



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:03 PM UTC

PDB ID : 1KTL / pdb_00001ktl
Title : The human non-classical major histocompatibility complex molecule HLA-E
Authors : Holmes, M.A.; Strong, R.K.
Deposited on : 2002-01-16
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

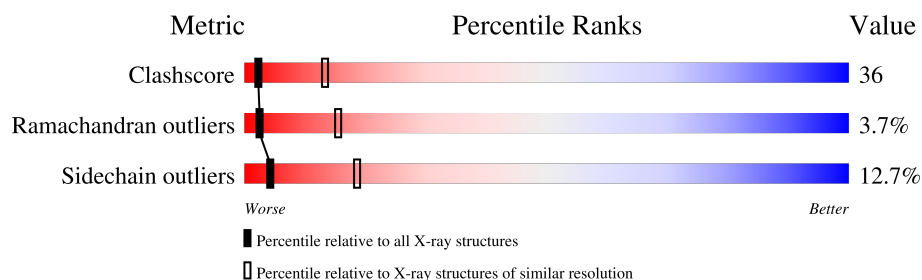
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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))
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	274	38% 42% 16% .
1	C	274	42% 39% 16% .
2	B	100	45% 42% 11% .
2	D	100	35% 50% 14% .
3	P	9	33% 44% 11% 11%
3	Q	9	33% 11% 44% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6211 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 HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2200	1376	389	428	7			
1	C	274	Total	C	N	O	S	0	0	0
			2212	1383	394	428	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	GLY	ARG	engineered mutation	UNP P13747
A	256	ALA	ARG	conflict	UNP P13747
C	107	GLY	ARG	engineered mutation	UNP P13747
C	256	ALA	ARG	conflict	UNP P13747

- Molecule 2 is a protein called BETA-2-MICROGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			828	526	139	159	4			
2	D	100	Total	C	N	O	S	0	0	0
			828	526	139	159	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	cloning artifact	UNP P01884
D	1	MET	-	cloning artifact	UNP P01884

- Molecule 3 is a protein called Peptide VTAPRTLTL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	9	Total	C	N	O	0	0	0
			69	45	12	12			
3	Q	9	Total	C	N	O	0	0	0
			69	45	12	12			

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



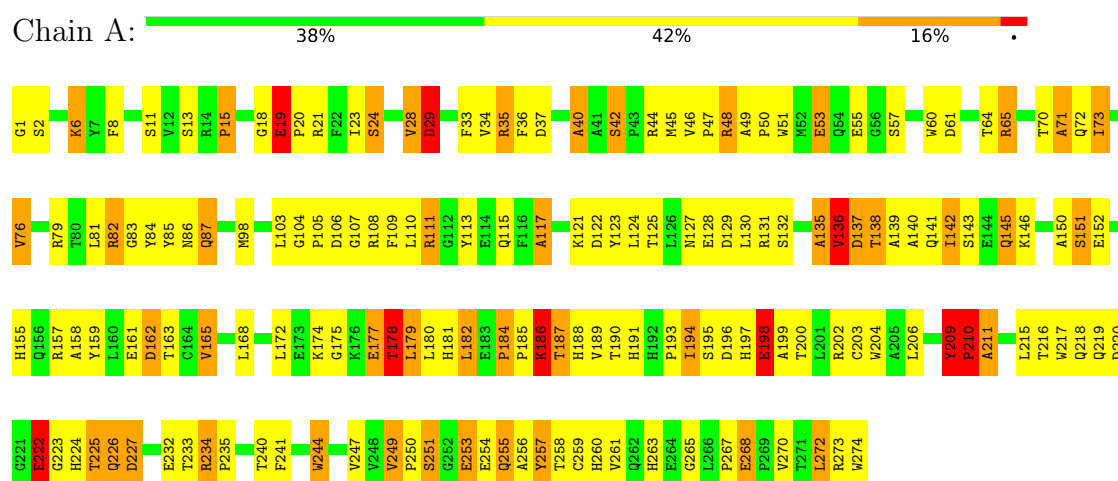
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

3 Residue-property plots

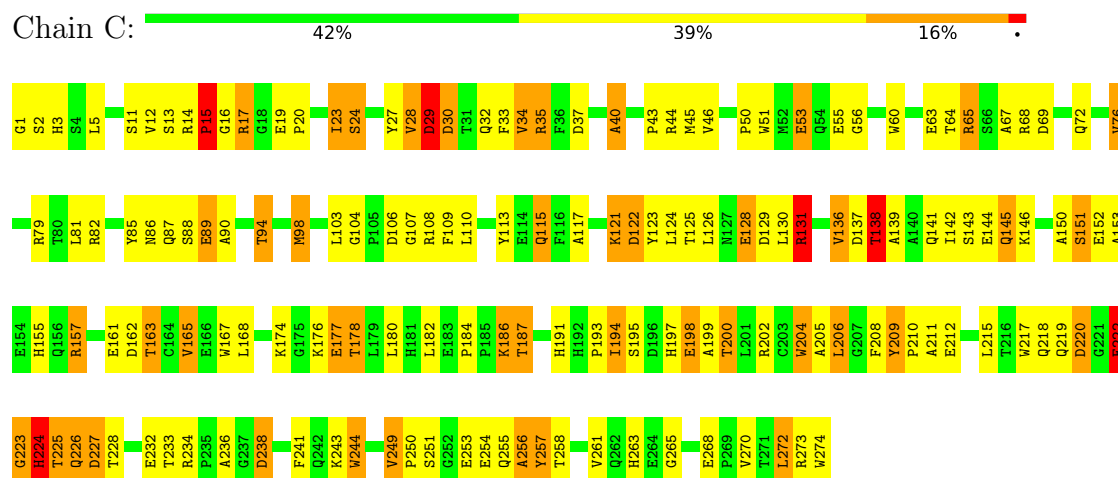
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, ALPHA CHAIN

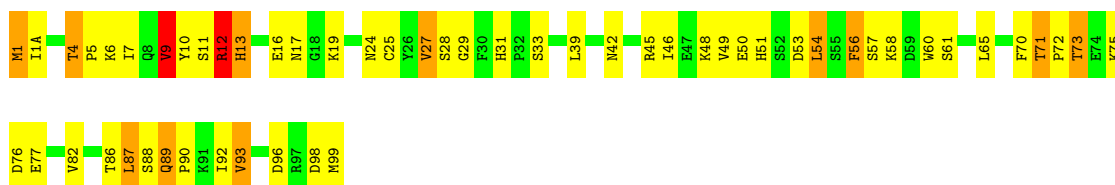


• Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, ALPHA CHAIN



• Molecule 2: BETA-2-MICROGLOBULIN





• Molecule 2: BETA-2-MICROGLOBULIN

Chain D: 35% 50% 14%



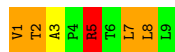
• Molecule 3: Peptide VTAPRTLTL

Chain P: 33% 44% 11% 11%



• Molecule 3: Peptide VTAPRTLTL

Chain Q: 33% 11% 44% 11%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	178.40 Å 178.40 Å 87.30 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (25.00-3.10)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.238 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6211	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	1.61	24/2265 (1.1%)	1.66	52/3082 (1.7%)
1	C	1.48	18/2278 (0.8%)	1.64	46/3099 (1.5%)
2	B	1.65	10/851 (1.2%)	1.55	15/1152 (1.3%)
2	D	1.42	4/851 (0.5%)	1.56	12/1152 (1.0%)
3	P	2.55	6/69 (8.7%)	2.87	8/93 (8.6%)
3	Q	1.78	1/69 (1.4%)	2.13	3/93 (3.2%)
All	All	1.56	63/6383 (1.0%)	1.65	136/8671 (1.6%)

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	2
1	C	0	3
3	P	0	1
3	Q	0	1
All	All	0	7

