



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 11:46 AM UTC

PDB ID : 5TEZ / pdb_00005tez
Title : TCR F50 recognizing M1-HLA-A2
Authors : Yang, X.; Mariuzza, R.A.
Deposited on : 2016-09-23
Resolution : 1.70 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

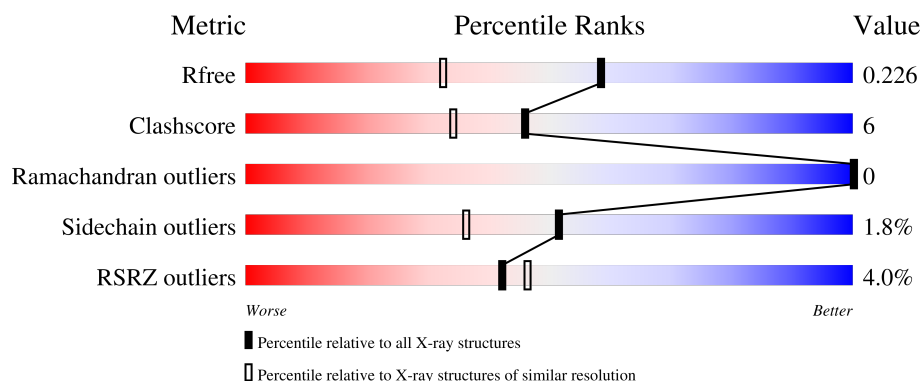
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	C	9	33% 67%
2	A	275	4% 34% 60% 5%
3	B	100	5% 37% 59%
4	I	208	5% 37% 56%
5	J	243	3% 35% 59%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7466 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 GLY-ILE-LEU-GLY-PHE-VAL-PHE-THR-LEU.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	C	9	Total	C	N	O	0	0	0
			68	49	9	10			

- Molecule 2 is a protein called HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	275	Total	C	N	O	S	0	0	0
			2246	1403	409	425	9			

- Molecule 3 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	100	Total	C	N	O	S	0	0	0
			834	531	141	159	3			

- Molecule 4 is a protein called TCR F50 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	202	Total	C	N	O	S	0	0	0
			1586	992	268	319	7			

- Molecule 5 is a protein called TCR F50 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	J	240	Total	C	N	O	S	0	0	0
			1927	1219	334	366	8			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	4	Total	O	0	0
			4	4		

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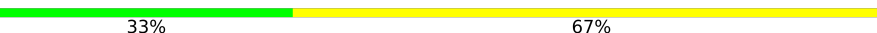
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	246	Total 246	O 246	0	0
6	B	125	Total 125	O 125	0	0
6	I	187	Total 187	O 187	0	0
6	J	243	Total 243	O 243	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

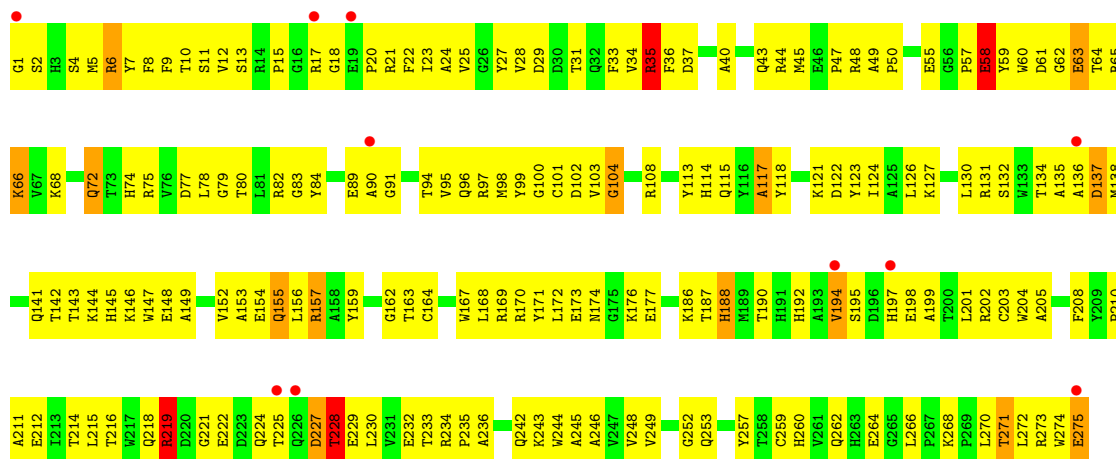
• Molecule 1: GLY-ILE-LEU-GLY-PHE-VAL-PHE-THR-LEU

Chain C: 



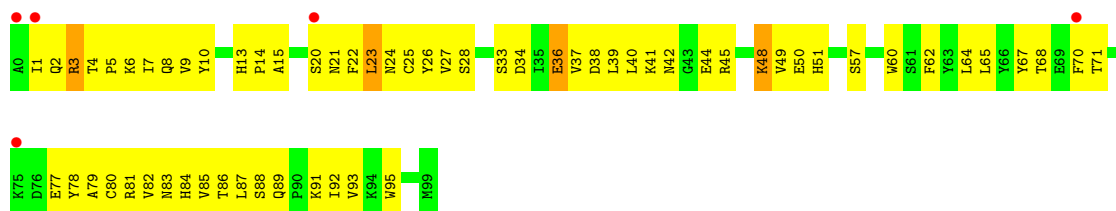
• Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain

Chain A: 



