



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:49 AM UTC

PDB ID : 3TBV / pdb_00003tbv
Title : CRYSTAL STRUCTURE OF THE MURINE CLASS I MAJOR HISTOCOMPATIBILITY COMPLEX H-2DB IN COMPLEX WITH THE LCMV-DERIVED GP33 ALTERED PEPTIDE ligand (A2G,V3P,Y4A)
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Deposited on : 2011-08-08
Resolution : 2.10 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

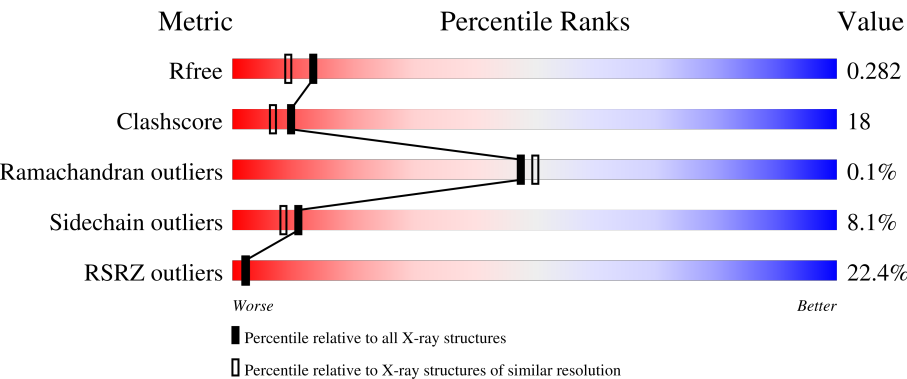
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	276	32% 66% 29% 5%
1	C	276	23% 70% 26% 5%
1	E	276	25% 68% 25% 5%
1	G	276	22% 67% 27%

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Mol	Chain	Length	Quality of chain
2	B	99	
2	D	99	
2	F	99	
2	H	99	
3	I	9	
3	J	9	
3	K	9	
3	L	9	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	F	100	-	-	X	-
5	GOL	E	341	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13548 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 H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2264	1430	400	425	9			
1	C	276	Total	C	N	O	S	0	0	0
			2264	1430	400	425	9			
1	E	276	Total	C	N	O	S	0	0	0
			2264	1430	400	425	9			
1	G	276	Total	C	N	O	S	0	0	0
			2264	1430	400	425	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			820	524	138	151	7			
2	D	99	Total	C	N	O	S	0	0	0
			820	524	138	151	7			
2	F	99	Total	C	N	O	S	0	0	0
			820	524	138	151	7			
2	H	99	Total	C	N	O	S	0	0	0
			820	524	138	151	7			

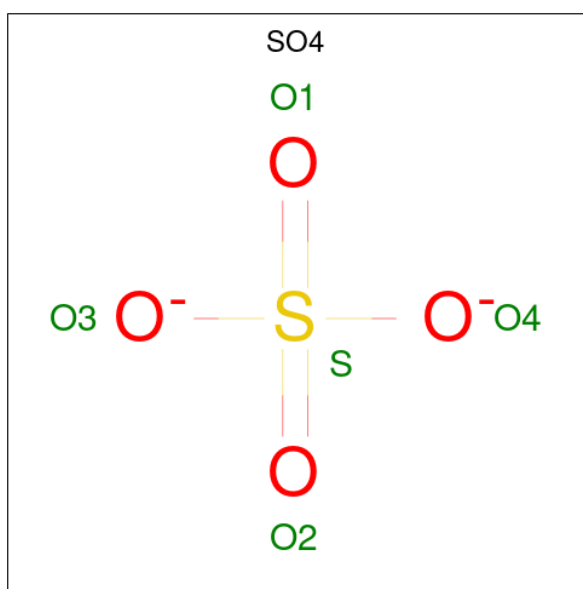
- Molecule 3 is a protein called Glycoprotein G1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	9	Total	C	N	O	S	0	0	0
			65	41	11	12	1			
3	J	9	Total	C	N	O	S	0	0	0
			65	41	11	12	1			
3	K	9	Total	C	N	O	S	0	0	0
			65	41	11	12	1			
3	L	9	Total	C	N	O	S	0	0	0
			65	41	11	12	1			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	2	GLY	ALA	engineered mutation	UNP P07399
I	3	PRO	VAL	engineered mutation	UNP P07399
I	4	ALA	TYR	engineered mutation	UNP P07399
I	9	MET	CYS	engineered mutation	UNP P07399
J	2	GLY	ALA	engineered mutation	UNP P07399
J	3	PRO	VAL	engineered mutation	UNP P07399
J	4	ALA	TYR	engineered mutation	UNP P07399
J	9	MET	CYS	engineered mutation	UNP P07399
K	2	GLY	ALA	engineered mutation	UNP P07399
K	3	PRO	VAL	engineered mutation	UNP P07399
K	4	ALA	TYR	engineered mutation	UNP P07399
K	9	MET	CYS	engineered mutation	UNP P07399
L	2	GLY	ALA	engineered mutation	UNP P07399
L	3	PRO	VAL	engineered mutation	UNP P07399
L	4	ALA	TYR	engineered mutation	UNP P07399
L	9	MET	CYS	engineered mutation	UNP P07399

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	132	Total	O	0	0
			132	132		

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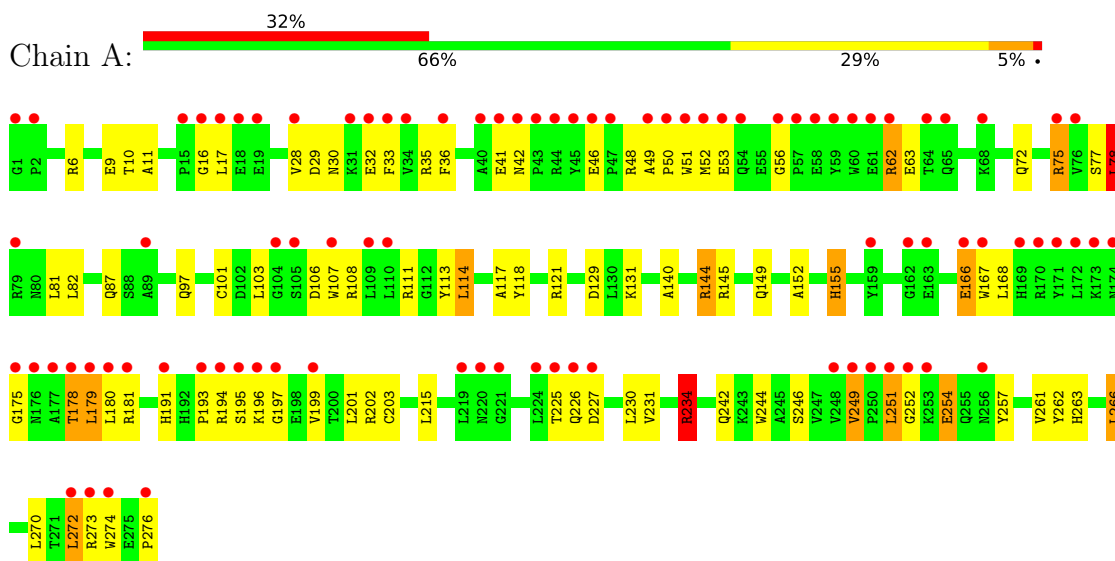
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	67	Total 67	O 67	0	0
6	C	164	Total 164	O 164	0	0
6	D	77	Total 77	O 77	0	0
6	E	154	Total 154	O 154	0	0
6	F	69	Total 69	O 69	0	0
6	G	128	Total 128	O 128	0	0
6	H	74	Total 74	O 74	0	0
6	I	4	Total 4	O 4	0	0
6	J	9	Total 9	O 9	0	0
6	K	10	Total 10	O 10	0	0
6	L	2	Total 2	O 2	0	0

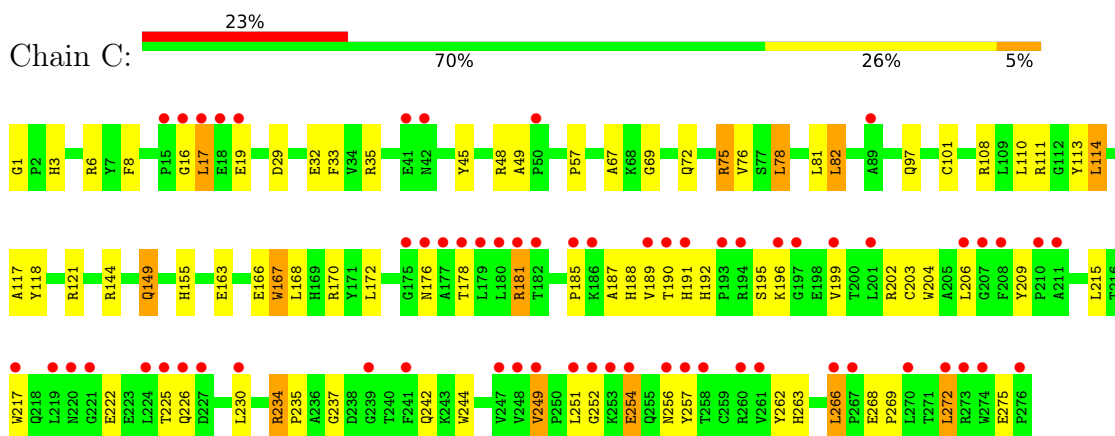
3 Residue-property plots

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: H-2 class I histocompatibility antigen, D-B alpha chain

