	172	ARG
1	H	188	VAL
1	H	204	THR
1	H	218	THR
1	J	11	GLU
1	J	44	ASP
1	J	48	SER
1	J	68	ASN
1	J	75	GLU
1	J	77	THR
1	J	78	LYS
1	J	104	GLU
1	J	133	SER
1	J	149	TYR
1	J	172	ARG
1	J	188	VAL
1	J	204	THR
1	K	14	ARG
1	K	44	ASP
1	K	48	SER
1	K	54	GLU
1	K	75	GLU

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Mol	Chain	Res	Type
1	K	130	LYS
1	K	149	TYR
1	K	163	ASN
1	K	188	VAL
1	K	218	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	65	HIS
1	A	106	GLN
1	A	186	HIS
1	A	217	ASN
1	B	19	ASN
1	B	31	HIS
1	B	68	ASN
1	B	161	ASN
1	B	217	ASN
1	C	19	ASN
1	C	68	ASN
1	C	159	ASN
1	C	186	HIS
1	D	31	HIS
1	D	34	ASN
1	D	68	ASN
1	D	141	ASN
1	D	186	HIS
1	D	200	GLN
1	E	68	ASN
1	E	200	GLN
1	F	63	ASN
1	F	65	HIS
1	F	68	ASN
1	F	120	GLN
1	F	186	HIS
1	G	68	ASN
1	H	28	ASN
1	H	85	ASN
1	H	120	GLN
1	H	159	ASN
1	J	68	ASN

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Mol	Chain	Res	Type
1	J	141	ASN
1	K	65	HIS
1	K	68	ASN
1	K	217	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	218/226 (96%)	0.36	2 (0%) 81 64	24, 36, 59, 81	0
1	B	221/226 (97%)	0.44	3 (1%) 73 54	21, 38, 63, 100	0
1	C	222/226 (98%)	0.44	4 (1%) 67 48	21, 39, 59, 79	0
1	D	219/226 (96%)	0.76	9 (4%) 41 25	33, 54, 82, 109	0
1	E	217/226 (96%)	0.67	14 (6%) 25 16	27, 49, 73, 113	0
1	F	221/226 (97%)	1.00	18 (8%) 18 11	26, 53, 80, 98	0
1	G	218/226 (96%)	0.98	21 (9%) 13 9	35, 56, 76, 89	0
1	H	218/226 (96%)	1.21	38 (17%) 4 3	36, 61, 85, 99	0
1	J	218/226 (96%)	0.87	15 (6%) 23 14	30, 50, 78, 87	0
1	K	219/226 (96%)	0.53	4 (1%) 67 48	23, 41, 64, 81	0
All	All	2191/2260 (96%)	0.73	128 (5%) 29 18	21, 48, 76, 113	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	218	THR	5.0
1	E	54	GLU	3.9
1	H	58	ILE	3.9
1	D	144	ASP	3.6
1	F	63	ASN	3.6
1	E	7	SER	3.6
1	G	28	ASN	3.6
1	H	68	ASN	3.5
1	H	42	VAL	3.5
1	G	187	ILE	3.5
1	F	55	ASN	3.5
1	H	62	ILE	3.5
1	K	219	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	69	ALA	3.3
1	H	83	SER	3.3
1	F	64	PRO	3.3
1	C	222	ALA	3.2
1	G	174	GLY	3.1
1	J	161	ASN	3.1
1	A	218	THR	3.1
1	B	54	GLU	3.1
1	G	27	THR	3.1
1	G	106	GLN	3.0
1	H	39	PHE	3.0
1	J	132	VAL	3.0
1	F	127	ILE	2.9
1	F	36	GLY	2.9
1	F	191	GLY	2.8
1	G	218	THR	2.8
1	H	46	PHE	2.8
1	H	52	GLY	2.7
1	E	161	ASN	2.7
1	F	161	ASN	2.7
1	H	8	ALA	2.7
1	H	99	ALA	2.7
1	C	90	ILE	2.7
1	D	219	VAL	2.6
1	H	7	SER	2.6
1	F	135	PHE	2.6
1	H	41	THR	2.6
1	J	214	ALA	2.6
1	B	159	ASN	2.6
1	H	66	LEU	2.6
1	D	89	LYS	2.6
1	G	134	PRO	2.5
1	G	133	SER	2.5
1	H	84	SER	2.5
1	F	92	CYS	2.5
1	H	111	ASN	2.5
1	K	1	MET	2.5
1	H	215	TRP	2.5
1	H	92	CYS	2.5
1	H	36	GLY	2.5
1	D	39	PHE	2.4
1	G	39	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	85	ASN	2.4
1	K	102	GLU	2.4
1	D	90	ILE	2.4
1	J	79	ILE	2.4
1	J	200	GLN	2.4
1	F	59	SER	2.4
1	G	84	SER	2.4
1	E	8	ALA	2.3
1	F	169	ALA	2.3
1	J	115	VAL	2.3
1	E	204	THR	2.3
1	G	22	ILE	2.3
1	F	163	ASN	2.3
1	D	130	LYS	2.3
1	F	187	ILE	2.3
1	C	53	VAL	2.3
1	G	5	LEU	2.3
1	G	167	ILE	2.3
1	E	3	TYR	2.3
1	G	141	ASN	2.3
1	H	216	ASP	2.3
1	G	177	ILE	2.2
1	J	164	THR	2.2
1	G	210	LYS	2.2
1	G	55	ASN	2.2
1	F	54	GLU	2.2
1	E	52	GLY	2.2
1	H	1	MET	2.2
1	H	38	PRO	2.2
1	H	40	LEU	2.2
1	H	130	LYS	2.2
1	J	213	ASN	2.2
1	D	40	LEU	2.2
1	E	208	LEU	2.2
1	H	67	ASP	2.2
1	G	65	HIS	2.2
1	A	200	GLN	2.2
1	D	34	ASN	2.2
1	E	55	ASN	2.2
1	F	28	ASN	2.2
1	H	37	LYS	2.2
1	J	38	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	32	ILE	2.1
1	E	90	ILE	2.1
1	J	32	ILE	2.1
1	D	35	SER	2.1
1	H	185	ALA	2.1
1	J	18	GLU	2.1
1	G	108	ILE	2.1
1	H	89	LYS	2.1
1	J	131	PHE	2.1
1	F	31	HIS	2.1
1	H	72	MET	2.1
1	C	200	GLN	2.1
1	G	114	LEU	2.1
1	E	183	ALA	2.1
1	H	74	GLU	2.1
1	E	133	SER	2.1
1	F	7	SER	2.1
1	H	48	SER	2.1
1	H	161	ASN	2.1
1	J	215	TRP	2.1
1	H	203	PHE	2.1
1	B	48	SER	2.0
1	H	59	SER	2.0
1	J	133	SER	2.0
1	H	187	ILE	2.0
1	E	195	TYR	2.0
1	F	136	VAL	2.0
1	H	77	THR	2.0
1	H	93	THR	2.0
1	H	197	GLU	2.0
1	K	9	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.