• Molecule 3: Beta-2-microglobulin

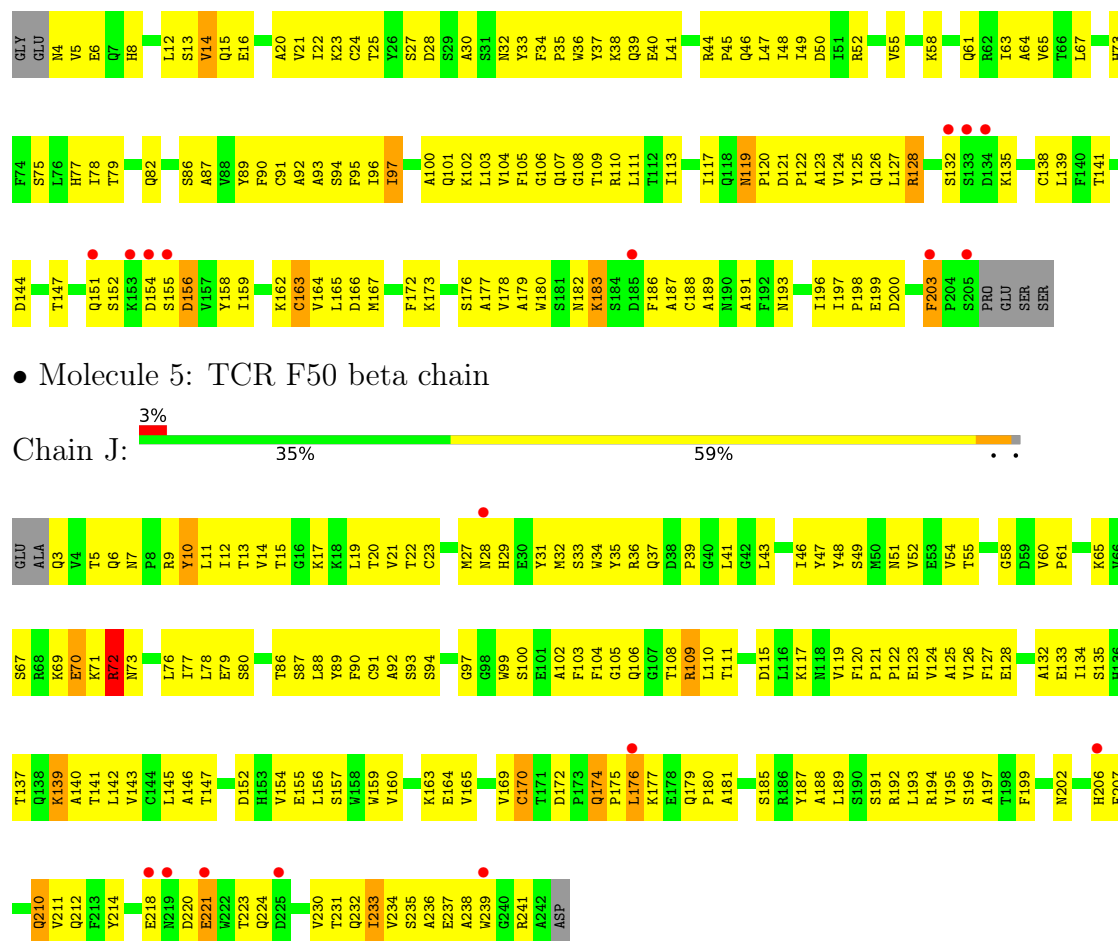
Chain B: 



• Molecule 4: TCR F50 alpha chain

Chain I: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.27Å 71.05Å 100.69Å 90.00° 96.22° 90.00°	Depositor
Resolution (Å)	37.92 – 1.70 37.92 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.1 (37.92-1.70) 98.1 (37.92-1.70)	Depositor EDS
R_{merge}	0.35	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.190 , 0.224 0.193 , 0.226	Depositor DCC
R_{free} test set	2000 reflections (1.96%)	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7466	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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	C	2.67	5/69 (7.2%)	0.85	0/90
2	A	2.54	177/2311 (7.7%)	1.05	4/3137 (0.1%)
3	B	2.50	61/857 (7.1%)	1.04	0/1159
4	I	2.59	117/1619 (7.2%)	1.09	1/2195 (0.0%)
5	J	2.58	152/1980 (7.7%)	1.04	0/2696
All	All	2.56	512/6836 (7.5%)	1.05	5/9277 (0.1%)