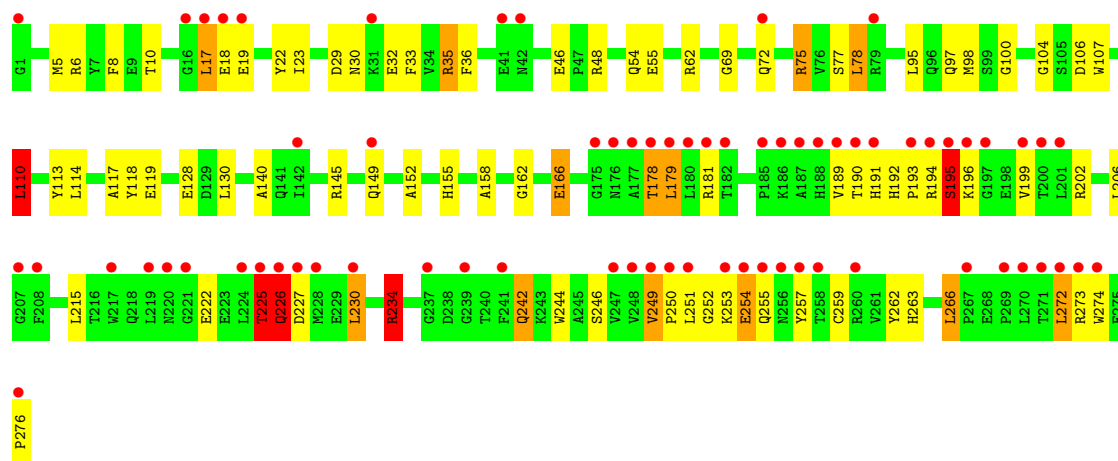


- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

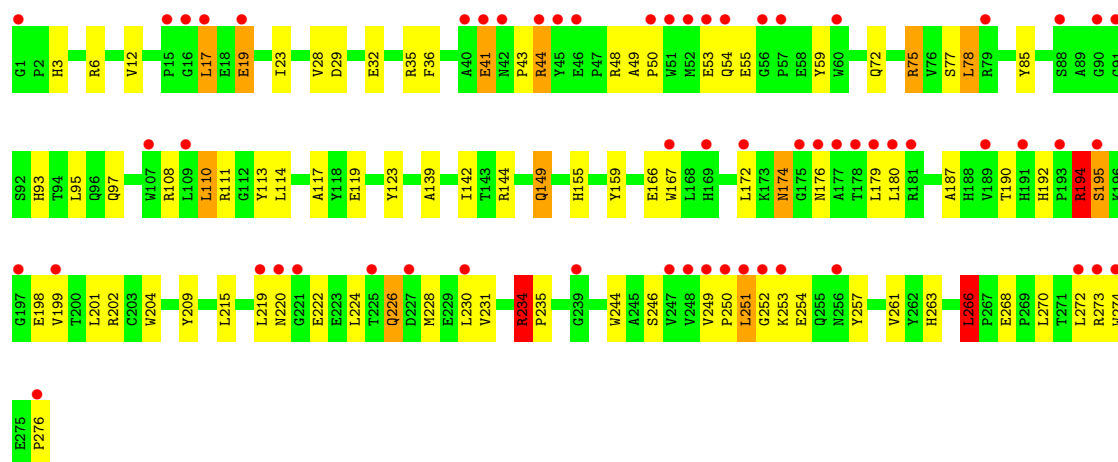


- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

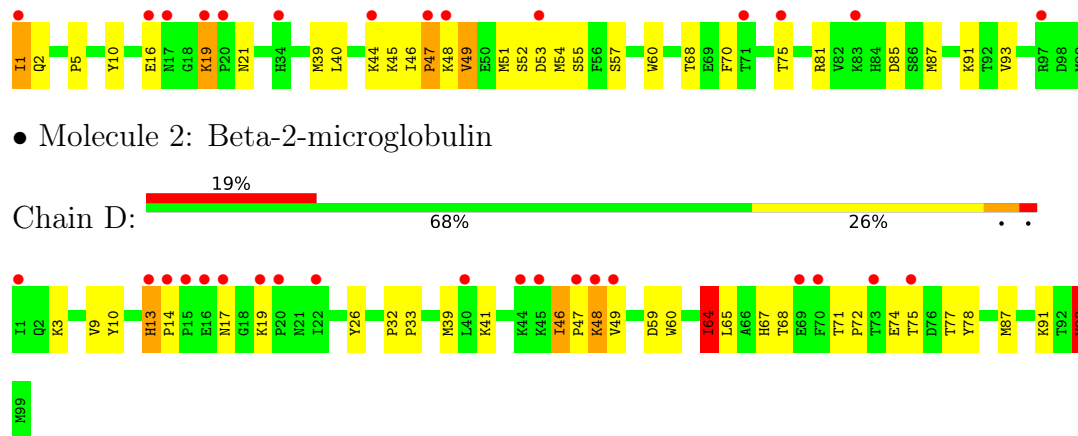




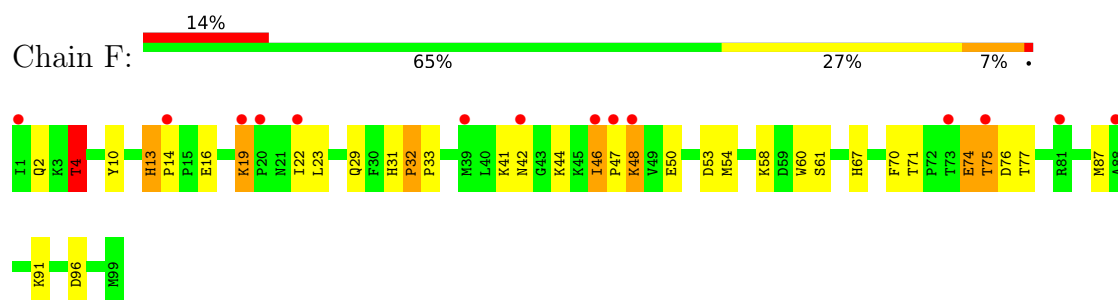
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



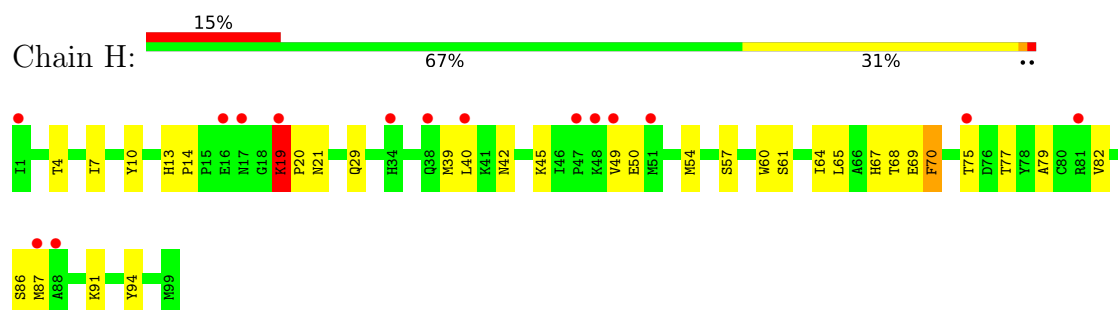
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



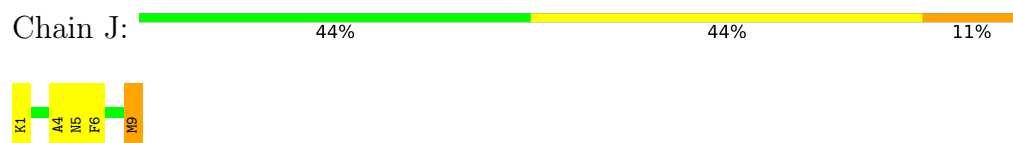
- Molecule 2: Beta-2-microglobulin



- Molecule 3: Glycoprotein G1



- Molecule 3: Glycoprotein G1



- Molecule 3: Glycoprotein G1



- Molecule 3: Glycoprotein G1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.58Å 126.47Å 102.11Å 90.00° 106.71° 90.00°	Depositor
Resolution (Å)	49.51 – 2.10 49.51 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.51-2.10) 99.1 (49.51-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.225 , 0.278 0.233 , 0.282	Depositor DCC
R_{free} test set	6806 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13548	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.04 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.1085e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SO4, GOL

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	1.12	5/2331 (0.2%)	1.16	15/3166 (0.5%)
1	C	1.08	2/2331 (0.1%)	1.20	12/3166 (0.4%)
1	E	1.13	4/2331 (0.2%)	1.19	12/3166 (0.4%)
1	G	1.07	3/2331 (0.1%)	1.16	17/3166 (0.5%)
2	B	1.22	1/846 (0.1%)	1.23	3/1148 (0.3%)
2	D	1.11	1/846 (0.1%)	1.35	9/1148 (0.8%)
2	F	1.21	1/846 (0.1%)	1.32	12/1148 (1.0%)
2	H	1.17	0/846	1.23	3/1148 (0.3%)
3	I	3.49	3/66 (4.5%)	1.66	1/86 (1.2%)
3	J	3.30	2/66 (3.0%)	1.43	1/86 (1.2%)
3	K	3.14	1/66 (1.5%)	1.39	0/86
3	L	2.06	1/66 (1.5%)	1.35	0/86
All	All	1.19	24/12972 (0.2%)	1.21	85/17600 (0.5%)

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	A	0	1
1	G	0	1
All	All	0	2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	9	MET	C-OXT	25.68	1.75	1.23
3	K	9	MET	C-OXT	23.17	1.69	1.23
3	J	9	MET	C-OXT	22.25	1.68	1.23
3	L	9	MET	C-OXT	12.14	1.47	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	4	ALA	CA-CB	9.64	1.67	1.53
1	E	152	ALA	N-CA	6.75	1.54	1.46
1	A	9	GLU	CA-C	-6.61	1.44	1.52
1	G	123	TYR	CA-C	6.33	1.59	1.53
1	E	140	ALA	CA-CB	-6.13	1.42	1.53
1	A	140	ALA	CA-CB	-6.04	1.43	1.53
2	B	49	VAL	CA-CB	5.62	1.60	1.54
3	I	6	PHE	N-CA	5.50	1.49	1.46
1	A	155	HIS	CA-C	5.41	1.59	1.52
1	C	49	ALA	C-O	-5.38	1.18	1.24
1	A	140	ALA	CA-C	5.33	1.59	1.52
2	F	22	ILE	CA-CB	5.32	1.61	1.54
2	D	3	LYS	C-O	5.30	1.30	1.24
1	E	69	GLY	CA-C	5.27	1.57	1.52
1	G	142	ILE	CA-CB	-5.22	1.48	1.54
3	I	6	PHE	CA-C	-5.20	1.50	1.53
1	E	158	ALA	N-CA	5.19	1.52	1.46
1	C	69	GLY	CA-C	5.14	1.57	1.52
1	G	12	VAL	N-CA	-5.14	1.40	1.46
1	A	152	ALA	N-CA	5.07	1.52	1.46