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	MET	SD-CE	12.42	2.10	1.79
1	A	225	THR	CA-CB	11.06	1.70	1.53
2	D	10	TYR	C-O	-10.07	1.11	1.23
1	A	42	SER	CA-C	8.69	1.61	1.52
2	D	1	MET	SD-CE	8.14	2.00	1.79
1	C	225	THR	C-O	8.10	1.33	1.23
3	P	5	ARG	CZ-NH1	-8.01	1.21	1.32
2	B	9	VAL	CA-CB	-7.92	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1	GLY	C-O	7.72	1.39	1.23
1	A	227	ASP	CA-C	-7.63	1.45	1.53
3	P	5	ARG	NE-CZ	-7.36	1.25	1.33
3	P	2	THR	CB-CG2	-7.25	1.28	1.52
1	A	142	ILE	CA-CB	-7.18	1.45	1.54
1	C	131	ARG	CZ-NH2	7.10	1.42	1.33
1	A	124	LEU	CA-C	-6.96	1.44	1.52
1	A	21	ARG	CZ-NH1	6.90	1.42	1.32
3	P	5	ARG	CG-CD	6.90	1.73	1.52
2	B	46	ILE	CA-CB	-6.84	1.46	1.54
2	B	27	VAL	CA-CB	-6.54	1.46	1.54
1	A	209	TYR	N-CA	6.45	1.52	1.46
2	B	12	ARG	CZ-NH2	-6.40	1.25	1.33
1	C	23	ILE	CA-CB	-6.29	1.45	1.55
2	B	7	ILE	C-O	-6.16	1.17	1.24
3	Q	5	ARG	NE-CZ	-6.06	1.26	1.33
1	A	222	GLU	CA-C	6.05	1.60	1.52
1	C	2	SER	N-CA	6.04	1.53	1.46
1	C	98	MET	CG-SD	6.03	1.95	1.80
1	A	136	VAL	CA-CB	-5.99	1.46	1.54
1	A	165	VAL	CA-CB	5.97	1.61	1.54
1	A	117	ALA	CA-CB	-5.93	1.43	1.53
1	C	138	THR	CA-C	5.82	1.60	1.52
1	A	24	SER	CA-C	5.75	1.59	1.52
1	C	122	ASP	CA-C	-5.67	1.45	1.52
1	A	139	ALA	CA-CB	-5.67	1.44	1.53
1	A	61	ASP	C-O	5.61	1.30	1.24
1	A	46	VAL	CA-CB	-5.59	1.50	1.55
1	C	184	PRO	CA-C	-5.57	1.47	1.52
1	C	28	VAL	CA-CB	-5.56	1.47	1.54
1	A	240	THR	CA-CB	-5.53	1.44	1.53
1	A	71	ALA	CA-CB	-5.46	1.44	1.53
1	C	34	VAL	CA-C	-5.46	1.47	1.52
1	C	1	GLY	N-CA	5.42	1.54	1.45
1	C	157	ARG	CG-CD	-5.38	1.36	1.52
3	P	2	THR	CA-CB	5.37	1.61	1.53
1	C	29	ASP	C-O	-5.33	1.17	1.24
1	A	209	TYR	CA-CB	-5.33	1.46	1.54
1	C	157	ARG	CZ-NH2	5.33	1.40	1.33
1	C	76	VAL	CA-C	-5.30	1.46	1.52
1	A	227	ASP	N-CA	-5.29	1.39	1.46
1	A	23	ILE	C-O	-5.27	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	56	PHE	C-O	-5.27	1.17	1.23
1	A	211	ALA	CA-CB	-5.24	1.44	1.53
1	A	23	ILE	CA-C	-5.18	1.46	1.52
2	D	36	GLU	CA-CB	-5.17	1.46	1.53
1	A	117	ALA	CA-C	-5.17	1.46	1.52
2	D	20	SER	CA-C	5.17	1.59	1.52
2	B	31	HIS	C-O	-5.16	1.18	1.24
2	B	12	ARG	CZ-NH1	-5.12	1.25	1.32
1	C	29	ASP	CA-C	-5.12	1.46	1.52
2	B	54	LEU	C-O	-5.11	1.17	1.23
3	P	1	VAL	C-O	-5.09	1.13	1.23
1	C	67	ALA	CA-CB	-5.05	1.45	1.53
1	A	233	THR	C-O	-5.01	1.18	1.23