All (512) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	135	ALA	CA-CB	-12.42	1.33	1.53
4	I	55	VAL	C-O	-10.74	1.13	1.24
5	J	36	ARG	CB-CG	-9.70	1.23	1.52
2	A	28	VAL	C-O	-9.66	1.13	1.24
3	B	13	HIS	C-O	-9.47	1.14	1.24
4	I	65	VAL	C-O	-9.28	1.14	1.24
5	J	143	VAL	C-O	-9.24	1.14	1.24
4	I	122	PRO	C-O	-9.03	1.13	1.23
2	A	8	PHE	C-O	-8.98	1.13	1.24
3	B	37	VAL	C-O	-8.98	1.14	1.24
5	J	193	LEU	C-O	-8.88	1.13	1.24
2	A	65	ARG	C-O	-8.74	1.13	1.24
2	A	10	THR	C-O	-8.66	1.14	1.24
2	A	12	VAL	C-O	-8.59	1.14	1.24
2	A	214	THR	C-O	-8.57	1.14	1.24
4	I	96	ILE	C-O	-8.44	1.14	1.24
5	J	12	ILE	C-O	-8.43	1.15	1.24
5	J	234	VAL	C-O	-8.42	1.15	1.24
1	C	3	LEU	C-O	-8.35	1.14	1.23
5	J	94	SER	C-O	-8.33	1.13	1.23
5	J	211	VAL	C-O	-8.27	1.15	1.24
5	J	88	LEU	C-O	-8.26	1.14	1.24
2	A	9	PHE	C-O	-8.25	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	36	ARG	C-O	-8.24	1.14	1.24
5	J	172	ASP	C-O	-8.21	1.14	1.24
5	J	122	PRO	C-O	-8.18	1.14	1.23
4	I	178	VAL	C-O	-8.18	1.15	1.24
3	B	89	GLN	C-O	-8.15	1.15	1.24
4	I	63	ILE	C-O	-8.08	1.14	1.24
5	J	21	VAL	C-O	-8.04	1.14	1.24
2	A	146	LYS	C-O	-7.99	1.15	1.24
4	I	87	ALA	C-O	-7.97	1.16	1.23
2	A	66	LYS	C-O	-7.88	1.14	1.24
5	J	97	GLY	C-O	-7.87	1.15	1.23
4	I	14	VAL	C-O	-7.87	1.15	1.23
2	A	91	GLY	C-O	-7.86	1.16	1.23
2	A	34	VAL	C-O	-7.84	1.15	1.23
2	A	134	THR	C-O	-7.83	1.15	1.24
5	J	170	CYS	C-O	-7.83	1.14	1.23
3	B	8	GLN	C-O	-7.81	1.14	1.23
2	A	124	ILE	C-O	-7.79	1.14	1.23
3	B	23	LEU	C-O	-7.79	1.14	1.24
2	A	235	PRO	C-O	-7.78	1.15	1.23
4	I	36	TRP	C-O	-7.77	1.14	1.24
4	I	50	ASP	C-O	-7.75	1.14	1.23
4	I	46	GLN	C-O	-7.74	1.15	1.23
2	A	95	VAL	C-O	-7.73	1.15	1.24
5	J	187	TYR	C-O	-7.71	1.14	1.23
4	I	139	LEU	C-O	-7.69	1.15	1.24
5	J	124	VAL	C-O	-7.69	1.16	1.24
4	I	78	ILE	C-O	-7.68	1.15	1.24
1	C	4	GLY	C-O	-7.67	1.17	1.24
3	B	91	LYS	C-O	-7.67	1.14	1.24
2	A	114	HIS	C-O	-7.66	1.14	1.23
4	I	45	PRO	C-O	-7.63	1.15	1.23
5	J	119	VAL	C-O	-7.58	1.15	1.24
5	J	5	THR	C-O	-7.56	1.15	1.24
5	J	105	GLY	C-O	-7.55	1.14	1.23
2	A	143	THR	C-O	-7.53	1.15	1.24
5	J	71	LYS	C-O	-7.50	1.15	1.24
4	I	113	ILE	C-O	-7.50	1.15	1.24
5	J	154	VAL	C-O	-7.50	1.16	1.23
2	A	167	TRP	C-O	-7.49	1.15	1.24
5	J	86	THR	C-O	-7.49	1.15	1.24
4	I	101	GLN	C-O	-7.46	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	11	SER	C-O	-7.46	1.15	1.24
3	B	65	LEU	C-O	-7.45	1.15	1.24
2	A	202	ARG	C-O	-7.43	1.15	1.24
5	J	197	ALA	C-O	-7.43	1.15	1.24
4	I	12	LEU	C-O	-7.40	1.15	1.23
5	J	199	PHE	C-O	-7.40	1.15	1.24
2	A	126	LEU	C-O	-7.37	1.15	1.24
5	J	7	ASN	C-O	-7.36	1.16	1.24
4	I	61	GLN	C-O	-7.36	1.14	1.24
4	I	52	ARG	C-O	-7.34	1.14	1.23
3	B	81	ARG	C-O	-7.33	1.15	1.24
2	A	61	ASP	C-O	-7.31	1.15	1.24
4	I	108	GLY	C-O	-7.31	1.15	1.24
3	B	36	GLU	C-O	-7.29	1.15	1.24
2	A	25	VAL	C-O	-7.24	1.16	1.23
2	A	103	VAL	C-O	-7.24	1.16	1.24
4	I	67	LEU	C-O	-7.23	1.15	1.24
5	J	160	VAL	C-O	-7.22	1.16	1.24
4	I	25	THR	C-O	-7.20	1.14	1.23
4	I	73	HIS	C-O	-7.20	1.15	1.23
5	J	78	LEU	C-O	-7.20	1.15	1.23
4	I	119	ASN	C-O	-7.20	1.15	1.24
4	I	47	LEU	C-O	-7.19	1.15	1.23
4	I	16	GLU	C-O	-7.18	1.15	1.23
5	J	37	GLN	C-O	-7.15	1.15	1.24
2	A	98	MET	C-O	-7.13	1.15	1.23
2	A	118	TYR	C-O	-7.12	1.15	1.24
2	A	234	ARG	C-O	-7.12	1.14	1.24
2	A	49	ALA	C-O	-7.10	1.16	1.24
5	J	6	GLN	C-O	-7.10	1.15	1.24
4	I	183	LYS	CG-CD	-7.09	1.31	1.52
5	J	197	ALA	CA-CB	-7.09	1.42	1.53
5	J	126	VAL	C-O	-7.08	1.16	1.24
3	B	25	CYS	C-O	-7.08	1.16	1.24
4	I	49	ILE	C-O	-7.07	1.14	1.24
5	J	188	ALA	C-O	-7.07	1.15	1.23
2	A	242	GLN	C-O	-7.06	1.15	1.23
5	J	152	ASP	C-O	-7.06	1.15	1.24
2	A	37	ASP	C-O	-7.05	1.16	1.24
2	A	36	PHE	C-O	-7.05	1.16	1.23
4	I	164	VAL	C-O	-7.02	1.16	1.24
4	I	106	GLY	C-O	-7.02	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	123	TYR	C-O	-7.00	1.14	1.23
3	B	26	TYR	C-O	-7.00	1.15	1.24
3	B	64	LEU	C-O	-7.00	1.15	1.23
4	I	105	PHE	C-O	-7.00	1.15	1.23
2	A	262	GLN	C-O	-7.00	1.15	1.24
3	B	15	ALA	C-O	-6.99	1.15	1.24
5	J	79	GLU	C-O	-6.99	1.15	1.24
4	I	90	PHE	C-O	-6.99	1.15	1.24
2	A	260	HIS	C-O	-6.99	1.16	1.24
2	A	24	ALA	C-O	-6.98	1.15	1.24
2	A	174	ASN	C-O	-6.98	1.15	1.24
2	A	96	GLN	C-O	-6.95	1.14	1.23
2	A	113	TYR	C-O	-6.95	1.15	1.23
2	A	232	GLU	C-O	-6.95	1.15	1.23
3	B	93	VAL	C-O	-6.95	1.16	1.24
4	I	39	GLN	C-O	-6.94	1.16	1.24
2	A	74	HIS	C-O	-6.94	1.15	1.24
4	I	6	GLU	C-O	-6.93	1.15	1.24
4	I	117	ILE	C-O	-6.93	1.16	1.24
4	I	141	THR	C-O	-6.93	1.15	1.23
4	I	177	ALA	C-O	-6.92	1.15	1.23
2	A	268	LYS	C-O	-6.91	1.15	1.24
4	I	41	LEU	C-O	-6.91	1.15	1.23
2	A	45	MET	C-O	-6.91	1.15	1.23
4	I	91	CYS	C-O	-6.91	1.15	1.23
5	J	237	GLU	C-O	-6.90	1.15	1.23
5	J	121	PRO	C-O	-6.89	1.16	1.24
2	A	57	PRO	C-O	-6.88	1.15	1.24
5	J	102	ALA	C-O	-6.88	1.15	1.24
5	J	17	LYS	C-O	-6.88	1.15	1.24
5	J	61	PRO	C-O	-6.86	1.16	1.24
5	J	77	ILE	C-O	-6.85	1.16	1.24
5	J	239	TRP	C-O	-6.85	1.15	1.23
5	J	134	ILE	C-O	-6.83	1.16	1.24
2	A	164	CYS	C-O	-6.83	1.16	1.24
3	B	28	SER	C-O	-6.79	1.15	1.23
5	J	155	GLU	C-O	-6.79	1.16	1.24
3	B	3	ARG	C-O	-6.78	1.16	1.24
2	A	219	ARG	C-O	-6.78	1.16	1.24
2	A	6	ARG	C-O	-6.78	1.15	1.23
5	J	235	SER	C-O	-6.76	1.15	1.23
4	I	102	LYS	C-O	-6.76	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5	PRO	C-O	-6.74	1.16	1.23
5	J	140	ALA	C-O	-6.74	1.16	1.24
5	J	19	LEU	C-O	-6.73	1.15	1.23
5	J	212	GLN	C-O	-6.72	1.16	1.24
5	J	90	PHE	C-O	-6.72	1.16	1.24
2	A	243	LYS	C-O	-6.72	1.15	1.23
2	A	205	ALA	C-O	-6.71	1.16	1.24
4	I	126	GLN	C-O	-6.68	1.16	1.24
5	J	165	VAL	C-O	-6.66	1.15	1.23
4	I	166	ASP	C-O	-6.65	1.16	1.24
4	I	37	TYR	C-O	-6.64	1.15	1.24
2	A	82	ARG	C-O	-6.64	1.16	1.24
4	I	58	LYS	C-O	-6.64	1.15	1.23
4	I	176	SER	C-O	-6.62	1.15	1.23
2	A	72	GLN	C-O	-6.62	1.16	1.24
2	A	13	SER	C-O	-6.62	1.15	1.23
2	A	21	ARG	C-O	-6.60	1.15	1.23
4	I	15	GLN	C-O	-6.59	1.15	1.23
5	J	202	ASN	C-O	-6.59	1.15	1.24
4	I	34	PHE	C-O	-6.57	1.17	1.24
2	A	132	SER	C-O	-6.57	1.15	1.23
4	I	144	ASP	C-O	-6.56	1.15	1.23
3	B	82	VAL	C-O	-6.55	1.17	1.24
5	J	9	ARG	C-O	-6.55	1.16	1.24
2	A	215	LEU	C-O	-6.54	1.16	1.24
5	J	80	SER	C-O	-6.54	1.17	1.24
