



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:15 AM UTC

PDB ID : 3BZF / pdb_00003bzf
Title : The human non-classical major histocompatibility complex molecule HLA-E
Authors : Hoare, H.L.; Sullivan, L.C.; Ely, L.K.; Beddoe, T.; Henderson, K.N.; Lin, J.;
Clements, C.S.; Reid, H.H.; Brooks, A.G.; Rossjohn, J.
Deposited on : 2008-01-17
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

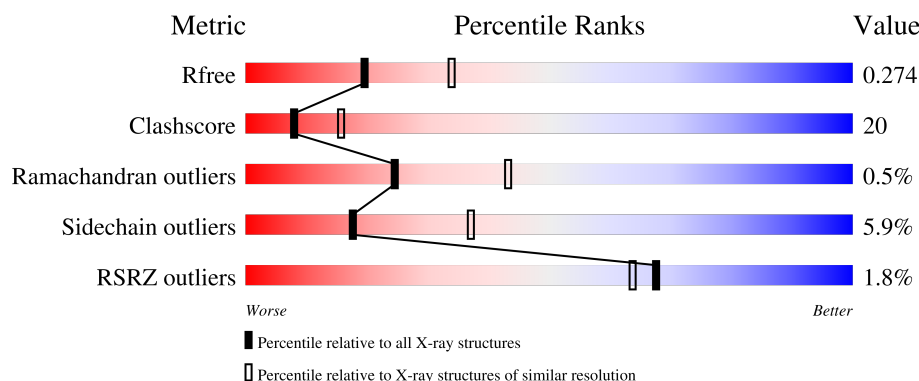
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	2% 46% 43% 9% .
1	C	276	3% 55% 32% 11% .
2	B	97	51% 42% 7%
2	D	97	% 52% 39% 8% .
3	P	9	33% 44% 22%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Q	9	78% 11% 11%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6516 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 E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2253	1409	405	432	7			
1	C	276	Total	C	N	O	S	0	0	0
			2253	1409	405	432	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	97	Total	C	N	O	S	0	0	0
			812	517	137	155	3			
2	D	97	Total	C	N	O	S	0	0	0
			812	517	137	155	3			

- Molecule 3 is a protein called leader peptide of HLA class I histocompatibility antigen, Cw-7 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	9	Total	C	N	O	S	0	0	0
			68	45	12	10	1			
3	Q	9	Total	C	N	O	S	0	0	0
			68	45	12	10	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	82	Total	O	0	0
			82	82		
4	B	42	Total	O	0	0
			42	42		
4	P	2	Total	O	0	0
			2	2		
4	C	85	Total	O	0	0
			85	85		

Continued on next page...

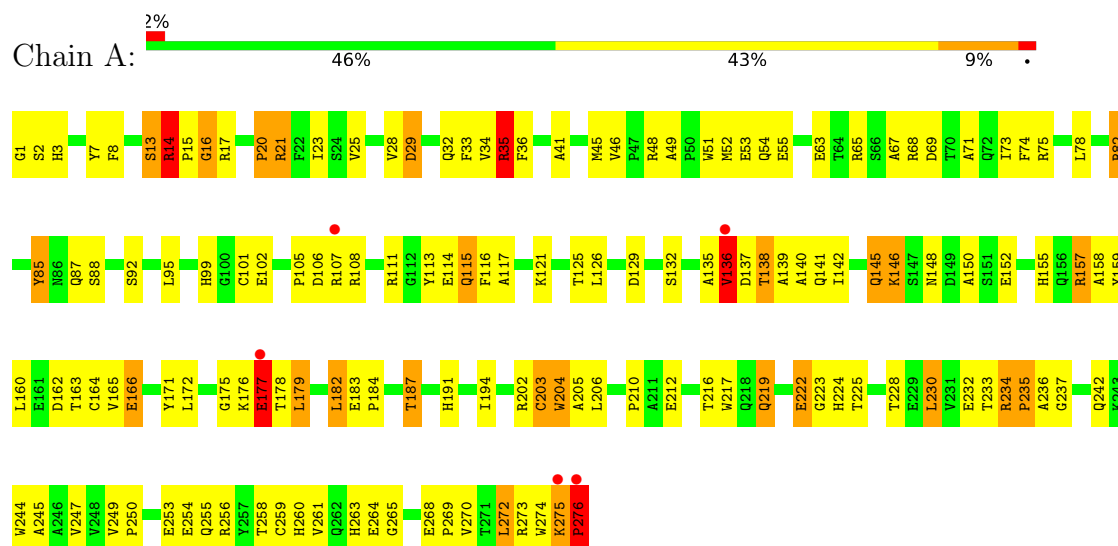
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	36	Total 36	O 36	0	0
4	Q	3	Total 3	O 3	0	0