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	225	THR	CB-CA-C	-15.75	83.94	110.56
1	C	16	GLY	N-CA-C	14.63	132.40	113.24
1	A	178	THR	CB-CA-C	11.27	132.85	110.42
1	A	234	ARG	NE-CZ-NH2	-9.76	110.42	119.20
3	I	6	PHE	N-CA-C	9.35	116.44	108.78
2	D	13	HIS	CA-C-N	-8.92	111.19	120.38
2	D	13	HIS	C-N-CA	-8.92	111.19	120.38
1	A	234	ARG	NE-CZ-NH1	8.02	129.52	121.50
2	F	71	THR	CA-C-N	-7.50	112.28	119.85
2	F	71	THR	C-N-CA	-7.50	112.28	119.85
1	E	234	ARG	NE-CZ-NH1	7.47	128.97	121.50
1	E	226	GLN	N-CA-C	7.42	126.60	110.80
1	C	78	LEU	N-CA-C	-7.37	103.25	111.28
1	G	234	ARG	CA-C-N	7.31	127.58	119.90
1	G	234	ARG	C-N-CA	7.31	127.58	119.90
1	E	234	ARG	NE-CZ-NH2	-7.15	112.76	119.20
1	C	1	GLY	CA-C-N	7.07	126.99	120.21
1	C	1	GLY	C-N-CA	7.07	126.99	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	64	ILE	CB-CA-C	-6.64	99.23	111.18
1	G	234	ARG	NE-CZ-NH2	-6.58	113.28	119.20
1	G	228	MET	N-CA-C	-6.44	100.02	110.20
1	A	56	GLY	CA-C-N	-6.43	112.37	119.19
1	A	56	GLY	C-N-CA	-6.43	112.37	119.19
1	G	266	LEU	CA-C-N	6.33	125.75	118.85
1	G	266	LEU	C-N-CA	6.33	125.75	118.85
2	D	46	ILE	CA-C-N	6.32	126.80	119.47
2	D	46	ILE	C-N-CA	6.32	126.80	119.47
1	C	82	LEU	N-CA-C	-6.20	104.52	111.28
1	G	234	ARG	NE-CZ-NH1	6.19	127.69	121.50
2	F	46	ILE	CA-C-N	6.00	125.48	119.24
2	F	46	ILE	C-N-CA	6.00	125.48	119.24
1	A	46	GLU	CA-C-N	-5.96	113.80	119.76
1	A	46	GLU	C-N-CA	-5.96	113.80	119.76
1	G	235	PRO	CB-CA-C	-5.90	104.32	111.46
1	C	181	ARG	N-CA-C	5.88	117.79	108.67
1	E	195	SER	CB-CA-C	-5.80	99.37	109.64
2	F	46	ILE	N-CA-C	-5.77	103.67	108.63
1	E	19	GLU	N-CA-C	5.73	118.91	109.58
1	G	110	LEU	N-CA-C	-5.71	106.35	113.55
1	E	225	THR	CA-C-N	5.71	132.44	121.54
1	E	225	THR	C-N-CA	5.71	132.44	121.54
1	G	195	SER	CB-CA-C	5.67	121.71	110.42
2	D	98	ASP	N-CA-C	-5.61	106.02	112.92
2	F	4	THR	CA-C-N	5.52	125.79	119.83
2	F	4	THR	C-N-CA	5.52	125.79	119.83
1	A	166	GLU	N-CA-C	-5.47	104.96	111.03
1	A	78	LEU	N-CA-C	-5.44	105.25	111.07
1	G	194	ARG	CA-C-N	5.42	131.89	121.54
1	G	194	ARG	C-N-CA	5.42	131.89	121.54
3	J	4	ALA	N-CA-C	-5.40	98.58	108.02
1	A	87	GLN	CA-C-N	-5.39	112.44	121.39
1	A	87	GLN	C-N-CA	-5.39	112.44	121.39
1	C	76	VAL	N-CA-C	-5.38	104.37	111.09
2	H	69	GLU	N-CA-C	-5.37	100.94	109.96
2	B	53	ASP	CA-C-N	5.33	129.88	121.56
2	B	53	ASP	C-N-CA	5.33	129.88	121.56
2	F	13	HIS	CA-C-N	-5.31	114.91	120.38
2	F	13	HIS	C-N-CA	-5.31	114.91	120.38
1	G	142	ILE	N-CA-C	-5.27	105.36	110.42
2	H	19	LYS	CA-C-N	-5.27	114.53	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	19	LYS	C-N-CA	-5.27	114.53	119.90
2	F	32	PRO	CA-C-N	5.24	124.85	119.56
2	F	32	PRO	C-N-CA	5.24	124.85	119.56
1	E	46	GLU	CA-C-N	-5.24	114.56	119.85
1	E	46	GLU	C-N-CA	-5.24	114.56	119.85
2	D	93	VAL	N-CA-C	5.24	116.26	108.46
1	E	35	ARG	NE-CZ-NH2	-5.23	114.49	119.20
1	C	163	GLU	N-CA-C	5.22	117.65	111.33
1	G	19	GLU	CB-CA-C	5.20	117.07	109.48
1	G	166	GLU	N-CA-C	-5.20	105.51	111.07
1	A	234	ARG	CD-NE-CZ	5.19	131.67	124.40
2	F	44	LYS	N-CA-C	5.19	117.70	109.24
1	C	256	ASN	N-CA-C	-5.17	106.82	113.02
1	C	8	PHE	CA-C-N	-5.15	115.22	122.94
1	C	8	PHE	C-N-CA	-5.15	115.22	122.94
1	A	42	ASN	CA-C-N	-5.12	114.04	119.98
1	A	42	ASN	C-N-CA	-5.12	114.04	119.98
1	E	110	LEU	N-CA-C	-5.11	107.17	113.41
2	B	5	PRO	CA-C-O	-5.09	115.54	121.34
1	C	167	TRP	N-CA-C	5.08	117.55	111.71
1	G	174	ASN	N-CA-C	5.06	117.91	111.69
1	A	82	LEU	N-CA-C	-5.04	105.86	111.36
1	G	144	ARG	N-CA-C	-5.03	105.68	111.07
2	D	71	THR	CA-C-N	-5.03	114.77	119.85
2	D	71	THR	C-N-CA	-5.03	114.77	119.85

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	GLY	Peptide
1	G	194	ARG	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	2264	0	2136	70	0
1	C	2264	0	2136	75	0
1	E	2264	0	2136	89	0
1	G	2264	0	2136	73	0
2	B	820	0	796	37	0
2	D	820	0	796	45	0
2	F	820	0	796	34	0
2	H	820	0	796	35	0
3	I	65	0	66	7	0
3	J	65	0	66	9	0
3	K	65	0	66	11	0
3	L	65	0	66	6	0
4	A	5	0	0	0	0
4	C	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	3	0
5	A	12	0	16	3	0
5	B	6	0	8	3	0
5	E	12	0	16	9	0
5	H	12	0	16	3	0
6	A	132	0	0	5	0
6	B	67	0	0	7	0
6	C	164	0	0	9	0
6	D	77	0	0	2	0
6	E	154	0	0	1	0
6	F	69	0	0	4	0
6	G	128	0	0	4	0
6	H	74	0	0	0	0
6	I	4	0	0	0	0
6	J	9	0	0	0	0
6	K	10	0	0	0	0
6	L	2	0	0	0	0
All	All	13548	0	12048	437	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 18.