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	VAL	N-CA-CB	-12.98	102.87	111.83
1	C	76	VAL	N-CA-C	-12.57	98.61	110.42
1	A	28	VAL	N-CA-C	-11.82	90.66	107.80
1	C	157	ARG	CG-CD-NE	11.38	137.03	112.00
1	C	249	VAL	N-CA-CB	-11.00	104.24	111.83
1	A	256	ALA	N-CA-C	-10.82	99.34	112.54
3	P	2	THR	N-CA-C	-10.76	97.18	110.41
1	A	76	VAL	N-CA-C	-10.72	100.34	110.42
1	C	256	ALA	N-CA-C	-10.38	100.63	113.18
1	C	28	VAL	N-CA-C	-10.21	93.00	107.80
3	P	5	ARG	NE-CZ-NH1	-10.01	111.49	121.50
3	P	5	ARG	CG-CD-NE	-9.80	90.44	112.00
1	C	186	LYS	N-CA-C	-8.82	95.73	109.76
1	C	184	PRO	CA-C-N	8.78	129.12	119.90
1	C	184	PRO	C-N-CA	8.78	129.12	119.90
2	B	33	SER	N-CA-C	8.60	123.42	113.19
1	A	179	LEU	N-CA-C	8.41	120.44	111.28
1	C	227	ASP	CA-C-N	-8.23	111.36	122.72
1	C	227	ASP	C-N-CA	-8.23	111.36	122.72
3	P	5	ARG	NE-CZ-NH2	8.18	126.56	119.20
1	A	139	ALA	N-CA-C	-7.82	102.84	111.36
1	C	107	GLY	N-CA-C	7.77	125.85	115.59
1	A	227	ASP	CA-C-N	-7.72	112.12	123.00
1	A	227	ASP	C-N-CA	-7.72	112.12	123.00
1	A	135	ALA	N-CA-C	-7.71	100.58	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	GLY	N-CA-C	7.64	125.48	115.47
1	C	146	LYS	N-CA-C	-7.50	103.10	111.28
1	A	223	GLY	N-CA-C	7.45	123.09	112.81
2	D	87	LEU	N-CA-C	7.45	121.17	107.99
1	C	30	ASP	N-CA-C	7.41	126.59	110.80
3	Q	5	ARG	CG-CD-NE	7.36	128.18	112.00
1	C	131	ARG	NE-CZ-NH2	7.32	125.78	119.20
1	A	257	TYR	N-CA-C	7.31	121.75	109.76
1	A	168	LEU	N-CA-C	-7.16	103.41	111.07
1	C	249	VAL	CA-C-N	7.04	128.09	120.13
1	C	249	VAL	C-N-CA	7.04	128.09	120.13
1	C	17	ARG	N-CA-C	6.98	125.67	110.80
1	A	186	LYS	N-CA-C	-6.95	99.99	110.28
1	A	197	HIS	N-CA-C	6.90	121.01	112.59
1	C	228	THR	N-CA-C	-6.82	98.13	109.24
1	C	89	GLU	N-CA-C	-6.74	104.93	113.02
2	D	13	HIS	CA-C-N	-6.73	112.82	119.76
2	D	13	HIS	C-N-CA	-6.73	112.82	119.76
2	D	89	GLN	CA-C-N	-6.70	112.88	119.78
2	D	89	GLN	C-N-CA	-6.70	112.88	119.78
1	C	204	TRP	N-CA-C	6.64	120.06	109.24
1	A	162	ASP	CA-C-O	6.53	124.32	119.68
1	C	143	SER	N-CA-C	-6.53	104.16	111.28
1	C	208	PHE	N-CA-C	6.46	120.08	110.52
1	C	223	GLY	N-CA-C	6.43	123.25	113.02
1	A	157	ARG	CG-CD-NE	-6.41	97.90	112.00
1	A	196	ASP	N-CA-C	-6.38	104.42	111.82
1	A	111	ARG	NE-CZ-NH1	-6.38	115.12	121.50
2	B	9	VAL	CA-C-N	-6.35	109.42	121.54
2	B	9	VAL	C-N-CA	-6.35	109.42	121.54
1	A	6	LYS	N-CA-C	6.34	119.83	109.06
1	C	131	ARG	CG-CD-NE	-6.20	98.37	112.00
1	C	168	LEU	N-CA-C	-6.19	104.44	111.07
1	A	46	VAL	N-CA-C	6.18	114.70	107.84
2	D	58	LYS	N-CA-C	6.18	118.82	111.71
2	B	89	GLN	CA-C-N	-6.16	113.60	119.89
2	B	89	GLN	C-N-CA	-6.16	113.60	119.89
2	B	13	HIS	CA-C-N	-6.12	113.46	119.76
2	B	13	HIS	C-N-CA	-6.12	113.46	119.76
3	Q	2	THR	N-CA-C	-6.10	102.90	110.41
1	A	253	GLU	N-CA-C	6.07	120.42	113.19
1	C	257	TYR	N-CA-C	6.06	119.34	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	LEU	CA-CB-CG	-6.03	95.21	116.30
1	A	184	PRO	CA-C-N	6.02	127.63	120.23
1	A	184	PRO	C-N-CA	6.02	127.63	120.23
1	A	137	ASP	CA-C-N	-5.96	111.17	121.66
1	A	137	ASP	C-N-CA	-5.96	111.17	121.66
1	C	131	ARG	NH1-CZ-NH2	-5.94	111.58	119.30
2	D	12	ARG	NE-CZ-NH2	5.91	124.52	119.20
1	C	253	GLU	N-CA-C	5.82	120.24	113.20
1	C	115	GLN	N-CA-C	5.79	118.20	109.23
1	C	142	ILE	CB-CA-C	-5.74	104.29	112.22
1	C	27	TYR	N-CA-C	5.74	118.81	109.06
3	Q	8	LEU	N-CA-C	-5.73	99.85	108.96
1	C	5	LEU	N-CA-C	-5.69	99.14	108.41
2	B	92	ILE	CA-C-N	-5.69	115.69	123.14
2	B	92	ILE	C-N-CA	-5.69	115.69	123.14
1	A	198	GLU	N-CA-C	5.68	117.04	108.46
1	A	185	PRO	N-CA-C	5.66	119.39	110.50
1	C	144	GLU	N-CA-C	5.65	117.11	111.07
1	C	79	ARG	N-CA-C	-5.63	104.78	111.03
2	B	28	SER	N-CA-C	5.62	117.33	108.96
2	B	70	PHE	N-CA-C	5.62	115.96	108.38
1	A	267	PRO	N-CA-C	-5.59	105.42	113.75
3	P	5	ARG	NH1-CZ-NH2	-5.58	112.04	119.30
1	C	56	GLY	N-CA-C	5.58	120.18	112.37
2	D	67	TYR	N-CA-C	5.56	117.29	108.79
1	A	223	GLY	O-C-N	5.55	129.05	123.11
1	A	249	VAL	CA-C-N	5.54	126.38	120.13
1	A	249	VAL	C-N-CA	5.54	126.38	120.13
1	A	49	ALA	CA-C-N	-5.53	112.92	119.84
1	A	49	ALA	C-N-CA	-5.53	112.92	119.84
2	D	25	CYS	CA-CB-SG	-5.47	101.83	114.40
1	C	3	HIS	N-CA-C	5.45	117.68	109.23
2	B	11	SER	N-CA-CB	-5.37	102.19	110.56
1	A	223	GLY	CA-C-N	5.37	131.79	121.54
1	A	223	GLY	C-N-CA	5.37	131.79	121.54
1	A	260	HIS	CA-C-N	-5.36	115.97	123.10
1	A	260	HIS	C-N-CA	-5.36	115.97	123.10
2	B	87	LEU	N-CA-C	5.35	117.14	108.41
1	C	142	ILE	N-CA-C	-5.34	105.32	110.72
2	D	45	ARG	NE-CZ-NH1	-5.33	116.17	121.50
1	A	82	ARG	N-CA-C	-5.32	105.59	111.71
1	A	234	ARG	N-CA-C	5.31	118.52	109.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	34	ASP	CA-C-N	-5.31	113.91	122.25
2	D	34	ASP	C-N-CA	-5.31	113.91	122.25
1	A	87	GLN	N-CA-C	5.27	118.00	109.40
1	A	162	ASP	CB-CA-C	-5.26	105.00	114.52
1	A	222	GLU	CA-C-N	-5.24	117.24	122.69
1	A	222	GLU	C-N-CA	-5.24	117.24	122.69
1	C	238	ASP	CA-C-N	-5.22	117.23	123.08
1	C	238	ASP	C-N-CA	-5.22	117.23	123.08
1	C	157	ARG	NH1-CZ-NH2	-5.21	112.53	119.30
1	C	139	ALA	N-CA-C	-5.19	105.71	111.36
1	A	24	SER	N-CA-CB	-5.17	102.34	110.77
1	A	225	THR	CA-C-N	5.17	131.41	121.54
1	A	225	THR	C-N-CA	5.17	131.41	121.54
1	A	19	GLU	N-CA-C	5.16	121.21	109.81
1	A	209	TYR	O-C-N	-5.11	117.85	121.83
2	B	82	VAL	N-CA-C	5.09	115.81	108.48
1	A	162	ASP	O-C-N	5.09	126.33	120.58
1	C	197	HIS	N-CA-C	5.08	119.44	112.88
1	C	126	LEU	N-CA-C	-5.08	101.69	109.76
2	B	33	SER	CA-CB-OG	-5.07	100.95	111.10
1	C	206	LEU	N-CA-C	5.07	117.50	109.50
3	P	2	THR	CA-CB-CG2	5.06	119.10	110.50
3	P	2	THR	CA-C-N	5.06	127.67	120.49
3	P	2	THR	C-N-CA	5.06	127.67	120.49
1	C	227	ASP	N-CA-C	5.03	118.18	107.67
1	A	143	SER	N-CA-C	-5.02	106.00	111.82
1	C	204	TRP	CB-CA-C	-5.01	101.49	109.75

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	209	TYR	Sidechain,Mainchain
1	C	113	TYR	Sidechain
1	C	131	ARG	Sidechain
1	C	209	TYR	Sidechain
3	P	5	ARG	Sidechain
3	Q	5	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	2200	0	2022	171	1
1	C	2212	0	2039	167	0
2	B	828	0	780	59	0
2	D	828	0	780	65	0
3	P	69	0	83	21	0
3	Q	69	0	83	19	0
4	A	5	0	0	1	0
All	All	6211	0	5787	431	1

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 36.