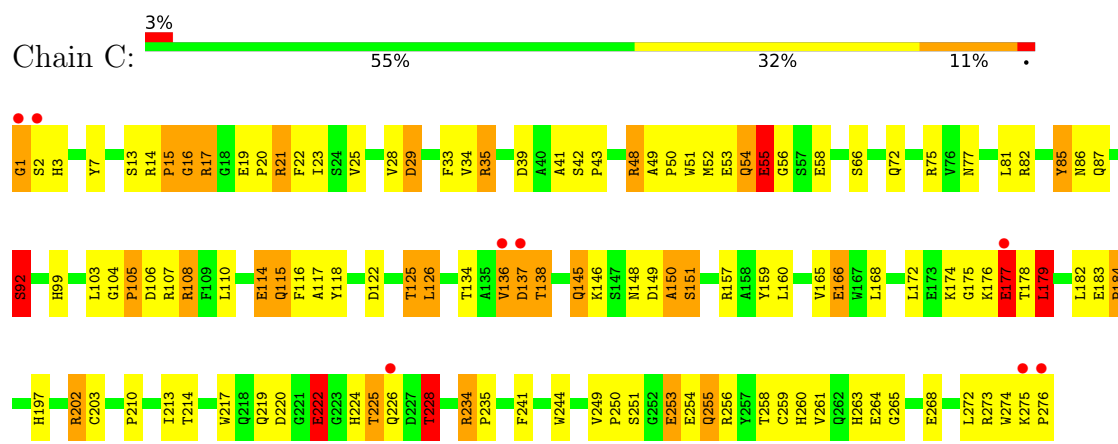
3 Residue-property plots

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.

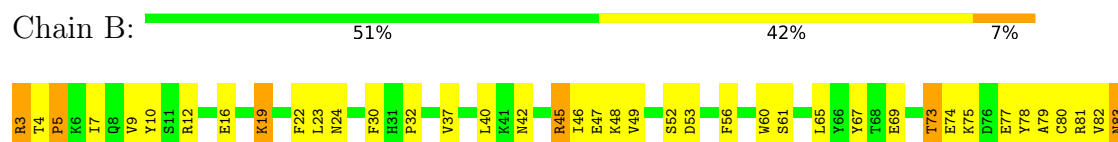
- Molecule 1: HLA class I histocompatibility antigen, alpha chain E



- Molecule 1: HLA class I histocompatibility antigen, alpha chain E

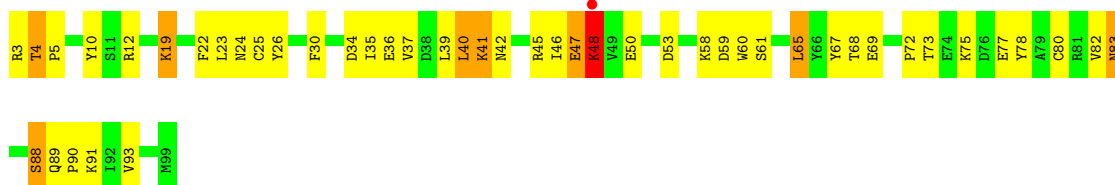


- Molecule 2: Beta-2-microglobulin

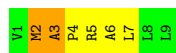




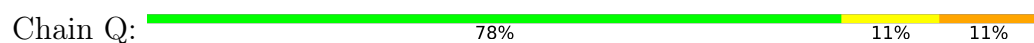
- Molecule 2: Beta-2-microglobulin



- Molecule 3: leader peptide of HLA class I histocompatibility antigen, Cw-7 alpha chain



- Molecule 3: leader peptide of HLA class I histocompatibility antigen, Cw-7 alpha chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.52Å 62.30Å 98.77Å 90.00° 106.15° 90.00°	Depositor
Resolution (Å)	29.60 – 2.50 29.60 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.60-2.50) 98.6 (29.60-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.40 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.269 0.208 , 0.274	Depositor DCC
R_{free} test set	1620 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6516	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	2.04	65/2320 (2.8%)	1.46	26/3155 (0.8%)
1	C	1.97	51/2320 (2.2%)	1.54	27/3155 (0.9%)
2	B	1.88	9/835 (1.1%)	1.34	4/1129 (0.4%)
2	D	1.91	11/835 (1.3%)	1.56	11/1129 (1.0%)
3	P	2.18	3/68 (4.4%)	1.71	2/90 (2.2%)
3	Q	1.77	0/68	1.84	2/90 (2.2%)
All	All	1.98	139/6446 (2.2%)	1.49	72/8748 (0.8%)