2	A	187	THR	C-O	-6.53	1.15	1.23
4	I	197	ILE	C-O	-6.52	1.16	1.24
5	J	241	ARG	C-O	-6.52	1.16	1.24
5	J	111	THR	C-O	-6.52	1.16	1.24
4	I	95	PHE	C-O	-6.52	1.16	1.23
5	J	181	ALA	C-O	-6.51	1.15	1.24
5	J	196	SER	C-O	-6.51	1.15	1.23
3	B	9	VAL	C-O	-6.51	1.17	1.24
5	J	233	ILE	C-O	-6.51	1.17	1.24
3	B	10	TYR	C-O	-6.50	1.16	1.23
2	A	199	ALA	CA-CB	-6.50	1.40	1.54
3	B	81	ARG	CD-NE	-6.50	1.37	1.46
5	J	191	SER	C-O	-6.48	1.16	1.23
5	J	51	ASN	C-O	-6.48	1.17	1.24
3	B	62	PHE	C-O	-6.48	1.15	1.23
3	B	68	THR	C-O	-6.47	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	92	ALA	C-O	-6.45	1.16	1.23
2	A	31	THR	C-O	-6.43	1.16	1.24
3	B	27	VAL	C-O	-6.43	1.16	1.24
5	J	104	PHE	C-O	-6.43	1.16	1.23
2	A	244	TRP	C-O	-6.42	1.15	1.23
2	A	142	THR	C-O	-6.41	1.16	1.24
4	I	38	LYS	C-O	-6.40	1.16	1.24
2	A	266	LEU	C-O	-6.38	1.17	1.24
2	A	148	GLU	C-O	-6.38	1.16	1.24
2	A	40	ALA	CA-CB	-6.38	1.43	1.53
2	A	18	GLY	C-O	-6.37	1.17	1.23
5	J	207	PHE	C-O	-6.36	1.16	1.24
5	J	22	THR	C-O	-6.35	1.16	1.23
5	J	41	LEU	C-O	-6.34	1.16	1.24
5	J	231	THR	C-O	-6.34	1.16	1.23
2	A	163	THR	C-O	-6.33	1.16	1.24
4	I	121	ASP	C-O	-6.32	1.16	1.24
2	A	7	TYR	C-O	-6.32	1.15	1.24
4	I	89	TYR	C-O	-6.32	1.16	1.24
2	A	192	HIS	C-O	-6.31	1.16	1.23
3	B	4	THR	C-O	-6.31	1.15	1.23
5	J	72	ARG	C-O	-6.29	1.16	1.24
2	A	249	VAL	C-O	-6.29	1.18	1.24
3	B	92	ILE	C-O	-6.29	1.17	1.24
5	J	117	LYS	C-O	-6.29	1.16	1.24
2	A	78	LEU	C-O	-6.28	1.16	1.24
3	B	95	TRP	C-O	-6.28	1.16	1.24
5	J	236	ALA	C-O	-6.28	1.16	1.23
5	J	159	TRP	C-O	-6.27	1.17	1.24
2	A	83	GLY	C-O	-6.26	1.16	1.23
2	A	157	ARG	C-O	-6.26	1.16	1.24
5	J	141	THR	C-O	-6.26	1.16	1.24
2	A	188	HIS	C-O	-6.25	1.16	1.23
5	J	10	TYR	C-O	-6.25	1.16	1.23
4	I	156	ASP	N-CA	-6.25	1.38	1.46
2	A	190	THR	C-O	-6.25	1.15	1.23
5	J	15	THR	C-O	-6.24	1.16	1.23
5	J	54	VAL	CA-CB	-6.23	1.46	1.54
5	J	230	VAL	C-O	-6.22	1.16	1.24
2	A	201	LEU	C-O	-6.21	1.16	1.24
4	I	193	ASN	C-O	-6.21	1.15	1.23
2	A	22	PHE	C-O	-6.20	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	33	SER	C-O	-6.20	1.16	1.23
5	J	156	LEU	C-O	-6.19	1.16	1.24
5	J	145	LEU	C-O	-6.18	1.17	1.24
3	B	21	ASN	C-O	-6.18	1.18	1.24
5	J	14	VAL	C-O	-6.17	1.15	1.24
4	I	86	SER	C-O	-6.16	1.16	1.24
3	B	83	ASN	C-O	-6.16	1.16	1.24
2	A	230	LEU	C-O	-6.16	1.17	1.24
5	J	210	GLN	C-O	-6.15	1.16	1.24
5	J	99	TRP	C-O	-6.14	1.16	1.24
4	I	79	THR	C-O	-6.14	1.16	1.23
4	I	196	ILE	C-O	-6.13	1.16	1.23
4	I	22	ILE	C-O	-6.13	1.17	1.24
3	B	2	GLN	C-O	-6.12	1.17	1.24
5	J	120	PHE	C-O	-6.11	1.16	1.24
5	J	194	ARG	C-O	-6.10	1.16	1.24
2	A	228	THR	CB-CG2	-6.10	1.32	1.52
2	A	229	GLU	C-O	-6.10	1.16	1.24
2	A	117	ALA	C-O	-6.09	1.16	1.23
5	J	47	TYR	C-O	-6.09	1.16	1.23
5	J	49	SER	C-O	-6.09	1.16	1.24
4	I	24	CYS	C-O	-6.08	1.16	1.24
4	I	127	LEU	C-O	-6.07	1.16	1.24
4	I	97	ILE	C-O	-6.07	1.17	1.24
1	C	2	ILE	C-O	-6.07	1.16	1.24
4	I	92	ALA	C-O	-6.07	1.16	1.23
4	I	191	ALA	CA-CB	-6.06	1.44	1.54
3	B	24	ASN	C-O	-6.06	1.16	1.24
5	J	214	TYR	C-O	-6.06	1.16	1.24
4	I	179	ALA	C-O	-6.05	1.16	1.23
2	A	94	THR	C-O	-6.04	1.17	1.24
5	J	127	PHE	C-O	-6.03	1.16	1.24
2	A	152	VAL	C-O	-6.01	1.17	1.24
2	A	47	PRO	C-O	-6.00	1.17	1.23
2	A	216	THR	C-O	-6.00	1.16	1.23
2	A	204	TRP	C-O	-6.00	1.16	1.24
4	I	138	CYS	C-O	-6.00	1.16	1.24
5	J	139	LYS	C-O	-6.00	1.16	1.23
5	J	195	VAL	C-O	-5.99	1.16	1.23
3	B	78	TYR	C-O	-5.99	1.16	1.23
4	I	109	THR	C-O	-5.98	1.17	1.24
5	J	125	ALA	C-O	-5.98	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	257	TYR	C-O	-5.97	1.16	1.24
4	I	94	SER	C-O	-5.95	1.16	1.24
2	A	270	LEU	C-O	-5.95	1.16	1.23
3	B	49	VAL	C-O	-5.95	1.17	1.24
4	I	28	ASP	C-O	-5.95	1.16	1.24
5	J	179	GLN	C-O	-5.95	1.17	1.24
2	A	20	PRO	C-O	-5.94	1.16	1.23
4	I	188	CYS	C-O	-5.94	1.16	1.24
3	B	7	ILE	C-O	-5.94	1.18	1.24
2	A	63	GLU	C-O	-5.93	1.17	1.24
2	A	169	ARG	C-O	-5.93	1.17	1.24
2	A	271	THR	C-O	-5.93	1.16	1.24
5	J	133	GLU	C-O	-5.93	1.17	1.24
2	A	64	THR	C-O	-5.92	1.17	1.24
5	J	103	PHE	C-O	-5.92	1.16	1.24
2	A	153	ALA	C-O	-5.91	1.17	1.24
3	B	38	ASP	C-O	-5.91	1.16	1.24
2	A	211	ALA	C-O	-5.90	1.16	1.24
2	A	224	GLN	C-O	-5.90	1.17	1.23
2	A	97	ARG	C-O	-5.88	1.17	1.23
2	A	80	THR	C-O	-5.88	1.17	1.24
2	A	62	GLY	C-O	-5.87	1.16	1.23
4	I	159	ILE	C-O	-5.87	1.18	1.24
2	A	177	GLU	C-O	-5.86	1.16	1.24
5	J	91	CYS	C-O	-5.86	1.16	1.23
4	I	82	GLN	C-O	-5.85	1.18	1.24
4	I	75	SER	C-O	-5.85	1.17	1.23
5	J	54	VAL	C-O	-5.84	1.17	1.24
5	J	206	HIS	C-O	-5.84	1.17	1.24
4	I	186	PHE	C-O	-5.84	1.17	1.23
2	A	170	ARG	C-O	-5.84	1.17	1.24
2	A	127	LYS	C-O	-5.84	1.15	1.23
4	I	14	VAL	CB-CG1	-5.84	1.33	1.52
5	J	55	THR	C-O	-5.83	1.16	1.23
3	B	67	TYR	C-O	-5.83	1.16	1.23
5	J	60	VAL	C-O	-5.82	1.17	1.24
2	A	79	GLY	C-O	-5.81	1.16	1.23
4	I	125	TYR	C-O	-5.81	1.16	1.23
2	A	49	ALA	CA-CB	-5.80	1.46	1.54
2	A	212	GLU	C-O	-5.80	1.17	1.24
4	I	5	VAL	C-O	-5.80	1.17	1.24
4	I	93	ALA	C-O	-5.80	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	162	LYS	C-O	-5.79	1.16	1.23
5	J	29	HIS	C-O	-5.78	1.17	1.24
2	A	23	ILE	C-O	-5.77	1.18	1.24
5	J	185	SER	C-O	-5.77	1.16	1.23
2	A	137	ASP	C-O	-5.76	1.16	1.23
4	I	123	ALA	CA-CB	-5.76	1.44	1.53
5	J	128	GLU	C-O	-5.76	1.16	1.23
2	A	2	SER	C-O	-5.75	1.16	1.23
2	A	154	GLU	C-O	-5.75	1.17	1.24
5	J	142	LEU	CG-CD2	-5.75	1.33	1.52
2	A	168	LEU	C-O	-5.75	1.17	1.24
2	A	50	PRO	C-O	-5.73	1.17	1.24
2	A	222	GLU	C-O	-5.73	1.17	1.24
5	J	32	MET	C-O	-5.73	1.16	1.23
3	B	44	GLU	C-O	-5.73	1.17	1.23
3	B	41	LYS	C-O	-5.73	1.17	1.24
5	J	180	PRO	C-O	-5.72	1.17	1.24
5	J	73	ASN	C-O	-5.72	1.17	1.24
4	I	64	ALA	C-O	-5.71	1.16	1.23
2	A	221	GLY	C-O	-5.69	1.16	1.24
3	B	57	SER	C-O	-5.69	1.16	1.23
4	I	173	LYS	C-O	-5.69	1.16	1.23
2	A	29	ASP	C-O	-5.67	1.18	1.24
5	J	135	SER	C-O	-5.67	1.17	1.24
2	A	138	MET	CB-CG	-5.66	1.35	1.52
5	J	189	LEU	C-O	-5.66	1.17	1.23
2	A	136	ALA	CA-CB	-5.64	1.44	1.53
4	I	103	LEU	C-O	-5.63	1.17	1.24
5	J	192	ARG	C-O	-5.63	1.16	1.24
5	J	67	SER	C-O	-5.63	1.17	1.23
4	I	183	LYS	CA-C	-5.63	1.45	1.52
2	A	171	TYR	C-O	-5.63	1.17	1.24
3	B	88	SER	C-O	-5.63	1.17	1.24
4	I	199	GLU	C-O	-5.62	1.17	1.24
5	J	70	GLU	C-O	-5.62	1.16	1.23