All (431) 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:B:1:MET:SD	2:B:1:MET:CE	2.10	1.39
1:A:115:GLN:HG2	1:A:125:THR:HG23	1.34	1.10
1:C:65:ARG:HH11	1:C:65:ARG:CB	1.69	1.06
1:A:65:ARG:HH21	1:C:145:GLN:NE2	1.56	1.02
1:A:263:HIS:HD2	1:A:265:GLY:H	1.10	1.00
1:C:65:ARG:HH11	1:C:65:ARG:HB2	1.26	0.97
1:C:35:ARG:HH11	1:C:35:ARG:HG2	1.30	0.96
3:P:5:ARG:HE	3:Q:5:ARG:HH21	1.15	0.93
1:A:65:ARG:HH11	1:A:65:ARG:CB	1.81	0.92
2:D:98:ASP:O	2:D:99:MET:HG3	1.69	0.92
1:C:152:GLU:CB	3:Q:7:LEU:HD11	2.00	0.92
1:C:65:ARG:HB2	1:C:65:ARG:NH1	1.85	0.89
1:A:263:HIS:CD2	1:A:265:GLY:H	1.89	0.89
1:C:263:HIS:CD2	1:C:265:GLY:H	1.91	0.88
1:C:115:GLN:HG2	1:C:125:THR:HG23	1.54	0.87
1:C:155:HIS:CE1	3:P:5:ARG:NH2	2.43	0.86
1:A:103:LEU:HD21	1:A:165:VAL:HG23	1.57	0.86
1:C:263:HIS:HD2	1:C:265:GLY:H	1.24	0.85
1:C:204:TRP:HE3	1:C:206:LEU:HD21	1.43	0.83
2:D:9:VAL:CG2	2:D:93:VAL:CG2	2.57	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:42:ASN:HD21	2:D:77:GLU:H	1.27	0.82
2:B:73:THR:HG22	2:B:75:LYS:H	1.45	0.81
1:A:109:PHE:CE2	1:A:161:GLU:HG2	2.17	0.80
2:B:9:VAL:CG2	2:B:93:VAL:HG22	2.10	0.80
2:D:4:THR:HG22	2:D:5:PRO:HD2	1.63	0.80
1:A:65:ARG:HH11	1:A:65:ARG:HB3	1.45	0.80
1:A:152:GLU:CB	3:P:7:LEU:HD11	2.11	0.79
2:D:42:ASN:ND2	2:D:77:GLU:H	1.81	0.79
1:C:193:PRO:HA	1:C:199:ALA:HA	1.63	0.79
1:C:35:ARG:HH11	1:C:35:ARG:CG	1.96	0.79
2:B:73:THR:HG22	2:B:75:LYS:N	1.98	0.79
1:A:50:PRO:HA	1:A:53:GLU:OE2	1.83	0.78
2:B:42:ASN:HD21	2:B:77:GLU:H	1.31	0.78
2:B:42:ASN:ND2	2:B:77:GLU:H	1.81	0.78
1:A:202:ARG:HG3	1:A:202:ARG:HH11	1.48	0.78
2:D:9:VAL:HG23	2:D:93:VAL:CG2	2.16	0.76
1:C:65:ARG:HH11	1:C:65:ARG:HB3	1.51	0.76
1:A:129:ASP:OD2	1:A:131:ARG:HG3	1.86	0.75
1:A:98:MET:HE2	2:B:60:TRP:CH2	2.21	0.75
1:A:65:ARG:HB2	1:A:65:ARG:NH1	2.00	0.75
1:C:109:PHE:CE2	1:C:161:GLU:HG2	2.22	0.75
1:C:138:THR:HA	1:C:141:GLN:HE21	1.52	0.74
1:C:152:GLU:CG	3:Q:7:LEU:HD13	2.18	0.74
1:C:44:ARG:HA	1:C:64:THR:HG23	1.69	0.74
1:A:79:ARG:HH11	1:C:72:GLN:NE2	1.84	0.74
1:C:117:ALA:HB2	2:D:60:TRP:CE2	2.23	0.74
1:A:204:TRP:HE3	1:A:206:LEU:HD21	1.51	0.73
2:D:29:GLY:HA2	2:D:61:SER:OG	1.89	0.73
1:C:152:GLU:CD	3:Q:7:LEU:HD13	2.14	0.73
1:C:152:GLU:HB2	3:Q:7:LEU:HD11	1.70	0.73
2:D:73:THR:HG22	2:D:75:LYS:H	1.54	0.73
2:B:49:VAL:HG12	2:B:50:GLU:N	2.04	0.72
1:A:145:GLN:HG3	1:A:146:LYS:N	2.05	0.72
1:C:152:GLU:CB	3:Q:7:LEU:CD1	2.68	0.71
1:A:65:ARG:HH21	1:C:145:GLN:HE22	1.38	0.71
2:D:42:ASN:HD22	2:D:77:GLU:HB2	1.56	0.71
1:A:255:GLN:CD	1:A:255:GLN:N	2.48	0.71
2:D:73:THR:HG22	2:D:75:LYS:N	2.06	0.71
3:P:5:ARG:HE	3:Q:5:ARG:NH2	1.87	0.70
1:A:65:ARG:CB	1:A:65:ARG:NH1	2.54	0.70
1:A:65:ARG:HH21	1:C:145:GLN:HE21	1.38	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:MET:HE2	2:B:60:TRP:CZ2	2.25	0.70
2:B:9:VAL:CG2	2:B:93:VAL:CG2	2.70	0.70
1:A:65:ARG:NH2	1:C:145:GLN:NE2	2.36	0.69
1:C:33:PHE:CD2	1:C:34:VAL:HG13	2.27	0.69
1:A:65:ARG:HH11	1:A:65:ARG:HB2	1.53	0.69
1:A:79:ARG:NH1	1:C:72:GLN:NE2	2.41	0.69
1:A:121:LYS:HG3	1:A:122:ASP:N	2.08	0.69
2:B:4:THR:HG23	2:B:86:THR:OG1	1.92	0.68
1:C:152:GLU:CG	3:Q:7:LEU:CD1	2.71	0.68
1:C:28:VAL:O	1:C:29:ASP:O	2.10	0.68
1:A:55:GLU:HA	1:A:55:GLU:OE1	1.92	0.68
1:A:152:GLU:HB2	3:P:7:LEU:HD11	1.75	0.68
1:A:79:ARG:NH2	4:A:275:SO4:O2	2.25	0.68
1:A:195:SER:OG	1:A:198:GLU:HG3	1.94	0.68
1:A:152:GLU:CB	3:P:7:LEU:CD1	2.71	0.67
1:C:193:PRO:HA	1:C:199:ALA:CB	2.25	0.67
1:C:204:TRP:CE3	1:C:206:LEU:HD21	2.29	0.67
1:C:50:PRO:HA	1:C:53:GLU:OE2	1.94	0.66
3:P:5:ARG:NE	3:Q:5:ARG:HH21	1.90	0.66
1:C:193:PRO:HA	1:C:199:ALA:CA	2.25	0.66
2:B:9:VAL:HG21	2:B:93:VAL:HG22	1.77	0.66
2:D:4:THR:CG2	2:D:5:PRO:HD2	2.26	0.66
2:D:96:ASP:O	2:D:98:ASP:N	2.29	0.65
1:C:35:ARG:NH1	1:C:46:VAL:HG21	2.11	0.65
1:A:225:THR:C	1:A:227:ASP:H	2.05	0.65
1:A:255:GLN:H	1:A:255:GLN:NE2	1.94	0.65
2:D:39:LEU:HB3	2:D:46:ILE:HD12	1.78	0.65
1:A:187:THR:HB	1:A:272:LEU:HD11	1.78	0.65
1:A:48:ARG:NH1	2:B:53:ASP:OD2	2.30	0.65
1:A:79:ARG:HD2	1:C:72:GLN:NE2	2.12	0.65
1:C:249:VAL:HG22	1:C:257:TYR:CE1	2.32	0.64
1:A:51:TRP:HB2	1:A:174:LYS:O	1.97	0.64
1:A:193:PRO:HA	1:A:199:ALA:HA	1.79	0.64
1:A:8:PHE:HB3	2:B:56:PHE:CE2	2.33	0.64
1:A:109:PHE:CD1	1:A:110:LEU:N	2.66	0.64
1:A:194:ILE:HD12	1:A:194:ILE:N	2.13	0.64
2:D:42:ASN:ND2	2:D:77:GLU:HB2	2.14	0.63
2:B:73:THR:CG2	2:B:75:LYS:H	2.11	0.63
1:A:81:LEU:HD21	1:A:123:TYR:CZ	2.34	0.63
1:A:145:GLN:HG3	1:A:146:LYS:H	1.60	0.63
1:A:182:LEU:HD23	1:A:210:PRO:HD3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:VAL:HG22	1:A:257:TYR:CE1	2.34	0.63
2:B:42:ASN:HD22	2:B:77:GLU:HB2	1.64	0.63
1:A:172:LEU:HD23	1:A:179:LEU:HD23	1.81	0.62