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	2
All	All	0	4

All (139) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	VAL	C-O	-10.33	1.13	1.24
1	C	56	GLY	CA-C	-9.36	1.42	1.52
2	B	49	VAL	C-O	-8.91	1.14	1.24
2	D	35	ILE	N-CA	-8.84	1.35	1.46
1	C	184	PRO	C-O	-8.19	1.17	1.24
2	B	80	CYS	N-CA	-7.95	1.36	1.46
1	A	177	GLU	CB-CG	7.91	1.76	1.52
1	A	35	ARG	C-O	-7.84	1.14	1.23
1	A	85	TYR	C-O	7.78	1.32	1.23
1	A	46	VAL	C-O	-7.74	1.18	1.24
1	C	116	PHE	CA-C	-7.57	1.43	1.52
1	A	101	CYS	C-O	-7.36	1.14	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	255	GLN	C-O	-7.33	1.14	1.24
2	D	48	LYS	C-O	7.32	1.33	1.24
1	C	150	ALA	C-O	-7.21	1.14	1.24
1	A	272	LEU	C-O	-7.18	1.14	1.23
1	A	68	ARG	CZ-NH1	-7.11	1.22	1.32
1	A	275	LYS	C-O	7.06	1.33	1.24
1	A	116	PHE	C-O	-7.02	1.15	1.24
1	A	63	GLU	N-CA	-6.96	1.37	1.46
1	A	29	ASP	C-O	-6.90	1.15	1.24
1	A	191	HIS	C-O	-6.85	1.16	1.24
1	A	235	PRO	C-O	-6.84	1.16	1.23
1	C	149	ASP	C-O	-6.78	1.16	1.24
2	B	73	THR	C-O	-6.76	1.15	1.23
1	A	228	THR	N-CA	6.74	1.53	1.45
1	C	86	ASN	CA-C	6.72	1.60	1.53
1	C	43	PRO	CA-CB	-6.65	1.48	1.53
2	D	34	ASP	C-N	-6.61	1.27	1.33
2	B	79	ALA	CA-CB	-6.59	1.42	1.53
1	C	134	THR	N-CA	6.53	1.54	1.46
1	C	159	TYR	C-O	-6.47	1.16	1.24
1	A	136	VAL	CA-CB	6.45	1.63	1.54
1	C	177	GLU	CD-OE1	6.43	1.37	1.25
1	A	171	TYR	C-O	-6.43	1.16	1.24
1	A	187	THR	C-O	-6.43	1.16	1.23
1	C	115	GLN	C-O	-6.40	1.16	1.23
2	D	58	LYS	C-O	-6.37	1.16	1.24
1	C	125	THR	C-O	-6.36	1.15	1.24
1	A	269	PRO	C-O	-6.35	1.16	1.23
1	C	166	GLU	CG-CD	6.34	1.67	1.52
1	A	65	ARG	CZ-NH2	-6.30	1.25	1.33
1	C	1	GLY	N-CA	6.29	1.55	1.45
1	C	17	ARG	NE-CZ	6.20	1.39	1.33
1	C	85	TYR	C-O	6.17	1.31	1.23
1	C	58	GLU	CD-OE1	6.16	1.37	1.25
1	C	16	GLY	C-O	-6.14	1.15	1.24
1	A	136	VAL	CB-CG1	6.13	1.72	1.52
1	C	25	VAL	CA-CB	6.13	1.62	1.54
1	C	145	GLN	CG-CD	6.09	1.67	1.52
1	C	75	ARG	CD-NE	6.08	1.54	1.46
1	C	48	ARG	CA-C	6.05	1.60	1.52
1	C	39	ASP	C-O	-6.01	1.16	1.24
1	A	219	GLN	CA-C	-6.01	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	228	THR	N-CA	6.00	1.52	1.45
1	A	177	GLU	CG-CD	6.00	1.67	1.52
1	C	148	ASN	C-O	-5.98	1.17	1.24
1	C	72	GLN	CD-NE2	5.95	1.45	1.33
1	A	75	ARG	CD-NE	5.94	1.54	1.46
1	A	142	ILE	CA-CB	-5.94	1.47	1.54
1	C	251	SER	C-O	-5.86	1.16	1.23
1	A	159	TYR	C-O	-5.84	1.17	1.24
1	A	232	GLU	CD-OE1	5.83	1.36	1.25
1	A	20	PRO	C-O	-5.82	1.16	1.23
1	C	54	GLN	CA-C	-5.82	1.46	1.52
1	C	122	ASP	N-CA	-5.77	1.38	1.46
1	A	212	GLU	C-O	-5.77	1.16	1.23
1	A	139	ALA	CA-CB	5.73	1.64	1.53