All (437) 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)
3:J:9:MET:OXT	3:J:9:MET:C	1.68	1.35
3:K:9:MET:C	3:K:9:MET:OXT	1.69	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:9:MET:OXT	3:I:9:MET:C	1.74	1.27
1:E:226:GLN:CD	1:E:226:GLN:O	1.75	1.27
1:E:226:GLN:O	1:E:226:GLN:NE2	1.94	0.98
2:D:49:VAL:HG23	2:D:67:HIS:O	1.63	0.97
1:E:226:GLN:CD	1:E:226:GLN:C	2.36	0.93
1:A:234:ARG:HD3	2:B:10:TYR:CE2	2.07	0.89
2:D:47:PRO:O	2:D:48:LYS:HD2	1.74	0.86
2:H:39:MET:HE1	2:H:68:THR:HB	1.56	0.86
1:C:234:ARG:HD3	2:D:10:TYR:CZ	2.11	0.85
1:C:167:TRP:CZ2	3:J:1:LYS:HE3	2.13	0.83
2:D:47:PRO:O	2:D:48:LYS:CD	2.28	0.82
2:D:39:MET:HE1	2:D:68:THR:CG2	2.09	0.81
1:A:230:LEU:C	1:A:230:LEU:HD12	2.05	0.81
2:F:87:MET:HE1	2:F:91:LYS:HB2	1.61	0.80
2:H:87:MET:HE1	2:H:91:LYS:HB2	1.63	0.79
2:B:87:MET:HE1	2:B:91:LYS:HD2	1.66	0.78
2:B:57:SER:OG	5:B:100:GOL:H31	1.83	0.78
1:G:234:ARG:HD3	2:H:10:TYR:CE2	2.19	0.78
2:F:74:GLU:OE2	2:F:74:GLU:HA	1.81	0.78
2:H:39:MET:HE1	2:H:68:THR:CB	2.15	0.77
5:E:340:GOL:O3	5:E:340:GOL:O1	1.98	0.77
2:D:39:MET:HE1	2:D:68:THR:HG22	1.67	0.76
1:E:97:GLN:HE22	3:K:5:ASN:HD21	1.34	0.76
1:E:202:ARG:HD2	1:E:244:TRP:CD2	2.21	0.76
1:E:145:ARG:HD3	5:E:341:GOL:H12	1.69	0.75
1:G:167:TRP:CE2	3:L:1:LYS:HD2	2.22	0.74
2:B:52:SER:HA	6:B:483:HOH:O	1.86	0.73
1:G:97:GLN:HE22	3:L:5:ASN:HD21	1.36	0.72
2:B:39:MET:HE2	2:B:49:VAL:HG13	1.72	0.72
2:D:39:MET:CE	2:D:68:THR:CG2	2.68	0.72
2:D:39:MET:HE2	2:D:49:VAL:CG2	2.20	0.72
1:G:249:VAL:HG22	1:G:257:TYR:CE2	2.25	0.71
2:D:64:ILE:HG22	2:D:65:LEU:N	2.05	0.70
2:H:39:MET:CE	2:H:68:THR:HB	2.20	0.70
1:C:226:GLN:O	1:C:226:GLN:NE2	2.24	0.70
2:B:87:MET:HE1	2:B:91:LYS:HB2	1.73	0.70
2:H:39:MET:HE1	2:H:68:THR:CG2	2.20	0.69
1:E:234:ARG:HD3	2:F:10:TYR:CZ	2.28	0.69
1:E:77:SER:HB3	3:K:9:MET:CG	2.23	0.69
2:D:39:MET:HE1	2:D:68:THR:CB	2.23	0.69
2:D:49:VAL:HG23	2:D:67:HIS:C	2.18	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:49:VAL:CG2	2:D:67:HIS:O	2.40	0.68
1:G:202:ARG:NH2	6:G:726:HOH:O	2.26	0.68
2:F:46:ILE:HG23	2:F:47:PRO:HD2	1.75	0.67
2:H:57:SER:OG	5:H:101:GOL:C1	2.43	0.67
1:E:32:GLU:OE2	1:E:35:ARG:HD2	1.95	0.67
2:D:39:MET:HE1	2:D:68:THR:HB	1.76	0.67
1:G:32:GLU:OE2	1:G:48:ARG:HD2	1.95	0.67
1:C:263:HIS:HB3	1:C:266:LEU:HD22	1.76	0.66
1:C:222:GLU:OE2	1:C:222:GLU:HA	1.95	0.66
1:C:230:LEU:HD12	1:C:230:LEU:C	2.21	0.66
1:G:230:LEU:C	1:G:230:LEU:HD12	2.21	0.65
2:D:87:MET:HE1	2:D:91:LYS:HD2	1.78	0.65
1:G:6:ARG:NH2	1:G:113:TYR:CE1	2.65	0.65
2:D:64:ILE:CG2	2:D:65:LEU:N	2.60	0.65
2:D:39:MET:HE2	2:D:49:VAL:HG21	1.79	0.64
1:C:202:ARG:HD2	1:C:244:TRP:CD2	2.32	0.64
2:H:39:MET:HE2	2:H:49:VAL:CG1	2.28	0.64
1:A:263:HIS:HB3	1:A:266:LEU:HD22	1.77	0.64
1:G:194:ARG:HB2	1:G:199:VAL:HA	1.80	0.64
2:F:87:MET:HE1	2:F:91:LYS:HD2	1.80	0.64
1:G:249:VAL:HG22	1:G:257:TYR:CZ	2.33	0.64
2:H:39:MET:HE2	2:H:49:VAL:CG2	2.27	0.63
1:C:32:GLU:OE2	1:C:48:ARG:HD2	1.99	0.63
1:E:226:GLN:OE1	1:E:227:ASP:HB2	1.98	0.63
1:A:32:GLU:OE2	1:A:48:ARG:HD2	1.99	0.63
1:G:176:ASN:O	1:G:180:LEU:HD22	2.00	0.62
2:H:39:MET:CE	2:H:68:THR:CG2	2.78	0.62
1:A:249:VAL:HG22	1:A:257:TYR:CZ	2.35	0.62
1:C:226:GLN:O	1:C:226:GLN:CD	2.41	0.62
2:D:39:MET:CE	2:D:49:VAL:HG21	2.29	0.62
2:H:57:SER:OG	5:H:101:GOL:H12	1.99	0.62
1:E:117:ALA:HB2	2:F:60:TRP:CE2	2.35	0.61
1:E:226:GLN:C	1:E:226:GLN:OE1	2.42	0.61
1:E:181:ARG:HD3	1:E:181:ARG:H	1.64	0.61
2:H:39:MET:HE2	2:H:49:VAL:HG22	1.83	0.61
1:E:97:GLN:NE2	3:K:5:ASN:HD21	1.98	0.61
2:B:87:MET:HE1	2:B:91:LYS:CD	2.29	0.60
1:A:230:LEU:C	1:A:230:LEU:CD1	2.73	0.60
1:C:111:ARG:HD3	1:C:113:TYR:CZ	2.36	0.60
1:A:175:GLY:O	1:A:179:LEU:HG	2.01	0.60
1:E:145:ARG:CD	5:E:341:GOL:H12	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:234:ARG:HD3	2:H:10:TYR:CZ	2.36	0.60
1:E:230:LEU:HD12	1:E:230:LEU:C	2.26	0.60
1:E:251:LEU:HD23	1:E:252:GLY:N	2.16	0.60
2:B:40:LEU:HD23	2:B:45:LYS:HA	1.83	0.60
1:E:145:ARG:HD3	5:E:341:GOL:C1	2.32	0.60
1:G:97:GLN:NE2	3:L:5:ASN:HD21	1.99	0.60
1:G:110:LEU:HD13	6:G:657:HOH:O	2.02	0.59
2:D:39:MET:HE2	2:D:49:VAL:HB	1.84	0.59
2:D:39:MET:HE2	2:D:49:VAL:CB	2.33	0.59
1:E:251:LEU:HD23	1:E:252:GLY:H	1.67	0.59
1:A:234:ARG:HD3	2:B:10:TYR:CZ	2.38	0.59
1:E:145:ARG:CD	5:E:341:GOL:C1	2.80	0.58
1:G:17:LEU:HD23	1:G:17:LEU:H	1.68	0.58
1:C:195:SER:N	6:C:866:HOH:O	2.35	0.58
1:C:97:GLN:HE22	3:J:5:ASN:HD21	1.52	0.58
2:H:39:MET:HE2	2:H:49:VAL:HG13	1.83	0.58
1:E:234:ARG:HD3	2:F:10:TYR:CE2	2.39	0.58
2:D:39:MET:CE	2:D:49:VAL:CG2	2.82	0.58
1:A:72:GLN:OE1	1:A:75:ARG:NH1	2.36	0.58
1:C:234:ARG:HD3	2:D:10:TYR:CE2	2.38	0.57
1:C:57:PRO:HD2	6:C:669:HOH:O	2.03	0.57
1:C:202:ARG:NH2	6:C:689:HOH:O	2.38	0.57
1:E:104:GLY:N	1:E:110:LEU:HD22	2.20	0.57
2:H:39:MET:HE1	2:H:68:THR:HG22	1.85	0.57
1:E:191:HIS:HB2	1:E:274:TRP:CZ3	2.40	0.57
1:E:17:LEU:H	1:E:17:LEU:HD23	1.70	0.56
2:F:87:MET:HE1	2:F:91:LYS:CB	2.34	0.56
1:G:155:HIS:HB3	3:L:6:PHE:CZ	2.40	0.56
2:H:7:ILE:CD1	2:H:82:VAL:HG21	2.36	0.56
1:C:167:TRP:CE2	3:J:1:LYS:HE3	2.39	0.56
1:G:201:LEU:O	1:G:246:SER:HA	2.05	0.56
2:F:4:THR:HG23	4:F:100:SO4:O4	2.05	0.56
1:G:263:HIS:HB3	1:G:266:LEU:HD22	1.89	0.55
2:B:87:MET:CE	2:B:91:LYS:HB2	2.35	0.55
2:D:39:MET:CE	2:D:68:THR:HB	2.36	0.55
1:G:111:ARG:HD3	1:G:113:TYR:OH	2.07	0.55
1:E:226:GLN:O	1:E:226:GLN:OE1	2.17	0.54
1:E:77:SER:HB3	3:K:9:MET:HG3	1.88	0.54
2:F:58:LYS:HE2	6:F:195:HOH:O	2.06	0.54
1:E:202:ARG:HD2	1:E:244:TRP:CE3	2.42	0.54
2:F:50:GLU:HB2	2:F:67:HIS:CE1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:GLU:HA	1:E:222:GLU:OE2	2.08	0.54
1:E:77:SER:HB3	3:K:9:MET:HG2	1.88	0.54
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.43	0.54
2:B:39:MET:HE1	2:B:68:THR:HG22	1.90	0.54
1:E:8:PHE:CE2	5:E:340:GOL:H11	2.43	0.54
2:H:4:THR:HG22	2:H:86:SER:HB2	1.90	0.54
1:C:251:LEU:HD23	1:C:252:GLY:N	2.22	0.53
1:G:194:ARG:CB	1:G:198:GLU:O	2.56	0.53
1:G:202:ARG:HD2	1:G:244:TRP:CD2	2.42	0.53
1:E:95:LEU:HD11	3:K:9:MET:HE3	1.90	0.53
2:F:47:PRO:O	2:F:48:LYS:HD3	2.07	0.53
1:E:206:LEU:HD23	1:E:242:GLN:HB3	1.90	0.53
1:C:155:HIS:HB3	3:J:6:PHE:CZ	2.43	0.53
1:E:250:PRO:HB2	1:E:253:LYS:HB2	1.90	0.53
1:G:159:TYR:C	1:G:159:TYR:CD2	2.86	0.53
1:G:202:ARG:HD3	1:G:246:SER:HB3	1.90	0.53
1:A:226:GLN:OE1	1:A:227:ASP:HB2	2.08	0.53
3:I:9:MET:OXT	3:I:9:MET:O	2.23	0.53
1:E:194:ARG:HG2	1:E:195:SER:H	1.73	0.53
1:A:111:ARG:HD3	1:A:113:TYR:OH	2.08	0.53
1:A:178:THR:HG22	6:A:723:HOH:O	2.08	0.53
1:G:230:LEU:C	1:G:230:LEU:CD1	2.82	0.53
2:B:57:SER:OG	5:B:100:GOL:C3	2.56	0.53
1:C:111:ARG:HD3	1:C:113:TYR:OH	2.09	0.53
2:D:39:MET:CE	2:D:68:THR:HG22	2.34	0.52
1:A:28:VAL:HB	6:A:664:HOH:O	2.08	0.52
1:G:274:TRP:NE1	1:G:276:PRO:HG3	2.24	0.52
1:A:197:GLY:O	1:A:251:LEU:HB2	2.10	0.52
1:E:202:ARG:CD	1:E:244:TRP:CE3	2.93	0.52
1:A:144:ARG:NH2	6:A:628:HOH:O	2.41	0.52
1:A:249:VAL:HG22	1:A:257:TYR:CE2	2.44	0.52
1:C:187:ALA:C	1:C:272:LEU:HD11	2.35	0.52
1:C:230:LEU:C	1:C:230:LEU:CD1	2.82	0.52
2:H:64:ILE:HG22	2:H:65:LEU:N	2.25	0.52
1:C:190:THR:OG1	1:C:192:HIS:HE1	1.92	0.52
1:C:226:GLN:O	1:C:226:GLN:CG	2.57	0.52
1:E:230:LEU:C	1:E:230:LEU:CD1	2.83	0.52
1:A:10:THR:HG22	1:A:11:ALA:N	2.24	0.52
1:A:77:SER:HB3	3:I:9:MET:HG2	1.92	0.51
1:A:202:ARG:HD3	1:A:244:TRP:CE3	2.45	0.51
1:E:181:ARG:HD3	1:E:181:ARG:N	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:13:HIS:O	2:H:14:PRO:C	2.52	0.51
1:A:33:PHE:C	1:A:48:ARG:HB2	2.36	0.51
1:A:234:ARG:HD2	1:A:242:GLN:OE1	2.10	0.51
1:A:251:LEU:HD23	1:A:252:GLY:N	2.26	0.51
1:E:249:VAL:HG22	1:E:257:TYR:CZ	2.45	0.51
2:F:96:ASP:C	2:F:96:ASP:OD1	2.52	0.51
2:B:57:SER:HG	5:B:100:GOL:H31	1.76	0.51
1:C:234:ARG:HD3	2:D:10:TYR:CE1	2.45	0.51
1:E:225:THR:HG22	1:E:225:THR:O	2.11	0.51
1:G:202:ARG:HD2	1:G:244:TRP:CE3	2.46	0.51
1:A:251:LEU:HD23	1:A:251:LEU:C	2.36	0.51
2:B:39:MET:CE	2:B:68:THR:CG2	2.89	0.51
1:C:209:TYR:C	1:C:209:TYR:CD2	2.88	0.50
2:D:46:ILE:HG23	2:D:47:PRO:HD2	1.93	0.50
1:E:194:ARG:CG	1:E:195:SER:H	2.23	0.50
1:C:111:ARG:HG2	1:C:113:TYR:CE1	2.45	0.50
1:C:192:HIS:CD2	2:D:98:ASP:CG	2.89	0.50
1:G:194:ARG:HB3	1:G:198:GLU:O	2.10	0.50
1:A:262:TYR:CD2	1:C:108:ARG:HD3	2.46	0.50
2:B:39:MET:HE2	2:B:49:VAL:HG22	1.92	0.50
2:F:46:ILE:CG2	2:F:47:PRO:HD2	2.41	0.50
1:A:262:TYR:CD1	1:A:262:TYR:N	2.80	0.50
2:B:39:MET:CE	2:B:68:THR:HG22	2.42	0.50
1:E:262:TYR:CG	1:G:108:ARG:HD3	2.47	0.50
2:F:4:THR:HG23	4:F:100:SO4:O3	2.11	0.50
2:H:21:ASN:HB3	2:H:70:PHE:CE1	2.46	0.50
1:A:78:LEU:HD12	6:A:350:HOH:O	2.10	0.50
2:B:46:ILE:HG23	2:B:47:PRO:HD2	1.93	0.50
1:G:176:ASN:OD1	1:G:180:LEU:HD21	2.12	0.50
1:A:251:LEU:C	1:A:251:LEU:CD2	2.85	0.49
1:E:202:ARG:HD3	1:E:246:SER:HB3	1.94	0.49
2:D:87:MET:HE1	2:D:91:LYS:HB2	1.93	0.49
1:E:23:ILE:HD12	2:F:54:MET:SD	2.52	0.49
1:G:224:LEU:HD12	1:G:226:GLN:HE22	1.77	0.49
1:C:167:TRP:CZ3	1:C:170:ARG:HD3	2.47	0.49
1:A:49:ALA:O	1:A:50:PRO:C	2.54	0.49
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.48	0.49
1:E:72:GLN:OE1	1:E:75:ARG:HD3	2.12	0.49
1:E:191:HIS:HB2	1:E:274:TRP:CH2	2.46	0.49
1:G:17:LEU:HD23	1:G:17:LEU:N	2.27	0.49
2:B:44:LYS:HB3	6:B:228:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:155:HIS:HB3	3:K:6:PHE:CZ	2.47	0.49
3:K:8:THR:O	3:K:9:MET:C	2.55	0.49
2:B:52:SER:N	6:B:483:HOH:O	2.46	0.49
1:E:29:ASP:O	1:E:30:ASN:HB2	2.13	0.49
2:F:4:THR:HG23	4:F:100:SO4:S	2.52	0.49
1:A:6:ARG:NH2	1:A:113:TYR:CE1	2.81	0.49
1:C:237:GLY:HA3	6:D:288:HOH:O	2.13	0.49
2:D:91:LYS:NZ	6:D:887:HOH:O	2.44	0.49
2:B:1:ILE:HB	6:B:396:HOH:O	2.13	0.49
2:B:39:MET:HE1	2:B:68:THR:HB	1.94	0.49
1:G:43:PRO:C	1:G:44:ARG:HG2	2.38	0.49
2:H:29:GLN:HA	2:H:61:SER:HB2	1.94	0.49
2:B:39:MET:HE1	2:B:68:THR:CG2	2.43	0.49
2:B:39:MET:HE1	2:B:68:THR:CB	2.42	0.49
1:A:193:PRO:HA	1:A:199:VAL:HG12	1.95	0.48
1:C:185:PRO:HG2	1:C:266:LEU:HD21	1.93	0.48
1:C:263:HIS:HB3	1:C:266:LEU:CD2	2.41	0.48
2:H:19:LYS:HE3	2:H:19:LYS:HB3	1.55	0.48
1:C:176:ASN:ND2	6:C:558:HOH:O	2.45	0.48
1:C:97:GLN:NE2	3:J:5:ASN:HD21	2.11	0.48