1:A:138:THR:HA	1:A:141:GLN:HG3	1.80	0.62
1:A:225:THR:O	1:A:227:ASP:N	2.31	0.62
2:D:9:VAL:CG2	2:D:93:VAL:HG23	2.27	0.62
2:B:49:VAL:CG1	2:B:50:GLU:N	2.63	0.62
1:A:193:PRO:HA	1:A:199:ALA:CB	2.29	0.62
2:B:4:THR:HG22	2:B:5:PRO:HD2	1.80	0.62
1:C:152:GLU:HB3	3:Q:7:LEU:HD11	1.80	0.62
1:C:215:LEU:CD2	1:C:261:VAL:HG22	2.30	0.62
2:D:9:VAL:CG2	2:D:93:VAL:HG22	2.28	0.62
1:C:202:ARG:NH2	2:D:99:MET:HE3	2.15	0.61
1:C:194:ILE:HD12	1:C:194:ILE:N	2.14	0.61
2:D:73:THR:CG2	2:D:75:LYS:H	2.11	0.61
1:A:72:GLN:HE21	1:C:76:VAL:HG13	1.64	0.61
1:A:187:THR:O	1:A:188:HIS:HB3	2.00	0.61
1:A:152:GLU:CG	3:P:7:LEU:HD13	2.30	0.61
1:C:137:ASP:O	1:C:141:GLN:HG3	2.01	0.61
2:D:16:GLU:HB3	2:D:19:LYS:CB	2.31	0.61
1:C:155:HIS:CE1	3:P:5:ARG:HH21	2.18	0.61
1:A:202:ARG:NH2	2:B:99:MET:HE3	2.16	0.61
1:C:212:GLU:HA	1:C:212:GLU:OE1	2.01	0.60
2:D:16:GLU:O	2:D:19:LYS:N	2.30	0.60
1:C:150:ALA:O	1:C:151:SER:CB	2.49	0.60
2:D:51:HIS:HA	2:D:65:LEU:O	2.01	0.60
1:C:162:ASP:O	1:C:163:THR:C	2.44	0.60
1:A:13:SER:HA	1:A:20:PRO:HB3	1.84	0.60
1:A:270:VAL:HG12	1:A:272:LEU:CD2	2.31	0.60
1:C:82:ARG:HE	1:C:89:GLU:HB2	1.66	0.60
1:C:98:MET:HE3	1:C:115:GLN:OE1	2.02	0.60
1:C:152:GLU:HG3	3:Q:7:LEU:CD1	2.32	0.60
1:C:155:HIS:CE1	3:P:5:ARG:HH22	2.19	0.60
1:C:81:LEU:HD21	1:C:123:TYR:CZ	2.36	0.59
2:B:98:ASP:C	2:B:99:MET:HG3	2.25	0.59
1:C:32:GLN:NE2	2:D:53:ASP:OD2	2.35	0.59
1:C:234:ARG:NH1	2:D:8:GLN:OE1	2.34	0.59
1:C:209:TYR:HA	1:C:210:PRO:O	2.03	0.59
1:C:35:ARG:HD3	2:D:53:ASP:CG	2.28	0.59
1:A:73:ILE:HD11	3:Q:8:LEU:HD22	1.84	0.59
1:C:255:GLN:H	1:C:255:GLN:NE2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLU:CD	1:A:174:LYS:NZ	2.60	0.58
1:A:152:GLU:HB3	3:P:7:LEU:HD11	1.85	0.58
1:C:51:TRP:HB2	1:C:174:LYS:O	2.03	0.58
1:C:98:MET:CE	1:C:115:GLN:OE1	2.51	0.58
1:A:250:PRO:HG2	1:A:253:GLU:OE2	2.03	0.58
1:C:65:ARG:CB	1:C:65:ARG:NH1	2.47	0.58
1:A:263:HIS:HD2	1:A:265:GLY:N	1.92	0.58
2:B:9:VAL:HG23	2:B:93:VAL:CG2	2.33	0.58
2:B:42:ASN:ND2	2:B:77:GLU:HB2	2.18	0.58
1:A:35:ARG:HG2	1:A:35:ARG:HH11	1.68	0.58
1:A:202:ARG:HG3	1:A:202:ARG:NH1	2.15	0.58
1:C:109:PHE:CD1	1:C:110:LEU:N	2.71	0.58
3:P:5:ARG:HH11	3:Q:5:ARG:HH21	1.52	0.58
1:A:79:ARG:HH11	1:C:72:GLN:HE21	1.52	0.57
1:A:194:ILE:HD11	1:A:200:THR:OG1	2.04	0.57
1:A:155:HIS:CE1	3:P:5:ARG:NH2	2.72	0.57
1:A:225:THR:C	1:A:227:ASP:N	2.62	0.57
1:C:89:GLU:O	1:C:89:GLU:HG2	2.04	0.57
1:C:234:ARG:HG3	2:D:10:TYR:CZ	2.39	0.57
1:A:249:VAL:HG22	1:A:257:TYR:CZ	2.39	0.57
1:C:211:ALA:HB2	1:C:241:PHE:CE1	2.40	0.57
2:D:25:CYS:HB2	2:D:39:LEU:HD21	1.87	0.57
2:D:73:THR:HG22	2:D:76:ASP:H	1.70	0.57
1:C:55:GLU:CD	1:C:174:LYS:NZ	2.63	0.57
1:A:6:LYS:HD2	1:A:113:TYR:OH	2.05	0.56
1:A:152:GLU:HB3	3:P:7:LEU:CD1	2.35	0.56
1:C:35:ARG:HG2	1:C:35:ARG:NH1	2.10	0.56
1:C:43:PRO:O	1:C:68:ARG:NH2	2.39	0.56
1:C:236:ALA:O	2:D:12:ARG:HD3	2.05	0.56
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.87	0.56
1:A:235:PRO:O	2:B:10:TYR:OH	2.19	0.56
1:A:109:PHE:CE2	1:A:161:GLU:HA	2.41	0.55
1:A:193:PRO:HA	1:A:199:ALA:CA	2.36	0.55
1:A:227:ASP:O	1:A:247:VAL:HG23	2.06	0.55
2:B:51:HIS:HA	2:B:65:LEU:O	2.07	0.55
1:A:109:PHE:HD1	1:A:110:LEU:N	2.03	0.55
1:C:45:MET:O	1:C:60:TRP:CE3	2.60	0.55
1:C:12:VAL:HG22	1:C:94:THR:HG23	1.89	0.55
1:C:194:ILE:HD11	1:C:200:THR:OG1	2.06	0.55
2:D:49:VAL:HG12	2:D:50:GLU:N	2.21	0.55
1:A:150:ALA:O	1:A:151:SER:CB	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:GLU:HB3	3:Q:7:LEU:CD1	2.38	0.54
1:C:249:VAL:HG13	1:C:250:PRO:HD2	1.90	0.54
1:C:117:ALA:HB2	2:D:60:TRP:CD2	2.44	0.53
1:A:204:TRP:CE3	1:A:206:LEU:HD21	2.37	0.53
2:D:9:VAL:HG23	2:D:93:VAL:HG23	1.85	0.53
1:A:136:VAL:O	1:A:136:VAL:CG1	2.56	0.53
2:D:98:ASP:C	2:D:99:MET:HG3	2.32	0.53
1:C:254:GLU:HG2	1:C:274:TRP:CE3	2.44	0.53
1:C:225:THR:CG2	1:C:226:GLN:N	2.72	0.53
2:B:4:THR:CG2	2:B:5:PRO:HD2	2.38	0.53
1:C:223:GLY:O	1:C:224:HIS:O	2.27	0.53
2:D:39:LEU:CB	2:D:46:ILE:HD12	2.37	0.53
1:C:35:ARG:CG	1:C:35:ARG:NH1	2.67	0.52
1:A:255:GLN:CD	1:A:255:GLN:H	2.15	0.52
1:C:55:GLU:HA	1:C:55:GLU:OE1	2.09	0.52
3:Q:2:THR:HG22	3:Q:3:ALA:N	2.23	0.52
3:Q:5:ARG:HH11	3:Q:5:ARG:CG	2.23	0.52
1:A:33:PHE:CD2	1:A:34:VAL:HG13	2.44	0.52
1:A:189:VAL:HG12	1:A:190:THR:N	2.24	0.52
1:C:128:GLU:O	1:C:130:LEU:HG	2.09	0.52
1:A:152:GLU:CD	3:P:7:LEU:HD13	2.35	0.52
1:A:35:ARG:HG3	1:A:36:PHE:N	2.20	0.52
1:C:13:SER:HA	1:C:20:PRO:HB3	1.92	0.52
2:D:49:VAL:CG1	2:D:50:GLU:N	2.72	0.52
1:C:88:SER:OG	1:C:90:ALA:HB3	2.10	0.52
2:B:29:GLY:HA2	2:B:61:SER:OG	2.11	0.52
1:C:35:ARG:HH12	1:C:46:VAL:HG21	1.74	0.52
1:A:1:GLY:O	1:A:105:PRO:HA	2.10	0.51
2:B:10:TYR:O	2:B:24:ASN:HB2	2.10	0.51
2:B:45:ARG:O	2:B:45:ARG:HG3	2.10	0.51