1	A	276	PRO	C-O	5.73	1.35	1.23
1	C	261	VAL	CA-CB	-5.72	1.46	1.54
1	C	23	ILE	C-O	-5.71	1.18	1.24
1	C	214	THR	N-CA	5.71	1.53	1.46
3	P	2	MET	SD-CE	-5.71	1.65	1.79
1	C	241	PHE	C-O	5.67	1.31	1.23
1	C	49	ALA	C-O	5.66	1.31	1.24
2	B	94	LYS	C-O	-5.66	1.17	1.23
1	C	166	GLU	CB-CG	5.61	1.69	1.52
3	P	3	ALA	C-O	-5.61	1.17	1.24
1	A	13	SER	C-O	-5.61	1.17	1.23
1	A	163	THR	C-O	-5.61	1.17	1.24
1	A	165	VAL	C-O	-5.60	1.17	1.24
1	C	58	GLU	CG-CD	5.58	1.66	1.52
1	A	142	ILE	C-O	-5.57	1.17	1.24
2	B	45	ARG	C-O	-5.56	1.17	1.23
1	C	114	GLU	CA-C	5.54	1.59	1.52
1	C	42	SER	C-O	5.53	1.30	1.24
2	D	19	LYS	CG-CD	5.53	1.69	1.52
1	A	203	CYS	N-CA	-5.52	1.39	1.46
2	D	48	LYS	CG-CD	5.50	1.69	1.52
1	A	25	VAL	C-O	-5.50	1.18	1.24
1	C	22	PHE	CA-C	-5.50	1.45	1.52
1	A	148	ASN	C-O	-5.42	1.17	1.24
1	A	41	ALA	CA-CB	5.41	1.61	1.53
1	A	237	GLY	N-CA	5.40	1.52	1.45
1	A	233	THR	C-O	-5.40	1.17	1.23
1	A	249	VAL	CA-C	5.40	1.58	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	91	LYS	C-O	-5.39	1.17	1.23
1	A	164	CYS	CA-C	-5.39	1.46	1.52
1	A	16	GLY	C-O	-5.38	1.16	1.23
1	A	69	ASP	N-CA	-5.35	1.40	1.46
2	D	65	LEU	C-O	-5.35	1.18	1.24
1	A	204	TRP	C-O	-5.33	1.17	1.24
1	C	197	HIS	C-O	-5.33	1.17	1.24
1	C	23	ILE	N-CA	5.33	1.52	1.46
1	C	66	SER	C-O	5.33	1.30	1.24
2	B	61	SER	C-O	-5.31	1.17	1.23
1	A	236	ALA	N-CA	-5.30	1.39	1.46
1	A	242	GLN	C-O	-5.29	1.17	1.23
2	D	61	SER	C-O	-5.29	1.17	1.23
1	A	247	VAL	CB-CG2	-5.28	1.35	1.52
1	A	166	GLU	CG-CD	5.26	1.65	1.52
1	C	19	GLU	C-O	-5.25	1.17	1.24
1	A	233	THR	N-CA	5.23	1.52	1.46
1	A	216	THR	N-CA	-5.20	1.39	1.45
2	D	30	PHE	N-CA	5.20	1.51	1.45
1	C	92	SER	C-O	-5.17	1.17	1.23
1	A	71	ALA	C-O	5.17	1.30	1.24
1	C	151	SER	CA-C	5.16	1.60	1.53
1	A	194	ILE	C-O	-5.15	1.18	1.23
1	A	75	ARG	CZ-NH2	-5.15	1.26	1.33
1	A	182	LEU	N-CA	-5.14	1.39	1.46
1	A	222	GLU	C-O	5.14	1.30	1.24
2	B	52	SER	C-O	-5.13	1.16	1.23
1	C	118	TYR	N-CA	-5.13	1.39	1.46
2	D	91	LYS	CA-C	-5.12	1.46	1.52
1	A	145	GLN	CG-CD	5.12	1.64	1.52
1	C	179	LEU	CA-CB	-5.09	1.44	1.53
1	A	113	TYR	N-CA	5.09	1.52	1.45
1	C	92	SER	CA-C	5.07	1.59	1.52
1	A	230	LEU	C-O	-5.06	1.18	1.23
2	D	26	TYR	CA-C	-5.05	1.46	1.52
1	A	194	ILE	CG1-CD1	5.04	1.71	1.51
1	C	148	ASN	CA-C	-5.03	1.46	1.52
1	A	157	ARG	C-O	-5.03	1.18	1.24
1	A	203	CYS	CA-CB	-5.03	1.46	1.53
1	A	261	VAL	CA-CB	-5.02	1.47	1.53
3	P	5	ARG	C-O	-5.01	1.18	1.23
1	C	55	GLU	C-N	-5.00	1.29	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	183	GLU	N-CA	-5.00	1.40	1.46