1:C:191:HIS:CE1	1:C:199:VAL:HG21	2.49	0.48
2:F:47:PRO:HG2	6:F:281:HOH:O	2.12	0.48
1:G:41:GLU:O	1:G:43:PRO:HD3	2.13	0.48
1:A:191:HIS:HB2	1:A:274:TRP:CZ3	2.48	0.48
1:A:234:ARG:HD3	2:B:10:TYR:CD2	2.48	0.48
2:F:87:MET:CE	2:F:91:LYS:HB2	2.36	0.48
1:A:145:ARG:HD3	5:A:341:GOL:H32	1.96	0.48
1:C:45:TYR:CE2	1:C:67:ALA:HB2	2.48	0.48
2:D:47:PRO:O	2:D:48:LYS:HD3	2.13	0.48
2:B:52:SER:CA	6:B:483:HOH:O	2.56	0.47
1:G:149:GLN:HE21	1:G:149:GLN:HA	1.79	0.47
1:A:225:THR:O	1:A:226:GLN:C	2.55	0.47
2:B:39:MET:CE	2:B:68:THR:HB	2.44	0.47
1:G:190:THR:OG1	1:G:192:HIS:HE1	1.96	0.47
2:H:19:LYS:O	2:H:20:PRO:C	2.57	0.47
1:A:167:TRP:CE2	3:I:1:LYS:HD2	2.49	0.47
1:E:72:GLN:OE1	1:E:75:ARG:NH1	2.47	0.47
1:C:206:LEU:HD23	1:C:242:GLN:HG2	1.96	0.47
2:D:39:MET:HE3	2:D:68:THR:HG21	1.96	0.47
1:E:178:THR:O	1:E:178:THR:CG2	2.60	0.47
1:G:261:VAL:HB	1:G:270:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ARG:NE	6:A:347:HOH:O	2.47	0.47
1:A:194:ARG:HG2	1:A:195:SER:H	1.80	0.47
2:B:87:MET:HE1	2:B:91:LYS:CB	2.45	0.47
2:D:59:ASP:O	2:D:60:TRP:HB2	2.15	0.47
1:G:72:GLN:OE1	1:G:75:ARG:NH1	2.48	0.47
1:A:29:ASP:O	1:A:30:ASN:HB2	2.16	0.46
1:C:168:LEU:O	1:C:172:LEU:HG	2.14	0.46
1:C:187:ALA:HB1	1:C:272:LEU:HD12	1.96	0.46
1:C:178:THR:O	1:C:178:THR:CG2	2.63	0.46
1:E:104:GLY:CA	1:E:110:LEU:HD22	2.46	0.46
1:A:17:LEU:HD12	1:A:17:LEU:N	2.30	0.46
1:A:191:HIS:HE1	1:A:254:GLU:OE1	1.97	0.46
1:E:262:TYR:CD2	1:G:108:ARG:HG2	2.50	0.46
5:A:340:GOL:O2	2:B:54:MET:O	2.34	0.46
1:G:44:ARG:HD2	6:G:533:HOH:O	2.16	0.46
1:G:54:GLN:O	1:G:55:GLU:C	2.58	0.46
1:A:178:THR:O	1:A:181:ARG:HB3	2.16	0.46
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.51	0.46
2:D:39:MET:HE3	2:D:68:THR:CG2	2.45	0.46
1:E:234:ARG:HD3	2:F:10:TYR:CE1	2.51	0.46
2:H:57:SER:OG	5:H:101:GOL:H11	2.15	0.46
1:G:187:ALA:HA	1:G:204:TRP:O	2.15	0.46
1:G:251:LEU:HD23	1:G:252:GLY:H	1.81	0.46
1:E:95:LEU:HD11	3:K:9:MET:CE	2.46	0.46
2:F:16:GLU:OE1	2:F:19:LYS:HD3	2.16	0.46
2:F:31:HIS:CD2	2:F:32:PRO:HA	2.51	0.46
3:J:9:MET:OXT	3:J:9:MET:O	2.22	0.45
1:C:144:ARG:NH2	6:C:394:HOH:O	2.49	0.45
1:C:178:THR:O	1:C:178:THR:HG22	2.17	0.45
1:C:226:GLN:CD	1:C:226:GLN:C	2.84	0.45
1:E:263:HIS:HB3	1:E:266:LEU:HD22	1.98	0.45
1:A:274:TRP:NE1	1:A:276:PRO:HG3	2.31	0.45
1:E:72:GLN:OE1	1:E:75:ARG:CD	2.64	0.45
1:E:35:ARG:NH2	2:F:53:ASP:HB3	2.31	0.45
1:A:191:HIS:HB2	1:A:274:TRP:CH2	2.52	0.45
1:E:202:ARG:HD2	1:E:244:TRP:CE2	2.51	0.45
1:E:262:TYR:CD1	1:G:108:ARG:HD3	2.51	0.45
1:G:174:ASN:ND2	6:G:387:HOH:O	2.50	0.45
2:H:7:ILE:HD11	2:H:82:VAL:HG21	1.99	0.45
1:C:17:LEU:CD1	6:C:385:HOH:O	2.64	0.45
1:A:201:LEU:O	1:A:246:SER:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:GLY:O	1:E:166:GLU:HB2	2.16	0.45
1:E:181:ARG:O	1:E:181:ARG:HG2	2.17	0.45
1:G:209:TYR:CD2	1:G:209:TYR:C	2.95	0.45
2:H:40:LEU:HD23	2:H:45:LYS:HA	1.99	0.45
1:C:195:SER:O	1:C:196:LYS:C	2.57	0.45
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.52	0.45
2:H:64:ILE:CG2	2:H:65:LEU:N	2.80	0.45
1:C:6:ARG:NH2	1:C:113:TYR:CE1	2.85	0.45
1:C:235:PRO:HD2	2:D:26:TYR:CE2	2.51	0.45
2:D:46:ILE:CG2	2:D:47:PRO:HD2	2.47	0.45
1:E:33:PHE:C	1:E:48:ARG:HB2	2.42	0.45
1:A:195:SER:O	1:A:196:LYS:C	2.60	0.44
1:C:181:ARG:H	1:C:181:ARG:HD3	1.82	0.44
1:G:219:LEU:O	1:G:220:ASN:C	2.60	0.44
1:A:194:ARG:CG	1:A:195:SER:H	2.30	0.44
2:B:39:MET:HE2	2:B:49:VAL:CG1	2.44	0.44
1:C:72:GLN:OE1	1:C:75:ARG:HD3	2.17	0.44
1:A:28:VAL:O	1:A:29:ASP:C	2.59	0.44
1:E:178:THR:O	1:E:178:THR:HG23	2.18	0.44
1:E:190:THR:OG1	1:E:192:HIS:HE1	2.00	0.44
5:E:340:GOL:H32	6:F:847:HOH:O	2.17	0.44
1:G:93:HIS:HA	1:G:119:GLU:OE1	2.17	0.44
1:G:250:PRO:HB2	1:G:253:LYS:HB2	1.99	0.44
1:E:8:PHE:CD1	1:E:98:MET:HG2	2.52	0.44
1:G:85:TYR:CZ	1:G:139:ALA:HB3	2.52	0.44
1:C:81:LEU:HD13	1:C:118:TYR:CD1	2.53	0.44
1:C:188:HIS:N	1:C:272:LEU:HD11	2.33	0.44
1:E:18:GLU:N	6:E:456:HOH:O	2.50	0.44
2:F:13:HIS:O	2:F:14:PRO:C	2.57	0.44
1:G:23:ILE:HD12	2:H:54:MET:SD	2.58	0.44
1:G:194:ARG:HB2	1:G:198:GLU:O	2.17	0.44
1:C:203:CYS:HB2	1:C:217:TRP:CZ2	2.53	0.44
2:D:9:VAL:HG23	2:D:93:VAL:HG22	2.00	0.44
1:E:6:ARG:NH2	1:E:113:TYR:CE1	2.86	0.44
1:E:17:LEU:H	1:E:17:LEU:CD2	2.29	0.44
1:E:274:TRP:NE1	1:E:276:PRO:HG3	2.33	0.44
1:G:179:LEU:HD12	1:G:179:LEU:O	2.18	0.44
1:A:225:THR:O	1:A:227:ASP:N	2.51	0.43
1:C:181:ARG:C	6:C:780:HOH:O	2.60	0.43
2:F:47:PRO:O	2:F:48:LYS:CD	2.66	0.43
2:H:39:MET:CE	2:H:68:THR:HG22	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:230:LEU:HD12	1:E:230:LEU:O	2.18	0.43
1:G:59:TYR:CD1	1:G:59:TYR:C	2.95	0.43
1:G:28:VAL:O	1:G:29:ASP:C	2.61	0.43
1:A:155:HIS:HB3	3:I:6:PHE:CZ	2.53	0.43
1:E:17:LEU:CD2	1:E:17:LEU:N	2.81	0.43
2:F:32:PRO:HB2	2:F:33:PRO:HD2	2.00	0.43
1:E:128:GLU:C	1:E:130:LEU:H	2.27	0.43
1:A:97:GLN:HE22	3:I:5:ASN:HD21	1.67	0.43
1:E:145:ARG:HE	5:E:341:GOL:C1	2.32	0.43
1:G:226:GLN:O	1:G:226:GLN:CG	2.66	0.43
1:C:3:HIS:HA	1:C:29:ASP:OD1	2.19	0.43
1:A:36:PHE:CD1	1:A:36:PHE:C	2.96	0.43
1:C:249:VAL:HG22	1:C:257:TYR:CE2	2.54	0.43
1:A:49:ALA:O	1:A:51:TRP:N	2.52	0.43
1:A:203:CYS:O	1:A:244:TRP:HA	2.19	0.43
2:B:51:MET:C	6:B:483:HOH:O	2.62	0.43
1:C:187:ALA:HA	1:C:204:TRP:O	2.18	0.43
1:C:190:THR:OG1	1:C:202:ARG:HB3	2.19	0.43
1:E:192:HIS:O	1:E:193:PRO:C	2.61	0.43
2:B:16:GLU:OE2	2:B:19:LYS:HE2	2.19	0.43
1:C:155:HIS:HB3	3:J:6:PHE:CE2	2.53	0.43
2:D:39:MET:SD	2:D:49:VAL:HG21	2.58	0.43
1:G:231:VAL:HG13	1:G:244:TRP:CZ2	2.54	0.43
1:C:181:ARG:O	1:C:181:ARG:HG2	2.18	0.42
2:D:41:LYS:HG3	2:D:78:TYR:CE2	2.54	0.42
2:F:48:LYS:HD3	2:F:48:LYS:HA	1.60	0.42
1:G:19:GLU:OE2	1:G:75:ARG:HD2	2.19	0.42
1:G:167:TRP:CZ2	3:L:1:LYS:HD2	2.54	0.42
1:E:178:THR:HG22	1:E:179:LEU:HD23	2.01	0.42
1:A:32:GLU:OE2	1:A:35:ARG:HD2	2.19	0.42
1:C:48:ARG:NH2	6:C:729:HOH:O	2.51	0.42
1:C:117:ALA:HB2	2:D:60:TRP:CE2	2.54	0.42
2:D:17:ASN:HA	2:D:72:PRO:O	2.19	0.42
1:E:10:THR:O	1:E:22:TYR:HA	2.20	0.42
1:E:77:SER:CB	3:K:9:MET:HG2	2.49	0.42
1:E:189:VAL:HG23	1:E:272:LEU:HD13	2.01	0.42
2:F:29:GLN:HA	2:F:61:SER:HB2	2.00	0.42
1:G:234:ARG:HD3	2:H:10:TYR:CD2	2.52	0.42
1:C:234:ARG:CD	2:D:10:TYR:CE2	3.02	0.42
1:E:262:TYR:CD2	1:G:108:ARG:HD3	2.55	0.42
1:G:3:HIS:CG	1:G:172:LEU:HD11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:ASP:HB2	6:B:109:HOH:O	2.20	0.42
1:E:106:ASP:O	1:E:107:TRP:HB2	2.20	0.42
1:A:97:GLN:NE2	3:I:5:ASN:HD21	2.17	0.42
1:E:78:LEU:HD13	1:E:95:LEU:HB2	2.01	0.42
1:G:172:LEU:HD23	1:G:179:LEU:HD11	2.01	0.42
1:A:103:LEU:HD11	1:A:168:LEU:HD23	2.01	0.42
2:B:39:MET:HE3	2:B:68:THR:CG2	2.50	0.42
1:E:36:PHE:CD1	1:E:36:PHE:C	2.97	0.42
1:A:63:GLU:OE2	1:A:63:GLU:HA	2.19	0.42
2:D:9:VAL:CG2	2:D:93:VAL:HG22	2.49	0.42
2:F:32:PRO:CB	2:F:33:PRO:HD2	2.50	0.42
2:F:41:LYS:O	2:F:42:ASN:C	2.62	0.42
1:A:272:LEU:HD23	1:A:272:LEU:HA	1.85	0.42
2:B:19:LYS:HB3	2:B:19:LYS:HE3	1.63	0.42
1:C:202:ARG:HG2	1:C:204:TRP:NE1	2.35	0.42
2:F:13:HIS:HA	6:F:366:HOH:O	2.20	0.42
1:E:145:ARG:CD	5:E:341:GOL:H11	2.49	0.42
1:G:266:LEU:HB3	1:G:268:GLU:O	2.20	0.42
1:C:189:VAL:HG23	1:C:272:LEU:HD13	2.01	0.41
2:D:32:PRO:CB	2:D:33:PRO:CD	2.98	0.41
2:D:39:MET:CE	2:D:68:THR:HG21	2.49	0.41
1:G:77:SER:HB3	3:L:9:MET:HG2	2.02	0.41
1:A:231:VAL:HG13	1:A:244:TRP:CZ2	2.55	0.41
5:A:340:GOL:O2	2:B:55:SER:HA	2.21	0.41
1:C:199:VAL:HG21	1:C:254:GLU:OE1	2.20	0.41
1:E:118:TYR:CD2	1:E:119:GLU:HG2	2.55	0.41
1:G:78:LEU:HD13	1:G:95:LEU:HB2	2.02	0.41
1:G:226:GLN:O	1:G:226:GLN:HG2	2.19	0.41
1:C:33:PHE:C	1:C:48:ARG:HB2	2.45	0.41
1:C:149:GLN:NE2	6:C:831:HOH:O	2.54	0.41
1:C:167:TRP:CE3	1:C:170:ARG:HD3	2.55	0.41
2:D:13:HIS:O	2:D:14:PRO:C	2.62	0.41
1:E:193:PRO:HA	1:E:199:VAL:HG12	2.03	0.41
2:F:75:THR:HG22	2:F:76:ASP:N	2.36	0.41
1:A:17:LEU:N	1:A:17:LEU:CD1	2.84	0.41
1:E:128:GLU:C	1:E:130:LEU:N	2.79	0.41
1:A:129:ASP:O	1:A:131:LYS:HG3	2.20	0.41
2:H:87:MET:HE1	2:H:91:LYS:HD2	2.02	0.41
1:A:108:ARG:HD3	1:C:262:TYR:CD2	2.56	0.41
1:E:272:LEU:HD23	1:E:272:LEU:HA	1.85	0.41
1:E:5:MET:O	1:E:100:GLY:HA3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:49:ALA:O	1:G:50:PRO:C	2.63	0.41
1:A:51:TRP:CZ3	1:A:52:MET:SD	3.14	0.41
1:A:226:GLN:O	1:A:227:ASP:C	2.63	0.41
1:C:114:LEU:HD23	1:C:114:LEU:HA	1.82	0.41
1:A:262:TYR:CG	1:C:108:ARG:HD3	2.55	0.41
1:C:268:GLU:HB2	1:C:269:PRO:CD	2.51	0.41
1:E:54:GLN:O	1:E:55:GLU:C	2.63	0.41
1:A:261:VAL:HB	1:A:270:LEU:HB2	2.03	0.41
1:G:36:PHE:CD1	1:G:36:PHE:C	2.99	0.41
1:C:167:TRP:CH2	3:J:1:LYS:HE3	2.53	0.40
1:E:254:GLU:O	1:E:255:GLN:HG2	2.21	0.40
2:F:23:LEU:HB2	2:F:70:PHE:CD1	2.56	0.40
1:G:41:GLU:N	1:G:41:GLU:CD	2.79	0.40
1:G:190:THR:OG1	1:G:192:HIS:CE1	2.74	0.40
1:G:274:TRP:CE2	1:G:276:PRO:HG3	2.56	0.40
2:H:39:MET:HE3	2:H:68:THR:CG2	2.51	0.40
2:H:79:ALA:HB2	2:H:94:TYR:CD1	2.57	0.40
1:A:106:ASP:O	1:A:107:TRP:HB2	2.21	0.40
1:C:266:LEU:HB3	1:C:268:GLU:O	2.21	0.40
2:F:16:GLU:CD	2:F:19:LYS:HE2	2.46	0.40
1:G:222:GLU:HA	1:G:222:GLU:OE2	2.22	0.40
2:H:50:GLU:HB2	2:H:67:HIS:CE1	2.56	0.40
1:A:114:LEU:HD23	1:A:114:LEU:HA	1.86	0.40
2:D:19:LYS:HB3	2:D:19:LYS:HE3	1.85	0.40
1:C:251:LEU:HD23	1:C:252:GLY:H	1.87	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	274/276 (99%)	257 (94%)	17 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	274/276 (99%)	260 (95%)	14 (5%)	0	100	100
1	E	274/276 (99%)	259 (94%)	15 (6%)	0	100	100
1	G	274/276 (99%)	261 (95%)	13 (5%)	0	100	100
2	B	97/99 (98%)	94 (97%)	2 (2%)	1 (1%)	12	9
2	D	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
2	F	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
2	H	97/99 (98%)	91 (94%)	5 (5%)	1 (1%)	12	9
3	I	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	J	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
3	K	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	L	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	1512/1536 (98%)	1433 (95%)	77 (5%)	2 (0%)	48	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	42	ASN
2	B	47	PRO