1:C:103:LEU:HA	1:C:108:ARG:O	2.10	0.51
2:D:9:VAL:HG21	2:D:93:VAL:CG2	2.39	0.51
1:C:69:ASP:O	1:C:72:GLN:HB2	2.10	0.51
2:D:29:GLY:HA2	2:D:61:SER:CB	2.40	0.51
2:B:9:VAL:HG21	2:B:93:VAL:CG2	2.39	0.51
1:C:219:GLN:O	1:C:220:ASP:C	2.52	0.51
1:A:83:GLY:O	1:A:84:TYR:C	2.53	0.51
1:C:37:ASP:HB3	1:C:40:ALA:HB2	1.92	0.51
1:C:219:GLN:O	1:C:219:GLN:HG3	2.10	0.51
1:A:121:LYS:CG	1:A:122:ASP:N	2.74	0.51
1:A:152:GLU:CG	3:P:7:LEU:CD1	2.89	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:MET:HE2	2:D:60:TRP:CH2	2.45	0.51
1:A:35:ARG:HD3	2:B:53:ASP:OD2	2.11	0.51
1:C:103:LEU:HD21	1:C:165:VAL:HG23	1.93	0.50
1:C:152:GLU:OE1	3:P:5:ARG:NH1	2.44	0.50
3:Q:5:ARG:HH11	3:Q:5:ARG:HG2	1.76	0.50
2:B:4:THR:HG22	2:B:5:PRO:CD	2.42	0.50
1:C:28:VAL:O	1:C:29:ASP:C	2.55	0.50
1:C:82:ARG:NE	1:C:89:GLU:HB2	2.26	0.50
2:D:16:GLU:O	2:D:17:ASN:C	2.55	0.50
1:A:203:CYS:HB2	1:A:217:TRP:CZ2	2.46	0.50
2:D:9:VAL:HA	2:D:24:ASN:O	2.12	0.50
1:C:176:LYS:C	1:C:178:THR:H	2.19	0.50
1:A:109:PHE:HE1	1:A:111:ARG:CA	2.25	0.50
1:C:176:LYS:O	1:C:178:THR:N	2.41	0.50
1:A:28:VAL:O	1:A:29:ASP:C	2.54	0.49
1:C:209:TYR:HA	1:C:210:PRO:C	2.36	0.49
1:A:135:ALA:HB1	1:A:140:ALA:CB	2.42	0.49
1:A:218:GLN:HB2	1:A:222:GLU:O	2.12	0.49
1:C:122:ASP:O	1:C:136:VAL:HG11	2.12	0.49
1:C:129:ASP:OD2	1:C:131:ARG:HB2	2.12	0.49
2:D:9:VAL:HG21	2:D:93:VAL:HG23	1.95	0.49
1:A:210:PRO:O	1:A:263:HIS:HE1	1.95	0.49
1:C:263:HIS:HD2	1:C:265:GLY:N	2.02	0.49
1:C:82:ARG:CG	1:C:87:GLN:O	2.61	0.49
1:C:109:PHE:CD1	1:C:109:PHE:C	2.90	0.49
2:B:39:LEU:HD23	2:B:39:LEU:HA	1.60	0.48
1:C:194:ILE:H	1:C:199:ALA:HA	1.77	0.48
1:A:184:PRO:HB3	1:A:265:GLY:O	2.13	0.48
1:C:194:ILE:HD13	1:C:199:ALA:C	2.38	0.48
3:P:5:ARG:HH11	3:Q:5:ARG:NH2	2.10	0.48
1:A:85:TYR:O	1:A:86:ASN:C	2.56	0.48
1:C:217:TRP:O	1:C:224:HIS:HA	2.13	0.48
1:C:219:GLN:HB3	1:C:257:TYR:CE2	2.49	0.48
1:A:175:GLY:O	1:A:179:LEU:HB2	2.14	0.48
1:A:109:PHE:CD2	1:A:161:GLU:HA	2.49	0.47
1:A:215:LEU:CD2	1:A:261:VAL:HG22	2.44	0.47
2:B:73:THR:HB	2:B:76:ASP:HB2	1.96	0.47
1:C:234:ARG:HG3	2:D:10:TYR:OH	2.14	0.47
1:A:35:ARG:HG2	1:A:35:ARG:NH1	2.27	0.47
1:A:186:LYS:HD3	1:A:186:LYS:N	2.28	0.47
1:A:129:ASP:OD2	1:A:131:ARG:CG	2.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:MET:O	1:C:60:TRP:HE3	1.97	0.47
1:A:104:GLY:C	1:A:106:ASP:N	2.71	0.47
1:A:109:PHE:CD1	1:A:109:PHE:C	2.93	0.47
1:C:157:ARG:HH21	1:C:157:ARG:HB3	1.79	0.47
1:C:236:ALA:HB3	1:C:238:ASP:OD1	2.15	0.47
2:D:79:ALA:HB2	2:D:94:LYS:HA	1.97	0.47
1:C:270:VAL:HG12	1:C:272:LEU:CD2	2.45	0.47
2:D:9:VAL:HG21	2:D:93:VAL:O	2.15	0.47
2:D:51:HIS:HB3	2:D:66:TYR:CD2	2.49	0.47
1:C:191:HIS:ND1	1:C:274:TRP:CH2	2.72	0.47
1:A:155:HIS:CE1	1:C:155:HIS:CE1	3.03	0.47
2:B:16:GLU:HG2	2:B:19:LYS:CB	2.45	0.47
1:C:202:ARG:HG3	1:C:202:ARG:HH11	1.80	0.47
1:C:244:TRP:C	1:C:244:TRP:HE3	2.23	0.47
2:D:39:LEU:C	2:D:46:ILE:HD12	2.39	0.47
1:C:44:ARG:HA	1:C:64:THR:CG2	2.41	0.47
1:C:194:ILE:N	1:C:194:ILE:CD1	2.77	0.47
1:A:82:ARG:HG3	1:A:87:GLN:HB2	1.98	0.46
1:A:127:ASN:HB2	1:A:132:SER:OG	2.14	0.46
2:B:16:GLU:O	2:B:17:ASN:C	2.58	0.46
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.97	0.46
1:C:109:PHE:CE2	1:C:161:GLU:HA	2.50	0.46
1:C:249:VAL:CG2	1:C:257:TYR:CE1	2.99	0.46
1:C:35:ARG:NH1	1:C:46:VAL:CG2	2.78	0.46
1:A:227:ASP:O	1:A:227:ASP:OD1	2.33	0.46
1:C:121:LYS:HG3	1:C:122:ASP:N	2.31	0.46
2:D:4:THR:HG22	2:D:5:PRO:CD	2.39	0.46
2:D:36:GLU:O	2:D:82:VAL:HA	2.16	0.46
1:A:103:LEU:CD2	1:A:165:VAL:HG23	2.38	0.46
1:C:180:LEU:HD23	1:C:180:LEU:HA	1.67	0.46
1:C:195:SER:OG	1:C:198:GLU:HG3	2.15	0.46
2:B:96:ASP:OD1	2:B:98:ASP:HB2	2.16	0.46
1:C:124:LEU:HD12	1:C:124:LEU:HA	1.73	0.46
1:A:145:GLN:CD	1:C:65:ARG:HH21	2.23	0.45
1:A:255:GLN:C	1:A:257:TYR:N	2.72	0.45
1:C:205:ALA:O	1:C:206:LEU:HD23	2.17	0.45
2:D:40:LEU:HD11	2:D:81:ARG:HB2	1.98	0.45
1:A:211:ALA:HB2	1:A:241:PHE:CE1	2.52	0.45
2:D:16:GLU:HG2	2:D:19:LYS:CB	2.47	0.45
1:A:98:MET:HE3	1:A:115:GLN:OE1	2.17	0.45
1:A:234:ARG:HG3	2:B:10:TYR:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:SER:O	1:A:44:ARG:N	2.44	0.45
1:A:109:PHE:HE1	1:A:111:ARG:HA	1.82	0.45
1:A:211:ALA:HB2	1:A:241:PHE:CD1	2.52	0.45
2:B:73:THR:CG2	2:B:76:ASP:H	2.30	0.45
1:A:135:ALA:HB1	1:A:140:ALA:HB3	1.97	0.45
1:A:162:ASP:O	1:A:163:THR:C	2.59	0.45
1:A:187:THR:O	1:A:188:HIS:CB	2.64	0.45
1:A:219:GLN:HG3	1:A:219:GLN:O	2.17	0.45
2:B:12:ARG:HG2	2:B:13:HIS:NE2	2.32	0.45
1:A:44:ARG:HA	1:A:64:THR:HG23	1.99	0.45
1:A:104:GLY:HA3	1:A:106:ASP:OD1	2.17	0.45
1:A:33:PHE:CD1	1:A:33:PHE:N	2.84	0.45
2:D:3:ARG:HG2	2:D:3:ARG:HH11	1.82	0.45
1:A:142:ILE:HG23	1:C:65:ARG:HE	1.82	0.44
1:A:158:ALA:O	1:A:159:TYR:C	2.60	0.44