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	55	GLU	N-CA-C	-10.52	88.39	110.80
2	D	47	GLU	CA-C-N	-9.47	103.46	121.54
2	D	47	GLU	C-N-CA	-9.47	103.46	121.54
1	A	276	PRO	N-CA-C	9.37	135.51	112.10
1	C	54	GLN	N-CA-C	-8.97	95.69	109.95
1	C	15	PRO	CB-CA-C	-8.69	97.23	111.56
1	C	202	ARG	CD-NE-CZ	8.51	136.31	124.40
2	D	41	LYS	CA-C-N	-8.43	110.30	122.19
2	D	41	LYS	C-N-CA	-8.43	110.30	122.19
1	C	202	ARG	NE-CZ-NH2	-8.33	111.70	119.20
1	A	15	PRO	N-CA-C	8.07	124.75	113.53
1	C	222	GLU	CA-C-O	7.88	130.68	121.46
3	Q	3	ALA	CA-C-N	7.87	127.51	119.56
3	Q	3	ALA	C-N-CA	7.87	127.51	119.56
1	C	55	GLU	CA-C-N	-7.72	115.60	122.47
1	C	55	GLU	C-N-CA	-7.72	115.60	122.47
1	C	104	GLY	CA-C-N	7.63	127.17	119.24
1	C	104	GLY	C-N-CA	7.63	127.17	119.24
1	A	254	GLU	N-CA-C	7.41	120.29	111.33
1	C	85	TYR	N-CA-C	-7.41	99.56	110.52
1	A	115	GLN	N-CA-C	7.39	119.98	108.96
1	A	85	TYR	N-CA-C	-7.33	98.37	110.17
1	C	138	THR	N-CA-C	-7.26	102.84	114.09
2	D	47	GLU	N-CA-C	-7.21	101.23	110.53
1	A	276	PRO	CB-CA-C	-7.17	96.48	110.10
1	C	41	ALA	N-CA-C	-7.16	103.48	111.28
1	C	115	GLN	N-CA-C	7.07	119.82	109.07
2	D	30	PHE	N-CA-C	6.88	120.81	110.14
1	C	222	GLU	O-C-N	-6.72	114.11	123.11
1	C	222	GLU	CA-C-N	-6.57	113.29	120.71
1	C	222	GLU	C-N-CA	-6.57	113.29	120.71
1	C	85	TYR	CA-C-N	-6.50	113.03	122.06
1	C	85	TYR	C-N-CA	-6.50	113.03	122.06
1	A	45	MET	N-CA-C	-6.27	100.56	109.96
1	A	49	ALA	CA-C-N	6.26	125.75	119.24
1	A	49	ALA	C-N-CA	6.26	125.75	119.24
1	A	150	ALA	N-CA-C	-6.24	105.43	113.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	138	THR	CA-C-O	6.13	125.72	118.79
2	B	46	ILE	CB-CA-C	-6.09	102.69	111.34
1	A	14	ARG	N-CA-C	-6.04	95.34	108.74
1	A	138	THR	N-CA-C	-6.02	105.76	114.12
3	P	3	ALA	CA-C-N	5.95	126.06	119.87
3	P	3	ALA	C-N-CA	5.95	126.06	119.87
1	C	172	LEU	N-CA-C	-5.76	105.00	111.28
2	B	5	PRO	N-CA-C	5.68	119.37	110.80
1	C	77	ASN	N-CA-C	5.53	116.99	111.07
1	C	213	ILE	N-CA-C	5.48	115.53	107.75
1	A	141	GLN	N-CA-C	5.47	117.68	111.11
1	A	205	ALA	CA-C-O	-5.45	114.62	120.46
1	A	32	GLN	N-CA-C	-5.34	102.57	110.48
2	D	40	LEU	CA-C-N	5.30	130.41	122.47
2	D	40	LEU	C-N-CA	5.30	130.41	122.47
1	A	206	LEU	N-CA-C	5.23	117.98	109.24
1	A	228	THR	CA-CB-OG1	-5.20	101.80	109.60
2	D	88	SER	N-CA-C	-5.20	106.04	112.38
1	A	137	ASP	CB-CA-C	5.19	120.74	110.42
2	D	47	GLU	CA-C-O	-5.18	115.98	121.94
1	A	85	TYR	CA-C-N	-5.16	114.89	122.06
1	A	85	TYR	C-N-CA	-5.16	114.89	122.06
1	A	160	LEU	N-CA-C	5.13	116.95	111.36
2	D	59	ASP	N-CA-C	5.12	119.29	113.19
1	A	146	LYS	N-CA-CB	-5.12	102.57	110.20
1	A	194	ILE	N-CA-C	-5.12	107.76	111.90
1	A	88	SER	N-CA-C	-5.10	102.47	110.17
1	C	126	LEU	N-CA-C	-5.10	102.14	110.20
1	C	160	LEU	N-CA-C	5.08	116.89	111.36
2	B	30	PHE	N-CA-C	5.08	117.60	110.14
2	B	19	LYS	N-CA-C	5.07	117.02	108.96
1	C	105	PRO	CA-N-CD	-5.07	104.91	112.00
1	A	184	PRO	O-C-N	5.06	123.53	121.15
1	C	254	GLU	N-CA-C	5.05	117.44	111.33
1	A	132	SER	N-CA-C	5.02	116.44	108.96