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	234/234 (100%)	213 (91%)	21 (9%)	9	6
1	C	234/234 (100%)	214 (92%)	20 (8%)	10	7
1	E	234/234 (100%)	210 (90%)	24 (10%)	7	4
1	G	234/234 (100%)	215 (92%)	19 (8%)	11	8
2	B	94/94 (100%)	87 (93%)	7 (7%)	13	10
2	D	94/94 (100%)	88 (94%)	6 (6%)	16	14
2	F	94/94 (100%)	87 (93%)	7 (7%)	13	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	94/94 (100%)	90 (96%)	4 (4%)	26	27
3	I	6/6 (100%)	6 (100%)	0	100	100
3	J	6/6 (100%)	6 (100%)	0	100	100
3	K	6/6 (100%)	6 (100%)	0	100	100
3	L	6/6 (100%)	6 (100%)	0	100	100
All	All	1336/1336 (100%)	1228 (92%)	108 (8%)	11	8

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLU
1	A	53	GLU
1	A	62	ARG
1	A	75	ARG
1	A	78	LEU
1	A	101	CYS
1	A	114	LEU
1	A	121	ARG
1	A	144	ARG
1	A	149	GLN
1	A	166	GLU
1	A	179	LEU
1	A	180	LEU
1	A	215	LEU
1	A	234	ARG
1	A	249	VAL
1	A	251	LEU
1	A	254	GLU
1	A	266	LEU
1	A	272	LEU
1	A	273	ARG
2	B	1	ILE
2	B	2	GLN
2	B	19	LYS
2	B	48	LYS
2	B	75	THR
2	B	81	ARG
2	B	93	VAL
1	C	17	LEU
1	C	19	GLU