1:A:191:HIS:NE2	1:A:199:ALA:CB	2.80	0.44
1:C:243:LYS:O	1:C:244:TRP:HB3	2.17	0.44
1:A:70:THR:O	1:A:71:ALA:C	2.58	0.44
1:C:182:LEU:HD23	1:C:182:LEU:HA	1.71	0.44
2:D:71:THR:HA	2:D:72:PRO:HD2	1.69	0.44
2:B:73:THR:HG22	2:B:76:ASP:H	1.82	0.44
1:C:219:GLN:HA	1:C:256:ALA:O	2.17	0.44
1:A:150:ALA:O	1:A:151:SER:HB2	2.17	0.44
2:B:6:LYS:HB2	2:B:6:LYS:HE3	1.89	0.44
2:B:57:SER:O	2:B:60:TRP:N	2.49	0.44
2:D:15:ALA:HB2	2:D:95:TRP:CZ2	2.52	0.44
1:A:255:GLN:N	1:A:255:GLN:NE2	2.63	0.44
1:C:131:ARG:HH11	1:C:157:ARG:NH1	2.16	0.44
1:A:79:ARG:NH1	1:C:72:GLN:HE22	2.15	0.44
1:A:225:THR:CG2	1:A:226:GLN:N	2.80	0.44
1:C:37:ASP:OD1	1:C:37:ASP:C	2.60	0.44
1:C:243:LYS:HG2	1:C:244:TRP:N	2.33	0.43
1:A:152:GLU:CB	3:P:7:LEU:HD13	2.48	0.43
2:B:16:GLU:HB3	2:B:19:LYS:CB	2.48	0.43
1:C:162:ASP:HB2	1:C:163:THR:H	1.45	0.43
1:A:47:PRO:HB3	1:A:60:TRP:CZ2	2.54	0.43
1:A:249:VAL:CG2	1:A:257:TYR:CE1	3.00	0.43
1:A:37:ASP:HB3	1:A:40:ALA:HB2	2.00	0.43
1:A:162:ASP:HB2	1:A:163:THR:H	1.42	0.43
1:C:104:GLY:C	1:C:106:ASP:N	2.73	0.43
1:A:121:LYS:HG3	1:A:122:ASP:H	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:GLU:CD	3:Q:1:VAL:HG12	2.43	0.43
1:A:65:ARG:NH2	1:C:145:GLN:HE21	2.08	0.43
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.54	0.43
1:A:142:ILE:HG23	1:C:65:ARG:NE	2.34	0.43
1:A:129:ASP:O	1:A:130:LEU:HB2	2.18	0.43
1:A:232:GLU:OE1	2:B:6:LYS:NZ	2.42	0.43
1:A:249:VAL:HA	1:A:250:PRO:HD3	1.80	0.43
1:C:128:GLU:C	1:C:130:LEU:N	2.75	0.43
1:C:244:TRP:C	1:C:244:TRP:CE3	2.97	0.43
1:A:137:ASP:OD2	1:A:138:THR:N	2.52	0.43
1:A:189:VAL:CG1	1:A:190:THR:N	2.82	0.43
1:A:194:ILE:N	1:A:194:ILE:CD1	2.80	0.43
2:B:29:GLY:HA2	2:B:61:SER:CB	2.49	0.43
1:A:24:SER:HB3	1:A:36:PHE:HB3	2.00	0.42
1:A:270:VAL:HG12	1:A:272:LEU:HD23	2.01	0.42
2:B:89:GLN:O	2:B:90:PRO:C	2.59	0.42
1:C:44:ARG:HH11	1:C:44:ARG:HD3	1.69	0.42
2:D:39:LEU:HD23	2:D:39:LEU:HA	1.70	0.42
1:A:35:ARG:HD3	2:B:53:ASP:CG	2.44	0.42
1:C:53:GLU:C	1:C:55:GLU:H	2.27	0.42
1:A:188:HIS:HA	1:A:272:LEU:HD12	2.01	0.42
1:C:187:THR:HB	1:C:272:LEU:HD11	2.01	0.42
1:C:255:GLN:CD	1:C:255:GLN:N	2.77	0.42
2:D:70:PHE:CD1	2:D:70:PHE:C	2.96	0.42
1:A:216:THR:O	1:A:259:CYS:HA	2.18	0.42
2:B:27:VAL:O	2:B:27:VAL:HG23	2.20	0.42
1:A:76:VAL:HG11	3:P:8:LEU:HD11	2.01	0.42
1:C:152:GLU:O	1:C:153:ALA:C	2.61	0.42
1:C:163:THR:O	1:C:167:TRP:HD1	2.03	0.42
1:C:232:GLU:O	1:C:233:THR:C	2.60	0.42
1:A:55:GLU:CD	1:A:174:LYS:HZ2	2.27	0.42
2:B:53:ASP:O	2:B:54:LEU:C	2.60	0.42
1:A:73:ILE:HG21	3:P:6:THR:HG23	2.01	0.42
2:B:17:ASN:OD1	2:B:73:THR:C	2.63	0.42
1:C:176:LYS:C	1:C:178:THR:N	2.77	0.42
1:C:85:TYR:O	1:C:86:ASN:C	2.61	0.42
2:B:49:VAL:CG1	2:B:50:GLU:H	2.33	0.42
1:C:109:PHE:HD1	1:C:110:LEU:N	2.18	0.42
1:C:255:GLN:NE2	1:C:255:GLN:N	2.66	0.42
1:A:191:HIS:ND1	1:A:274:TRP:CH2	2.75	0.42
1:A:244:TRP:CE3	1:A:244:TRP:C	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:PRO:O	1:A:251:SER:C	2.61	0.42
1:C:109:PHE:CD2	1:C:161:GLU:HA	2.55	0.42
1:C:136:VAL:O	1:C:136:VAL:CG1	2.66	0.42
2:D:6:LYS:O	2:D:27:VAL:HA	2.19	0.42
1:A:198:GLU:CB	1:A:249:VAL:O	2.68	0.41
2:D:72:PRO:HB2	2:D:97:ARG:NH1	2.34	0.41
2:D:96:ASP:O	2:D:97:ARG:C	2.63	0.41
2:B:45:ARG:O	2:B:45:ARG:CG	2.67	0.41
1:C:225:THR:C	1:C:227:ASP:N	2.78	0.41
2:D:38:ASP:O	2:D:80:CYS:HA	2.20	0.41
2:D:89:GLN:O	2:D:90:PRO:C	2.60	0.41
1:A:137:ASP:H	1:A:140:ALA:HB3	1.84	0.41
1:C:211:ALA:HB2	1:C:241:PHE:CD1	2.55	0.41
1:C:218:GLN:HB2	1:C:222:GLU:O	2.20	0.41
1:A:181:HIS:CE1	1:A:182:LEU:O	2.73	0.41
2:B:71:THR:HA	2:B:72:PRO:HD2	1.77	0.41
1:C:23:ILE:HG22	1:C:24:SER:N	2.36	0.41
1:C:150:ALA:O	1:C:151:SER:HB2	2.21	0.41
1:A:8:PHE:HD2	2:B:56:PHE:CE1	2.39	0.41
1:A:121:LYS:HB2	2:B:1(A):ILE:HG13	2.02	0.41
1:A:45:MET:O	1:A:60:TRP:CE3	2.73	0.41
1:A:109:PHE:HE2	1:A:161:GLU:HA	1.84	0.41
1:A:177:GLU:O	1:A:178:THR:C	2.64	0.41
1:C:122:ASP:HB3	1:C:136:VAL:HG21	2.03	0.41
2:D:56:PHE:HA	2:D:62:PHE:HA	2.03	0.41
2:D:21:ASN:O	2:D:69:GLU:HG3	2.20	0.41
1:A:108:ARG:O	1:A:109:PHE:C	2.64	0.41
1:C:82:ARG:HD2	1:C:88:SER:C	2.45	0.41
1:C:270:VAL:HG12	1:C:272:LEU:HD23	2.02	0.41
2:D:96:ASP:C	2:D:98:ASP:N	2.79	0.41
1:A:209:TYR:HA	1:A:210:PRO:C	2.45	0.41
1:C:225:THR:O	1:C:227:ASP:N	2.54	0.40
1:A:222:GLU:H	1:A:222:GLU:HG3	1.57	0.40
1:C:15:PRO:O	1:C:16:GLY:C	2.64	0.40
1:C:212:GLU:OE1	1:C:212:GLU:CA	2.66	0.40
2:D:53:ASP:O	2:D:54:LEU:C	2.64	0.40
2:D:67:TYR:CD1	2:D:67:TYR:N	2.88	0.40
1:A:37:ASP:C	1:A:37:ASP:OD1	2.64	0.40
1:C:88:SER:C	1:C:90:ALA:H	2.29	0.40
1:A:155:HIS:NE2	1:C:151:SER:HB3	2.37	0.40
1:A:194:ILE:H	1:A:199:ALA:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:LEU:O	2:B:88:SER:C	2.61	0.40