2	A	58	GLU	C-O	-5.62	1.17	1.24
4	I	13	SER	C-O	-5.62	1.16	1.24
2	A	199	ALA	C-O	-5.61	1.17	1.23
3	B	45	ARG	C-O	-5.61	1.17	1.24
3	B	34	ASP	C-O	-5.61	1.17	1.23
2	A	99	TYR	C-O	-5.61	1.17	1.23
2	A	159	TYR	C-O	-5.60	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	35	TYR	C-O	-5.60	1.16	1.23
4	I	111	LEU	C-O	-5.58	1.17	1.24
5	J	89	TYR	C-O	-5.58	1.17	1.23
2	A	122	ASP	C-O	-5.58	1.17	1.23
2	A	59	TYR	C-O	-5.57	1.17	1.24
2	A	156	LEU	C-O	-5.57	1.17	1.24
2	A	5	MET	C-O	-5.55	1.17	1.24
2	A	197	HIS	C-O	-5.55	1.19	1.24
5	J	34	TRP	C-O	-5.55	1.16	1.24
5	J	123	GLU	C-O	-5.55	1.17	1.23
5	J	106	GLN	C-O	-5.55	1.16	1.24
2	A	144	LYS	C-O	-5.54	1.17	1.24
3	B	50	GLU	C-O	-5.54	1.16	1.23
5	J	39	PRO	C-O	-5.54	1.16	1.24
5	J	115	ASP	C-O	-5.54	1.17	1.23
2	A	130	LEU	C-O	-5.53	1.15	1.23
5	J	31	TYR	C-O	-5.52	1.17	1.24
5	J	100	SER	C-O	-5.52	1.16	1.24
5	J	147	THR	C-O	-5.52	1.16	1.23
3	B	87	LEU	C-O	-5.51	1.17	1.24
5	J	146	ALA	C-O	-5.51	1.17	1.24
5	J	232	GLN	C-O	-5.51	1.17	1.23
3	B	22	PHE	C-O	-5.51	1.17	1.23
4	I	110	ARG	C-O	-5.50	1.17	1.24
4	I	147	THR	C-O	-5.50	1.17	1.24
2	A	108	ARG	C-O	-5.50	1.17	1.23
5	J	137	THR	C-O	-5.50	1.17	1.24
2	A	218	GLN	C-O	-5.50	1.17	1.23
2	A	44	ARG	C-O	-5.49	1.17	1.23
5	J	69	LYS	C-O	-5.49	1.16	1.24
2	A	33	PHE	C-O	-5.48	1.18	1.24
2	A	121	LYS	C-O	-5.48	1.16	1.23
4	I	30	ALA	CA-CB	-5.47	1.44	1.53
5	J	224	GLN	C-O	-5.47	1.16	1.23
2	A	4	SER	C-O	-5.46	1.17	1.23
4	I	40	GLU	C-O	-5.45	1.16	1.23
5	J	46	ILE	C-O	-5.45	1.17	1.24
2	A	147	TRP	C-O	-5.45	1.17	1.24
4	I	132	SER	CA-C	-5.45	1.46	1.52
3	B	77	GLU	C-O	-5.45	1.17	1.24
2	A	252	GLY	C-O	-5.44	1.16	1.24
3	B	79	ALA	C-O	-5.44	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	187	ALA	C-O	-5.44	1.17	1.23
4	I	44	ARG	C-O	-5.44	1.16	1.23
2	A	68	LYS	C-O	-5.43	1.17	1.24
3	B	6	LYS	C-O	-5.42	1.17	1.23
4	I	203	PHE	C-O	-5.42	1.17	1.24
3	B	85	VAL	C-O	-5.42	1.17	1.24
2	A	146	LYS	CB-CG	-5.41	1.36	1.52
5	J	11	LEU	C-O	-5.41	1.17	1.23
2	A	274	TRP	C-O	-5.41	1.17	1.23
5	J	220	ASP	C-O	-5.41	1.17	1.23
2	A	15	PRO	C-O	-5.39	1.17	1.23
5	J	43	LEU	C-O	-5.39	1.17	1.24
3	B	39	LEU	C-O	-5.39	1.17	1.23
2	A	176	LYS	C-O	-5.38	1.17	1.24
5	J	169	VAL	C-O	-5.38	1.18	1.24
2	A	12	VAL	CA-CB	-5.38	1.47	1.54
4	I	35	PRO	C-O	-5.38	1.17	1.23
2	A	162	GLY	C-O	-5.37	1.16	1.23
2	A	208	PHE	C-O	-5.37	1.17	1.23
3	B	71	THR	C-O	-5.37	1.20	1.25
4	I	23	LYS	C-O	-5.37	1.17	1.24
4	I	198	PRO	C-O	-5.37	1.16	1.23
3	B	84	HIS	C-O	-5.36	1.17	1.23
2	A	246	ALA	C-O	-5.36	1.17	1.23
4	I	77	HIS	C-O	-5.36	1.17	1.24
3	B	81	ARG	CZ-NH2	-5.35	1.26	1.33
5	J	223	THR	CB-CG2	-5.35	1.34	1.52
5	J	65	LYS	C-O	-5.34	1.17	1.23
2	A	48	ARG	C-O	-5.34	1.16	1.24
2	A	43	GLN	C-O	-5.33	1.16	1.23
2	A	115	GLN	C-O	-5.33	1.17	1.23
5	J	164	GLU	C-O	-5.32	1.17	1.23
2	A	233	THR	C-O	-5.32	1.17	1.23
1	C	6	VAL	C-O	-5.31	1.18	1.23
1	C	8	THR	C-O	-5.31	1.17	1.23
5	J	76	LEU	C-O	-5.30	1.17	1.24
2	A	264	GLU	C-O	-5.29	1.17	1.24
2	A	135	ALA	C-O	-5.29	1.18	1.23
5	J	58	GLY	C-O	-5.29	1.17	1.24
5	J	109	ARG	C-O	-5.27	1.17	1.23
5	J	48	TYR	C-O	-5.26	1.17	1.23
4	I	189	ALA	C-O	-5.25	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	110	LEU	C-O	-5.25	1.17	1.24
2	A	104	GLY	C-O	-5.25	1.17	1.23
2	A	195	SER	C-O	-5.24	1.18	1.24
4	I	33	TYR	C-O	-5.24	1.17	1.23
5	J	108	THR	C-O	-5.24	1.18	1.24
5	J	93	SER	C-O	-5.23	1.17	1.23
2	A	137	ASP	CA-C	-5.23	1.45	1.53
3	B	51	HIS	C-O	-5.21	1.17	1.23
4	I	107	GLN	C-O	-5.21	1.17	1.24
2	A	176	LYS	CB-CG	-5.20	1.36	1.52
3	B	42	ASN	C-O	-5.20	1.17	1.23
4	I	123	ALA	C-O	-5.20	1.17	1.23
5	J	13	THR	C-O	-5.19	1.17	1.23
4	I	135	LYS	C-O	-5.19	1.17	1.24
2	A	248	VAL	C-O	-5.19	1.18	1.24
4	I	163	CYS	C-O	-5.19	1.17	1.23
4	I	120	PRO	C-O	-5.18	1.17	1.23
5	J	238	ALA	C-O	-5.18	1.17	1.23
3	B	14	PRO	C-O	-5.18	1.16	1.23
2	A	275	GLU	CG-CD	-5.17	1.39	1.52
2	A	186	LYS	C-O	-5.17	1.17	1.24
3	B	20	SER	C-O	-5.16	1.17	1.23
4	I	100	ALA	C-O	-5.16	1.17	1.23
5	J	52	VAL	C-O	-5.16	1.19	1.24
4	I	21	VAL	C-O	-5.15	1.18	1.24
4	I	155	SER	CB-OG	-5.15	1.31	1.42
2	A	253	GLN	C-O	-5.15	1.17	1.24
2	A	203	CYS	C-O	-5.14	1.17	1.24
5	J	176	LEU	N-CA	-5.14	1.39	1.46
4	I	180	TRP	C-O	-5.13	1.17	1.23
2	A	101	CYS	C-O	-5.13	1.17	1.23
5	J	157	SER	C-O	-5.13	1.17	1.23
2	A	27	TYR	C-O	-5.13	1.17	1.23
4	I	20	ALA	C-O	-5.12	1.17	1.24
5	J	23	CYS	C-O	-5.12	1.18	1.23
2	A	173	GLU	C-O	-5.12	1.18	1.24
3	B	86	THR	C-O	-5.12	1.17	1.24
2	A	77	ASP	C-O	-5.12	1.18	1.24
2	A	100	GLY	C-O	-5.11	1.16	1.23
2	A	245	ALA	C-O	-5.09	1.17	1.23
2	A	55	GLU	C-O	-5.09	1.17	1.23
2	A	149	ALA	C-O	-5.08	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	172	LEU	C-O	-5.08	1.17	1.24
5	J	174	GLN	C-O	-5.08	1.17	1.24
5	J	177	LYS	C-O	-5.08	1.17	1.24
2	A	259	CYS	C-O	-5.07	1.17	1.24
2	A	60	TRP	C-O	-5.07	1.18	1.24
5	J	132	ALA	C-O	-5.07	1.18	1.24
5	J	163	LYS	C-O	-5.06	1.17	1.24
4	I	128	ARG	C-O	-5.06	1.18	1.23
4	I	104	VAL	C-O	-5.05	1.18	1.24
2	A	211	ALA	CA-CB	-5.05	1.45	1.53
5	J	37	GLN	CD-OE1	-5.04	1.14	1.23
2	A	205	ALA	CA-CB	-5.03	1.45	1.53
2	A	141	GLN	C-O	-5.03	1.17	1.24
4	I	165	LEU	C-O	-5.03	1.17	1.23
4	I	167	MET	C-O	-5.03	1.16	1.23
3	B	33	SER	C-O	-5.02	1.17	1.24
2	A	35	ARG	C-O	-5.02	1.17	1.23
3	B	80	CYS	C-O	-5.02	1.17	1.24
2	A	236	ALA	CA-CB	-5.02	1.45	1.53
3	B	40	LEU	C-O	-5.02	1.17	1.24
5	J	87	SER	C-O	-5.01	1.18	1.24
4	I	48	ILE	C-O	-5.01	1.19	1.24
2	A	155	GLN	C-O	-5.01	1.18	1.24
5	J	20	THR	C-O	-5.00	1.18	1.24
2	A	84	TYR	C-O	-5.00	1.17	1.24
2	A	210	PRO	CB-CG	-5.00	1.31	1.51
4	I	27	SER	C-O	-5.00	1.17	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	90	ALA	CA-C-N	-7.75	115.53	122.43
2	A	90	ALA	C-N-CA	-7.75	115.53	122.43
2	A	197	HIS	N-CA-CB	-6.34	104.19	111.79
2	A	91	GLY	N-CA-C	5.49	120.10	112.57
4	I	27	SER	N-CA-C	5.14	119.63	112.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	68	0	75	1	0
2	A	2246	0	2096	34	0
3	B	834	0	799	6	0
4	I	1586	0	1523	27	0
5	J	1927	0	1849	18	0
6	A	246	0	0	12	2
6	B	125	0	0	3	1
6	C	4	0	0	0	0
6	I	187	0	0	7	3
6	J	243	0	0	3	0
All	All	7466	0	6342	74	3