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Mol	Chain	Res	Type
1	C	35	ARG
1	C	75	ARG
1	C	78	LEU
1	C	82	LEU
1	C	101	CYS
1	C	110	LEU
1	C	114	LEU
1	C	121	ARG
1	C	149	GLN
1	C	166	GLU
1	C	215	LEU
1	C	225	THR
1	C	234	ARG
1	C	249	VAL
1	C	254	GLU
1	C	266	LEU
1	C	272	LEU
1	C	275	GLU
2	D	48	LYS
2	D	64	ILE
2	D	74	GLU
2	D	75	THR
2	D	77	THR
2	D	93	VAL
1	E	17	LEU
1	E	62	ARG
1	E	75	ARG
1	E	78	LEU
1	E	110	LEU
1	E	114	LEU
1	E	149	GLN
1	E	166	GLU
1	E	178	THR
1	E	179	LEU
1	E	195	SER
1	E	196	LYS
1	E	215	LEU
1	E	225	THR
1	E	226	GLN
1	E	230	LEU
1	E	234	ARG
1	E	242	GLN

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Mol	Chain	Res	Type
1	E	249	VAL
1	E	254	GLU
1	E	259	CYS
1	E	266	LEU
1	E	272	LEU
1	E	273	ARG
2	F	2	GLN
2	F	4	THR
2	F	19	LYS
2	F	48	LYS
2	F	74	GLU
2	F	75	THR
2	F	77	THR
1	G	17	LEU
1	G	35	ARG
1	G	41	GLU
1	G	44	ARG
1	G	53	GLU
1	G	75	ARG
1	G	78	LEU
1	G	114	LEU
1	G	149	GLN
1	G	194	ARG
1	G	195	SER
1	G	215	LEU
1	G	226	GLN
1	G	234	ARG
1	G	251	LEU
1	G	254	GLU
1	G	266	LEU
1	G	272	LEU
1	G	273	ARG
2	H	19	LYS
2	H	70	PHE
2	H	75	THR
2	H	77	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	54	GLN

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Mol	Chain	Res	Type
1	A	97	GLN
1	A	155	HIS
1	A	176	ASN
1	A	192	HIS
2	B	2	GLN
1	C	30	ASN
1	C	54	GLN
1	C	176	ASN
1	C	191	HIS
1	C	192	HIS
1	C	220	ASN
1	C	256	ASN
2	D	2	GLN
2	D	34	HIS
1	E	30	ASN
1	E	54	GLN
1	E	97	GLN
1	E	127	ASN
1	E	149	GLN
1	E	188	HIS
1	E	192	HIS
1	E	218	GLN
2	F	13	HIS
1	G	54	GLN
1	G	97	GLN
1	G	149	GLN
1	G	174	ASN
1	G	192	HIS
1	G	226	GLN
2	H	2	GLN
2	H	67	HIS
3	J	5	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GOL	H	100	-	5,5,5	0.51	0	5,5,5	1.10	0
5	GOL	H	101	-	5,5,5	0.58	0	5,5,5	0.75	0
5	GOL	A	340	-	5,5,5	0.75	0	5,5,5	0.89	0
5	GOL	A	341	-	5,5,5	0.69	0	5,5,5	0.31	0
4	SO4	F	100	-	4,4,4	0.44	0	6,6,6	0.44	0
4	SO4	E	339	-	4,4,4	0.24	0	6,6,6	0.37	0
5	GOL	E	340	-	5,5,5	0.68	0	5,5,5	1.68	2 (40%)
5	GOL	E	341	-	5,5,5	0.41	0	5,5,5	0.47	0
4	SO4	A	339	-	4,4,4	0.27	0	6,6,6	0.30	0
5	GOL	B	100	-	5,5,5	0.61	0	5,5,5	1.01	1 (20%)
4	SO4	C	339	-	4,4,4	0.34	0	6,6,6	0.99	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	H	100	-	-	3/4/4/4	-
5	GOL	H	101	-	-	0/4/4/4	-
5	GOL	A	340	-	-	2/4/4/4	-
5	GOL	A	341	-	-	4/4/4/4	-
5	GOL	E	340	-	-	0/4/4/4	-
5	GOL	E	341	-	-	4/4/4/4	-
5	GOL	B	100	-	-	0/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	340	GOL	C3-C2-C1	-2.72	101.83	111.80
5	E	340	GOL	O2-C2-C3	2.23	118.40	109.18
5	B	100	GOL	O3-C3-C2	2.10	119.83	110.38

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	340	GOL	C1-C2-C3-O3
5	A	341	GOL	O1-C1-C2-C3
5	E	341	GOL	C1-C2-C3-O3
5	H	100	GOL	O1-C1-C2-C3
5	A	341	GOL	C1-C2-C3-O3
5	E	341	GOL	O1-C1-C2-C3
5	A	340	GOL	O2-C2-C3-O3
5	A	341	GOL	O1-C1-C2-O2
5	E	341	GOL	O2-C2-C3-O3
5	E	341	GOL	O1-C1-C2-O2
5	H	100	GOL	O1-C1-C2-O2
5	A	341	GOL	O2-C2-C3-O3
5	H	100	GOL	O2-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	101	GOL	3	0
5	A	340	GOL	2	0
5	A	341	GOL	1	0
4	F	100	SO4	3	0
5	E	340	GOL	3	0
5	E	341	GOL	6	0
5	B	100	GOL	3	0

5.7 Other polymers

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	276/276 (100%)	1.45	89 (32%) 1 1	20, 52, 113, 192	0
1	C	276/276 (100%)	1.02	63 (22%) 2 2	20, 47, 112, 203	0
1	E	276/276 (100%)	1.16	70 (25%) 1 2	20, 46, 129, 193	0
1	G	276/276 (100%)	1.18	60 (21%) 2 2	19, 51, 116, 190	0
2	B	99/99 (100%)	0.84	14 (14%) 6 6	25, 41, 72, 101	0
2	D	99/99 (100%)	1.18	19 (19%) 3 3	24, 47, 82, 95	0
2	F	99/99 (100%)	1.12	14 (14%) 6 6	25, 46, 73, 100	0
2	H	99/99 (100%)	1.10	15 (15%) 5 5	26, 44, 74, 95	0
3	I	9/9 (100%)	0.46	0 100 100	30, 35, 51, 54	0
3	J	9/9 (100%)	-0.13	0 100 100	22, 29, 33, 38	0
3	K	9/9 (100%)	-0.30	0 100 100	20, 30, 36, 36	0
3	L	9/9 (100%)	0.24	0 100 100	25, 29, 45, 53	0
All	All	1536/1536 (100%)	1.14	344 (22%) 2 2	19, 47, 112, 203	0

All (344) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	1	ILE	9.8
2	D	1	ILE	8.3
1	A	179	LEU	8.0
1	G	179	LEU	7.6
1	E	179	LEU	7.0
1	C	179	LEU	6.9
2	B	1	ILE	6.9
1	G	178	THR	6.8
1	A	57	PRO	6.5
1	A	178	THR	6.4
2	H	1	ILE	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	172	LEU	5.9
1	A	175	GLY	5.5
1	G	17	LEU	5.4
1	E	180	LEU	5.4
1	E	178	THR	5.4
1	C	180	LEU	5.3
1	E	219	LEU	5.3
1	G	180	LEU	5.2
1	A	180	LEU	5.1
1	A	51	TRP	5.1
1	E	177	ALA	5.1
1	C	272	LEU	5.1
1	E	248	VAL	5.0
1	C	17	LEU	5.0
1	G	177	ALA	4.9
1	E	17	LEU	4.9
1	C	193	PRO	4.8
1	G	51	TRP	4.8
1	E	256	ASN	4.8
1	A	89	ALA	4.7
1	E	272	LEU	4.7
1	E	193	PRO	4.7
1	A	195	SER	4.7
1	E	251	LEU	4.7
2	D	47	PRO	4.7
1	A	60	TRP	4.6
1	C	178	THR	4.6
1	E	189	VAL	4.6
1	E	199	VAL	4.5
1	G	251	LEU	4.5
2	F	75	THR	4.5
1	C	16	GLY	4.5
1	A	177	ALA	4.5
1	G	16	GLY	4.4
1	E	186	LYS	4.4
1	G	57	PRO	4.3
1	A	40	ALA	4.2
1	E	187	ALA	4.2
1	A	249	VAL	4.2
1	C	219	LEU	4.2
1	E	257	TYR	4.2
1	A	52	MET	4.2