All (1) 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)
1:A:111:ARG:NH1	1:A:268:GLU:OE2[5_555]	2.08	0.12

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	272/274 (99%)	232 (85%)	25 (9%)	15 (6%)	1	9
1	C	272/274 (99%)	231 (85%)	30 (11%)	11 (4%)	2	13
2	B	98/100 (98%)	92 (94%)	6 (6%)	0	100	100
2	D	98/100 (98%)	85 (87%)	11 (11%)	2 (2%)	6	25
3	P	7/9 (78%)	7 (100%)	0	0	100	100
3	Q	7/9 (78%)	7 (100%)	0	0	100	100
All	All	754/766 (98%)	654 (87%)	72 (10%)	28 (4%)	2	15

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	GLU
1	A	222	GLU
1	A	224	HIS
1	A	226	GLN
1	C	29	ASP
1	C	177	GLU
1	C	222	GLU

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Mol	Chain	Res	Type
1	C	224	HIS
1	C	226	GLN
2	D	97	ARG
1	A	15	PRO
1	A	29	ASP
1	A	254	GLU
1	C	15	PRO
1	A	2	SER
1	A	178	THR
1	C	30	ASP
1	C	40	ALA
1	C	163	THR
1	C	178	THR
1	C	220	ASP
1	A	40	ALA
1	A	57	SER
1	A	220	ASP
2	D	17	ASN
1	A	18	GLY
1	A	19	GLU
1	A	210	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	229/234 (98%)	200 (87%)	29 (13%)	4	18
1	C	231/234 (99%)	199 (86%)	32 (14%)	3	15
2	B	93/95 (98%)	85 (91%)	8 (9%)	10	34
2	D	93/95 (98%)	83 (89%)	10 (11%)	6	25
3	P	8/8 (100%)	6 (75%)	2 (25%)	0	2
3	Q	8/8 (100%)	5 (62%)	3 (38%)	0	0
All	All	662/674 (98%)	578 (87%)	84 (13%)	4	18

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	15	PRO
1	A	19	GLU
1	A	29	ASP
1	A	35	ARG
1	A	48	ARG
1	A	53	GLU
1	A	65	ARG
1	A	73	ILE
1	A	128	GLU
1	A	136	VAL
1	A	138	THR
1	A	145	GLN
1	A	151	SER
1	A	178	THR
1	A	182	LEU
1	A	186	LYS
1	A	187	THR
1	A	194	ILE
1	A	198	GLU
1	A	210	PRO
1	A	222	GLU
1	A	244	TRP
1	A	251	SER
1	A	255	GLN
1	A	258	THR
1	A	268	GLU
1	A	272	LEU
1	A	273	ARG
2	B	4	THR
2	B	9	VAL
2	B	12	ARG
2	B	48	LYS
2	B	58	LYS
2	B	71	THR
2	B	73	THR
2	B	93	VAL
1	C	11	SER
1	C	14	ARG
1	C	15	PRO
1	C	17	ARG
1	C	19	GLU

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Mol	Chain	Res	Type
1	C	24	SER
1	C	29	ASP
1	C	35	ARG
1	C	53	GLU
1	C	65	ARG
1	C	94	THR
1	C	121	LYS
1	C	128	GLU
1	C	136	VAL
1	C	138	THR
1	C	145	GLN
1	C	151	SER
1	C	165	VAL
1	C	177	GLU
1	C	186	LYS
1	C	187	THR
1	C	194	ILE
1	C	198	GLU
1	C	200	THR
1	C	222	GLU
1	C	224	HIS
1	C	244	TRP
1	C	251	SER
1	C	258	THR
1	C	268	GLU
1	C	272	LEU
1	C	273	ARG
2	D	4	THR
2	D	11	SER
2	D	12	ARG
2	D	14	PRO
2	D	45	ARG
2	D	58	LYS
2	D	70	PHE
2	D	71	THR
2	D	73	THR
2	D	93	VAL
3	P	1	VAL
3	P	5	ARG
3	Q	1	VAL
3	Q	5	ARG
3	Q	7	LEU

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

Mol	Chain	Res	Type
1	A	72	GLN
1	A	87	GLN
1	A	127	ASN
1	A	148	ASN
1	A	155	HIS
1	A	181	HIS
1	A	218	GLN
1	A	219	GLN
1	A	255	GLN
1	A	263	HIS
2	B	2	GLN
2	B	42	ASN
2	B	89	GLN
1	C	72	GLN
1	C	87	GLN
1	C	127	ASN
1	C	141	GLN
1	C	145	GLN
1	C	155	HIS
1	C	218	GLN
1	C	255	GLN
1	C	263	HIS
2	D	2	GLN
2	D	42	ASN
2	D	89	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
4	SO4	A	275	-	4,4,4	1.04	0	6,6,6	0.32	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	275	SO4	1	0

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.