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 (74) 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)
2:A:58:GLU:HG2	6:A:359:HOH:O	1.44	1.18
2:A:35:ARG:NH1	6:A:301:HOH:O	2.00	0.95
2:A:75:ARG:NH1	6:A:302:HOH:O	2.08	0.86
4:I:156:ASP:OD2	4:I:183:LYS:NZ	2.11	0.83
4:I:154:ASP:OD2	6:I:301:HOH:O	1.97	0.83
2:A:1:GLY:N	6:A:303:HOH:O	2.10	0.82
4:I:163:CYS:HG	5:J:170:CYS:CB	1.97	0.78
5:J:109:ARG:NH2	6:J:301:HOH:O	2.15	0.77
3:B:3:ARG:NH2	6:B:101:HOH:O	2.04	0.76
2:A:58:GLU:H	2:A:58:GLU:CD	1.94	0.74
4:I:182:ASN:ND2	6:I:306:HOH:O	2.21	0.73
4:I:119:ASN:OD1	6:I:302:HOH:O	2.06	0.72
4:I:124:VAL:HB	4:I:203:PHE:CD2	2.27	0.68
2:A:17:ARG:NH1	2:A:89:GLU:OE2	2.26	0.68
4:I:154:ASP:OD1	6:I:304:HOH:O	2.12	0.67
2:A:17:ARG:NH1	2:A:89:GLU:CD	2.53	0.67
4:I:124:VAL:HB	4:I:203:PHE:CE2	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:163:CYS:CB	5:J:170:CYS:HG	2.07	0.66
2:A:72:GLN:OE1	2:A:75:ARG:NH2	2.32	0.63
2:A:137:ASP:HB3	6:A:307:HOH:O	2.00	0.62
4:I:158:TYR:CD1	5:J:176:LEU:HD21	2.35	0.61
4:I:4:ASN:HA	6:I:314:HOH:O	2.00	0.60
2:A:58:GLU:OE1	6:A:304:HOH:O	2.16	0.60
2:A:273:ARG:NE	2:A:275:GLU:OE2	2.29	0.60
2:A:17:ARG:NE	2:A:89:GLU:OE1	2.36	0.59
5:J:10:TYR:CE1	5:J:109:ARG:HD2	2.39	0.57
2:A:275:GLU:HG2	6:A:326:HOH:O	2.03	0.57
4:I:151:GLN:HG2	4:I:152:SER:N	2.22	0.54
4:I:151:GLN:HG2	4:I:152:SER:H	1.72	0.54
2:A:145:HIS:HE1	6:A:441:HOH:O	1.91	0.53
4:I:8:HIS:O	6:I:305:HOH:O	2.19	0.53
2:A:17:ARG:CZ	2:A:89:GLU:CD	2.81	0.53
3:B:3:ARG:NH1	6:B:103:HOH:O	2.29	0.53
2:A:188:HIS:HD2	6:A:394:HOH:O	1.92	0.53
5:J:221:GLU:H	5:J:221:GLU:CD	2.16	0.53
4:I:163:CYS:CB	5:J:170:CYS:SG	2.95	0.51
4:I:163:CYS:HB3	5:J:170:CYS:SG	2.51	0.51
5:J:72:ARG:NH1	6:J:308:HOH:O	2.44	0.49
4:I:128:ARG:HD2	6:I:319:HOH:O	2.11	0.49
4:I:124:VAL:CB	4:I:203:PHE:CE2	2.95	0.49
2:A:219:ARG:HB3	2:A:219:ARG:CZ	2.43	0.48
4:I:156:ASP:OD2	4:I:183:LYS:CE	2.61	0.48
3:B:48:LYS:O	3:B:48:LYS:HG3	2.15	0.47
2:A:225:THR:O	2:A:228:THR:HB	2.15	0.47
2:A:17:ARG:HH11	2:A:89:GLU:CD	2.23	0.46
2:A:227:ASP:N	2:A:227:ASP:OD1	2.47	0.46
2:A:104:GLY:HA3	6:A:400:HOH:O	2.16	0.46
5:J:3:GLN:N	6:J:314:HOH:O	2.49	0.46
2:A:194:VAL:HG22	2:A:198:GLU:HB2	1.98	0.45
2:A:131:ARG:HH21	2:A:157:ARG:NH2	2.15	0.45
2:A:117:ALA:HB2	3:B:60:TRP:CE2	2.52	0.44
4:I:163:CYS:HB3	5:J:170:CYS:HG	1.79	0.44
2:A:75:ARG:NH2	6:A:317:HOH:O	2.50	0.44
2:A:63:GLU:OE2	2:A:66:LYS:NZ	2.47	0.44
3:B:23:LEU:HB2	3:B:70:PHE:CD1	2.54	0.43
2:A:58:GLU:CD	2:A:58:GLU:N	2.71	0.43
5:J:210:GLN:HG3	5:J:233:ILE:HG23	1.99	0.43
2:A:17:ARG:NH1	2:A:89:GLU:OE1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:75:ARG:HG2	2:A:75:ARG:HH11	1.84	0.42
4:I:163:CYS:SG	5:J:170:CYS:CB	3.02	0.42
2:A:155:GLN:OE1	4:I:32:ASN:HB2	2.20	0.42
3:B:36:GLU:OE2	6:B:102:HOH:O	2.22	0.41
4:I:97:ILE:HD13	4:I:97:ILE:HG21	1.61	0.41
4:I:200:ASP:OD1	4:I:200:ASP:N	2.45	0.41
4:I:163:CYS:HG	5:J:170:CYS:HG	0.83	0.41
5:J:27:MET:O	5:J:28:ASN:HB3	2.21	0.41
2:A:17:ARG:NE	2:A:89:GLU:CD	2.79	0.41
2:A:271:THR:C	2:A:272:LEU:HD23	2.46	0.41
4:I:172:PHE:CE2	5:J:139:LYS:HE2	2.56	0.41
2:A:137:ASP:HB2	6:A:413:HOH:O	2.19	0.41
4:I:163:CYS:SG	5:J:170:CYS:HB2	2.61	0.41
1:C:9:LEU:C	1:C:9:LEU:HD12	2.46	0.40
5:J:174:GLN:HA	5:J:175:PRO:HD3	1.87	0.40
2:A:6:ARG:NH2	2:A:102:ASP:OD1	2.52	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:528:HOH:O	6:I:377:HOH:O[1_455]	2.07	0.13
6:B:194:HOH:O	6:I:453:HOH:O[1_455]	2.12	0.08
6:A:454:HOH:O	6:I:471:HOH:O[2_8411]	2.19	0.01