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Mol	Chain	Res	Type	RSRZ
1	G	175	GLY	4.1
1	E	274	TRP	4.1
1	E	224	LEU	4.1
1	E	258	THR	4.0
2	F	47	PRO	4.0
1	C	177	ALA	4.0
2	H	75	THR	4.0
1	A	56	GLY	3.9
1	A	199	VAL	3.9
1	A	59	TYR	3.9
2	B	48	LYS	3.9
1	C	239	GLY	3.8
1	G	199	VAL	3.8
1	A	107	TRP	3.8
1	C	257	TYR	3.8
1	E	276	PRO	3.8
1	G	41	GLU	3.8
1	A	219	LEU	3.7
1	A	79	ARG	3.7
1	A	193	PRO	3.7
1	E	249	VAL	3.7
1	G	193	PRO	3.7
1	A	227	ASP	3.7
1	E	182	THR	3.7
1	C	224	LEU	3.6
1	G	19	GLU	3.6
1	C	248	VAL	3.6
1	C	227	ASP	3.6
1	E	269	PRO	3.6
1	G	249	VAL	3.6
1	G	40	ALA	3.6
1	C	175	GLY	3.6
1	E	255	GLN	3.6
1	E	226	GLN	3.5
1	A	41	GLU	3.5
1	A	33	PHE	3.5
1	A	50	PRO	3.5
1	A	251	LEU	3.5
1	G	15	PRO	3.4
1	C	276	PRO	3.4
1	A	62	ARG	3.4
1	E	195	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	196	LYS	3.4
1	E	42	ASN	3.4
1	A	44	ARG	3.4
1	C	196	LYS	3.4
1	A	171	TYR	3.3
1	A	1	GLY	3.3
1	C	249	VAL	3.3
1	C	274	TRP	3.3
1	G	60	TRP	3.3
1	A	16	GLY	3.3
2	D	49	VAL	3.3
1	A	65	GLN	3.3
1	E	16	GLY	3.2
1	E	175	GLY	3.2
1	E	201	LEU	3.2
1	G	42	ASN	3.2
1	G	272	LEU	3.2
1	G	90	GLY	3.2
1	E	227	ASP	3.2
1	C	207	GLY	3.2
1	G	276	PRO	3.2
1	A	42	ASN	3.2
1	C	266	LEU	3.2
1	C	241	PHE	3.2
1	C	258	THR	3.2
1	C	267	PRO	3.2
1	A	226	GLN	3.2
1	G	248	VAL	3.1
1	E	208	PHE	3.1
1	C	186	LYS	3.1
1	A	110	LEU	3.1
2	D	48	LYS	3.1
2	H	48	LYS	3.1
1	A	17	LEU	3.1
1	C	251	LEU	3.1
1	A	256	ASN	3.1
1	E	188	HIS	3.0
1	G	189	VAL	3.0
1	A	252	GLY	3.0
1	C	176	ASN	3.0
1	E	176	ASN	3.0
1	G	1	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	253	LYS	3.0
2	F	19	LYS	3.0
1	A	34	VAL	3.0
1	A	272	LEU	3.0
1	C	254	GLU	3.0
1	A	274	TRP	3.0
1	G	45	TYR	3.0
2	D	19	LYS	3.0
2	F	48	LYS	3.0
1	A	58	GLU	3.0
1	C	256	ASN	3.0
1	E	194	ARG	2.9
1	C	89	ALA	2.9
1	E	270	LEU	2.9
1	E	207	GLY	2.9
1	E	181	ARG	2.9
1	A	18	GLU	2.9
1	C	42	ASN	2.9
1	A	196	LYS	2.9
1	C	211	ALA	2.9
1	C	247	VAL	2.9
2	D	75	THR	2.9
2	H	47	PRO	2.9
1	C	208	PHE	2.9
1	A	54	GLN	2.8
1	C	181	ARG	2.8
1	A	53	GLU	2.8
1	C	185	PRO	2.8
1	C	252	GLY	2.8
1	A	46	GLU	2.8
1	E	247	VAL	2.8
1	G	225	THR	2.8
1	G	191	HIS	2.8
1	C	225	THR	2.8
1	A	45	TYR	2.8
2	H	88	ALA	2.8
1	A	224	LEU	2.8
1	A	173	LYS	2.8
1	E	185	PRO	2.8
2	B	47	PRO	2.8
1	A	75	ARG	2.7
1	A	174	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	221	GLY	2.7
1	G	253	LYS	2.7
1	C	182	THR	2.7
1	C	260	ARG	2.7
1	E	142	ILE	2.7
1	E	149	GLN	2.7
1	E	191	HIS	2.7
1	C	19	GLU	2.7
1	G	221	GLY	2.7
1	A	225	THR	2.7
1	E	190	THR	2.7
1	C	189	VAL	2.7
1	E	19	GLU	2.7
1	E	41	GLU	2.7
1	C	221	GLY	2.7
1	G	197	GLY	2.7
1	A	181	ARG	2.7
1	C	190	THR	2.7
1	E	267	PRO	2.7
1	C	253	LYS	2.7
1	A	273	ARG	2.7
1	E	273	ARG	2.7
2	B	75	THR	2.6
1	A	43	PRO	2.6
1	G	176	ASN	2.6
1	G	256	ASN	2.6
1	A	105	SER	2.6
1	A	167	TRP	2.6
1	E	271	THR	2.6
1	A	109	LEU	2.6
2	B	20	PRO	2.6
1	A	248	VAL	2.6
1	G	52	MET	2.6
2	H	34	HIS	2.6
2	D	17	ASN	2.6
1	E	200	THR	2.6
1	G	107	TRP	2.6
1	C	201	LEU	2.6
1	G	50	PRO	2.6
1	C	273	ARG	2.6
2	B	97	ARG	2.6
1	A	169	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	191	HIS	2.6
1	A	220	ASN	2.6
2	H	19	LYS	2.6
1	C	217	TRP	2.6
1	G	195	SER	2.6
1	E	230	LEU	2.5
1	E	217	TRP	2.5
1	G	274	TRP	2.5
2	D	45	LYS	2.5
1	E	18	GLU	2.5
2	F	14	PRO	2.5
2	H	87	MET	2.5
1	E	31	LYS	2.5
1	G	247	VAL	2.5
1	A	176	ASN	2.5
1	A	61	GLU	2.5
1	E	72	GLN	2.5
1	A	64	THR	2.5
1	E	225	THR	2.5
1	A	47	PRO	2.5
1	E	250	PRO	2.5
2	F	20	PRO	2.5
1	C	206	LEU	2.5
1	C	230	LEU	2.5
1	A	36	PHE	2.5
2	B	83	LYS	2.5
1	E	260	ARG	2.5
1	A	197	GLY	2.5
1	A	28	VAL	2.4
1	C	50	PRO	2.4
1	A	49	ALA	2.4
1	E	237	GLY	2.4
1	A	166	GLU	2.4
1	C	18	GLU	2.4
1	C	199	VAL	2.4
1	G	172	LEU	2.4
1	C	226	GLN	2.4
1	G	54	GLN	2.4
2	D	20	PRO	2.4
2	B	34	HIS	2.4
1	G	46	GLU	2.3
2	D	40	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	17	ASN	2.3
1	E	197	GLY	2.3
2	B	19	LYS	2.3
1	G	169	HIS	2.3
1	A	276	PRO	2.3
2	F	73	THR	2.3
1	E	254	GLU	2.3
1	C	220	ASN	2.3
1	G	220	ASN	2.3
1	E	221	GLY	2.3
1	E	239	GLY	2.3
2	F	39	MET	2.3
1	C	261	VAL	2.3
1	A	162	GLY	2.3
1	A	194	ARG	2.3
1	G	239	GLY	2.3
1	G	181	ARG	2.3
1	G	91	GLY	2.3
2	B	44	LYS	2.3
1	G	219	LEU	2.3
1	C	210	PRO	2.2
2	B	17	ASN	2.2
1	A	31	LYS	2.2
1	A	104	GLY	2.2
1	E	228	MET	2.2
1	G	53	GLU	2.2
1	A	2	PRO	2.2
1	E	1	GLY	2.2
1	A	19	GLU	2.2
1	A	170	ARG	2.2
1	G	167	TRP	2.2
2	F	42	ASN	2.2
1	C	15	PRO	2.2
1	E	241	PHE	2.2
2	B	16	GLU	2.2
1	A	191	HIS	2.2
2	H	40	LEU	2.2
1	A	253	LYS	2.2
1	G	227	ASP	2.2
1	G	250	PRO	2.1
2	D	70	PHE	2.1
2	H	81	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	88	SER	2.1
1	A	159	TYR	2.1
1	C	41	GLU	2.1
2	D	16	GLU	2.1
2	D	69	GLU	2.1
2	B	71	THR	2.1
2	D	14	PRO	2.1
2	D	15	PRO	2.1
2	D	22	ILE	2.1
2	F	22	ILE	2.1
1	G	252	GLY	2.1
2	H	49	VAL	2.1
2	F	88	ALA	2.1
1	G	109	LEU	2.1
2	H	51	MET	2.1
1	C	194	ARG	2.1
1	C	197	GLY	2.1
1	G	230	LEU	2.1
1	A	250	PRO	2.1
1	G	44	ARG	2.1
2	D	13	HIS	2.1
2	D	73	THR	2.1
1	A	76	VAL	2.1
1	A	32	GLU	2.0
1	A	163	GLU	2.0
2	H	16	GLU	2.0
2	B	53	ASP	2.0
1	E	79	ARG	2.0
1	G	79	ARG	2.0
1	G	273	ARG	2.0
1	A	68	LYS	2.0
2	D	44	LYS	2.0
1	G	56	GLY	2.0
2	F	46	ILE	2.0
1	E	220	ASN	2.0
1	C	270	LEU	2.0
2	H	38	GLN	2.0
2	F	81	ARG	2.0
1	A	15	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	A	341	6/6	0.72	0.17	51,60,64,65	0
4	SO4	F	100	5/5	0.73	0.12	68,70,84,91	0
5	GOL	B	100	6/6	0.77	0.17	58,65,75,78	0
5	GOL	E	341	6/6	0.81	0.11	46,49,54,73	0
5	GOL	H	101	6/6	0.81	0.14	48,58,59,66	0
4	SO4	C	339	5/5	0.86	0.13	56,61,74,80	0
5	GOL	H	100	6/6	0.88	0.16	50,53,60,65	0
4	SO4	E	339	5/5	0.88	0.11	66,70,76,84	0
5	GOL	A	340	6/6	0.91	0.13	41,54,66,71	0
4	SO4	A	339	5/5	0.91	0.10	50,70,79,88	0
5	GOL	E	340	6/6	0.92	0.12	35,50,56,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.