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	ARG	Mainchain
1	A	275	LYS	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	C	222	GLU	Mainchain
1	C	275	LYS	Mainchain

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	2253	0	2098	92	0
1	C	2253	0	2098	81	0
2	B	812	0	772	42	0
2	D	812	0	774	37	0
3	P	68	0	83	6	0
3	Q	68	0	83	2	0
4	A	82	0	0	6	0
4	B	42	0	0	4	0
4	C	85	0	0	9	0
4	D	36	0	0	2	0
4	P	2	0	0	2	0
4	Q	3	0	0	2	0
All	All	6516	0	5908	238	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 20.

All (238) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLU:CB	1:A:177:GLU:CG	1.76	1.61
1:C:228:THR:CG2	4:C:415:HOH:O	1.97	1.13
1:C:15:PRO:O	1:C:17:ARG:NH1	1.82	1.11
2:D:47:GLU:HB2	2:D:48:LYS:HD3	1.35	1.08
1:A:121:LYS:HD2	4:A:339:HOH:O	1.53	1.06
1:C:48:ARG:NH1	2:D:53:ASP:OD2	1.87	1.06
2:D:47:GLU:O	2:D:48:LYS:HB2	1.49	1.06
1:C:228:THR:HG21	4:C:415:HOH:O	1.58	1.00
1:A:16:GLY:H	1:A:17:ARG:NH1	1.59	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:ARG:HD3	4:C:378:HOH:O	1.60	0.99
2:D:47:GLU:HB2	2:D:48:LYS:CD	1.92	0.97
1:A:16:GLY:H	1:A:17:ARG:HH11	0.98	0.92
1:C:54:GLN:O	1:C:55:GLU:HB2	1.74	0.88
2:D:47:GLU:O	2:D:48:LYS:CB	2.14	0.85
1:A:21:ARG:NE	1:A:23:ILE:HD11	1.90	0.84
1:A:121:LYS:HE2	4:A:317:HOH:O	1.78	0.82
2:D:83:ASN:ND2	2:D:90:PRO:HB3	1.95	0.81
1:C:136:VAL:O	1:C:137:ASP:CG	2.24	0.81
2:B:73:THR:HG22	2:B:74:GLU:N	1.96	0.81
1:A:82:ARG:O	1:A:85:TYR:O	2.00	0.80
1:C:250:PRO:HB2	1:C:253:GLU:HG3	1.64	0.78
1:A:108:ARG:HH11	1:A:108:ARG:HB2	1.50	0.77
2:B:73:THR:HG22	2:B:74:GLU:H	1.49	0.76
1:C:202:ARG:HD2	1:C:244:TRP:CD2	2.20	0.75
1:C:222:GLU:OE2	4:C:414:HOH:O	2.05	0.75
1:C:225:THR:C	1:C:228:THR:OG1	2.30	0.74
1:A:21:ARG:HE	1:A:23:ILE:HD11	1.49	0.74
1:A:202:ARG:HD2	1:A:244:TRP:CD2	2.23	0.73
1:C:35:ARG:NH1	2:D:53:ASP:OD1	2.21	0.72
1:A:234:ARG:HD3	2:B:10:TYR:CE2	2.25	0.72
1:A:16:GLY:N	1:A:17:ARG:HH11	1.81	0.72
1:A:263:HIS:CD2	1:A:265:GLY:H	2.08	0.71
1:A:234:ARG:HD3	2:B:10:TYR:CZ	2.26	0.70
1:C:234:ARG:HD3	2:D:10:TYR:CZ	2.26	0.70
1:A:108:ARG:HB2	1:A:108:ARG:NH1	2.07	0.69
1:C:263:HIS:CD2	1:C:265:GLY:H	2.10	0.69
1:C:52:MET:HE2	1:C:52:MET:HA	1.75	0.69
1:A:48:ARG:NH1	2:B:53:ASP:OD2	2.26	0.68
1:C:225:THR:C	1:C:228:THR:HG1	2.02	0.68
1:C:106:ASP:OD1	1:C:108:ARG:HG3	1.92	0.68
1:A:13:SER:HA	1:A:20:PRO:HB3	1.77	0.67
1:C:13:SER:HA	1:C:20:PRO:HB3	1.75	0.67
1:A:250:PRO:HB2	1:A:253:GLU:HG3	1.75	0.67