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	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	A	273/275 (99%)	267 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
4	I	200/208 (96%)	195 (98%)	5 (2%)	0	100	100
5	J	238/243 (98%)	234 (98%)	4 (2%)	0	100	100
All	All	816/835 (98%)	798 (98%)	18 (2%)	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	C	7/7 (100%)	7 (100%)	0	100	100
2	A	231/231 (100%)	225 (97%)	6 (3%)	40	23
3	B	94/94 (100%)	92 (98%)	2 (2%)	47	30
4	I	182/187 (97%)	181 (100%)	1 (0%)	81	76
5	J	213/215 (99%)	209 (98%)	4 (2%)	50	34
All	All	727/734 (99%)	714 (98%)	13 (2%)	51	36

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	35	ARG
2	A	58	GLU
2	A	194	VAL
2	A	219	ARG
2	A	227	ASP
2	A	228	THR
3	B	1	ILE
3	B	48	LYS
4	I	14	VAL
5	J	70	GLU
5	J	72	ARG
5	J	218	GLU

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Mol	Chain	Res	Type
5	J	221	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	145	HIS
2	A	188	HIS
2	A	262	GLN
3	B	13	HIS
4	I	15	GLN
4	I	73	HIS
4	I	119	ASN
4	I	182	ASN
5	J	45	GLN
5	J	219	ASN
5	J	224	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 ⓘ

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	C	9/9 (100%)	-0.11	0 100 100	15, 17, 20, 22	0
2	A	275/275 (100%)	0.20	10 (3%) 46 50	14, 23, 40, 50	0
3	B	100/100 (100%)	0.30	5 (5%) 34 38	15, 22, 42, 47	0
4	I	202/208 (97%)	0.23	10 (4%) 34 38	14, 21, 39, 59	0
5	J	240/243 (98%)	0.06	8 (3%) 49 53	15, 21, 35, 56	0
All	All	826/835 (98%)	0.18	33 (3%) 42 46	14, 22, 39, 59	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	J	28	ASN	3.6
2	A	194	VAL	3.5
3	B	0	ALA	3.4
4	I	133	SER	3.4
4	I	205	SER	3.2
5	J	219	ASN	3.0
4	I	132	SER	2.8
2	A	1	GLY	2.7
2	A	225	THR	2.6
3	B	70	PHE	2.6
2	A	197	HIS	2.6
3	B	1	ILE	2.5
2	A	136	ALA	2.5
4	I	203	PHE	2.5
5	J	225	ASP	2.5
5	J	221	GLU	2.5
4	I	151	GLN	2.4
4	I	155	SER	2.3
5	J	218	GLU	2.3
4	I	134	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
4	I	154	ASP	2.3
5	J	206	HIS	2.2
2	A	90	ALA	2.2
3	B	75	LYS	2.2
5	J	176	LEU	2.1
5	J	239	TRP	2.1
2	A	19	GLU	2.0
4	I	185	ASP	2.0
2	A	17	ARG	2.0
3	B	20	SER	2.0
4	I	153	LYS	2.0
2	A	275	GLU	2.0
2	A	226	GLN	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.