3:P:6:ALA:O	4:P:115:HOH:O	2.12	0.67
1:C:54:GLN:O	1:C:54:GLN:CD	2.39	0.66
1:A:106:ASP:O	1:A:107:ARG:HB2	1.95	0.65
1:A:255:GLN:OE1	1:A:273:ARG:HD3	1.97	0.65
1:A:16:GLY:N	1:A:17:ARG:NH1	2.39	0.65
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.32	0.64
1:C:175:GLY:O	1:C:179:LEU:HB2	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ASP:C	1:A:166:GLU:OE1	2.42	0.63
1:A:244:TRP:HZ2	2:B:99:MET:HE2	1.64	0.63
1:A:13:SER:O	1:A:92:SER:HB2	1.98	0.62
3:Q:3:ALA:HB1	4:Q:12:HOH:O	1.98	0.62
1:C:157:ARG:HD3	4:C:357:HOH:O	2.00	0.62
1:C:15:PRO:C	1:C:17:ARG:NH1	2.57	0.62
2:B:73:THR:HG21	2:B:75:LYS:NZ	2.15	0.62
1:C:125:THR:HG22	1:C:126:LEU:O	2.00	0.62
1:C:1:GLY:N	1:C:107:ARG:HE	1.97	0.61
1:C:82:ARG:O	1:C:85:TYR:O	2.17	0.61
1:A:125:THR:HG22	1:A:126:LEU:O	2.01	0.61
1:A:244:TRP:CZ2	2:B:99:MET:HE2	2.36	0.61
1:A:155:HIS:HE1	4:A:326:HOH:O	1.84	0.60
2:D:46:ILE:HG22	2:D:47:GLU:O	2.02	0.60
1:A:235:PRO:HG2	2:B:65:LEU:HD22	1.84	0.60
2:D:24:ASN:HB3	2:D:65:LEU:HD11	1.84	0.59
1:A:157:ARG:HD3	4:A:321:HOH:O	2.02	0.59
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.84	0.59
2:D:47:GLU:HB2	2:D:48:LYS:CG	2.32	0.59
2:D:40:LEU:HD23	2:D:45:ARG:HA	1.84	0.59
2:D:47:GLU:O	2:D:48:LYS:C	2.36	0.59
1:C:13:SER:O	1:C:92:SER:HB2	2.02	0.59
2:D:25:CYS:CB	2:D:80:CYS:SG	2.91	0.59
1:C:234:ARG:HD3	2:D:10:TYR:CE1	2.38	0.58
1:A:108:ARG:HH11	1:A:108:ARG:CB	2.15	0.58
1:C:50:PRO:O	1:C:53:GLU:HB2	2.04	0.58
1:A:1:GLY:N	1:A:107:ARG:HE	2.02	0.58
1:C:182:LEU:HD13	1:C:264:GLU:HG2	1.86	0.57
1:C:28:VAL:O	1:C:29:ASP:HB2	2.05	0.57
2:D:42:ASN:ND2	2:D:77:GLU:H	2.03	0.57
2:B:9:VAL:CG2	2:B:93:VAL:HG22	2.35	0.56
1:A:175:GLY:O	1:A:179:LEU:HB2	2.04	0.56
1:C:117:ALA:HB2	2:D:60:TRP:CE2	2.40	0.56
1:C:99:HIS:HB3	1:C:114:GLU:HG3	1.88	0.56
2:D:22:PHE:CE1	2:D:69:GLU:HG2	2.41	0.56
2:B:73:THR:CG2	2:B:74:GLU:N	2.67	0.56
1:A:253:GLU:O	1:A:256:ARG:HB2	2.06	0.55
1:C:106:ASP:OD2	1:C:108:ARG:NH1	2.39	0.55
1:A:99:HIS:HB3	1:A:114:GLU:HG3	1.88	0.55
2:D:19:LYS:O	2:D:72:PRO:HD2	2.06	0.55
2:B:42:ASN:ND2	2:B:77:GLU:H	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:ARG:HD3	2:D:10:TYR:CE2	2.41	0.55
1:A:82:ARG:HG2	1:A:87:GLN:HB2	1.89	0.55
1:A:225:THR:HG22	1:A:225:THR:O	2.07	0.55
1:C:54:GLN:O	1:C:54:GLN:CG	2.53	0.54
2:B:3:ARG:HB2	2:B:3:ARG:HH11	1.73	0.54
1:A:17:ARG:N	1:A:17:ARG:HD3	2.22	0.54
2:D:41:LYS:O	2:D:42:ASN:HB2	2.07	0.54
3:P:4:PRO:HD2	4:P:41:HOH:O	2.08	0.54
1:A:177:GLU:CG	1:A:177:GLU:CA	2.77	0.54
1:C:203:CYS:HB2	1:C:217:TRP:CZ2	2.43	0.53
2:D:42:ASN:HD21	2:D:77:GLU:H	1.55	0.53
1:A:33:PHE:CD2	1:A:34:VAL:HG13	2.44	0.53
1:A:182:LEU:HD13	1:A:264:GLU:HG2	1.91	0.53
1:C:82:ARG:HG2	1:C:87:GLN:HB2	1.90	0.53
1:A:102:GLU:OE2	1:A:111:ARG:NH1	2.42	0.52
1:A:219:GLN:HG2	1:A:224:HIS:CD2	2.45	0.52
1:C:274:TRP:CH2	1:C:276:PRO:HB3	2.44	0.52
1:A:219:GLN:HG3	1:A:219:GLN:O	2.09	0.52
3:Q:4:PRO:HD2	4:Q:12:HOH:O	2.08	0.52
1:C:210:PRO:O	1:C:263:HIS:HE1	1.92	0.52
1:C:226:GLN:HG2	4:C:423:HOH:O	2.08	0.52
1:A:162:ASP:HB3	1:A:166:GLU:OE1	2.10	0.51
1:A:177:GLU:CD	1:A:178:THR:HG23	2.36	0.51
2:B:73:THR:CG2	2:B:74:GLU:H	2.21	0.51
2:B:81:ARG:HD2	4:B:127:HOH:O	2.09	0.51
1:C:17:ARG:HD3	1:C:17:ARG:N	2.25	0.51
1:C:225:THR:O	1:C:228:THR:OG1	2.13	0.51
1:C:106:ASP:O	1:C:107:ARG:HB2	2.11	0.51
1:A:203:CYS:HB2	1:A:217:TRP:CZ2	2.47	0.50
2:B:73:THR:HG21	2:B:75:LYS:HZ1	1.75	0.50
1:C:35:ARG:C	1:C:35:ARG:HD2	2.36	0.50
2:B:83:ASN:ND2	2:B:90:PRO:HB3	2.27	0.50
1:A:21:ARG:HE	1:A:23:ILE:CD1	2.19	0.49
1:C:103:LEU:HG	1:C:168:LEU:HD23	1.93	0.49
1:A:67:ALA:HB2	3:P:2:MET:HE1	1.93	0.49
1:A:121:LYS:CE	4:A:317:HOH:O	2.48	0.49
1:C:258:THR:OG1	1:C:260:HIS:HE1	1.96	0.49
2:B:23:LEU:O	2:B:67:TYR:HA	2.13	0.49
1:C:219:GLN:HG2	1:C:224:HIS:CD2	2.48	0.48
1:C:7:TYR:HB2	1:C:99:HIS:CE1	2.48	0.48
2:D:39:LEU:HD23	2:D:68:THR:HG22	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:ASN:HD21	2:B:77:GLU:H	1.61	0.48
2:D:41:LYS:HB3	4:D:109:HOH:O	2.13	0.48
2:D:41:LYS:O	2:D:42:ASN:C	2.52	0.47
1:A:106:ASP:O	1:A:107:ARG:CB	2.62	0.47
2:D:37:VAL:HG22	2:D:82:VAL:HG22	1.96	0.47
1:C:150:ALA:O	1:C:151:SER:HB3	2.15	0.47
2:B:9:VAL:HG23	2:B:93:VAL:HG22	1.97	0.47
1:A:16:GLY:C	1:A:17:ARG:HD3	2.39	0.47
2:B:40:LEU:O	2:B:78:TYR:HA	2.15	0.47
2:B:48:LYS:C	4:B:132:HOH:O	2.57	0.47
1:C:219:GLN:HG3	1:C:219:GLN:O	2.15	0.47
1:C:253:GLU:O	1:C:256:ARG:HB2	2.14	0.47
2:B:22:PHE:CZ	2:B:69:GLU:HG2	2.50	0.47
2:B:32:PRO:HB2	4:B:110:HOH:O	2.14	0.47
1:A:230:LEU:HD12	1:A:245:ALA:HB2	1.97	0.46
1:C:202:ARG:CD	1:C:244:TRP:CE3	2.98	0.46
1:A:52:MET:HE2	1:A:52:MET:HA	1.97	0.46
1:A:177:GLU:OE2	1:A:178:THR:OG1	2.28	0.46
1:C:16:GLY:C	1:C:17:ARG:HD3	2.39	0.46
1:A:36:PHE:CD1	1:A:36:PHE:C	2.93	0.46
1:A:210:PRO:O	1:A:263:HIS:HE1	1.98	0.46
2:D:73:THR:HG22	2:D:75:LYS:HG2	1.96	0.46
2:D:83:ASN:HD21	2:D:90:PRO:HB3	1.75	0.46
1:A:145:GLN:NE2	1:A:146:LYS:HB2	2.30	0.46
1:A:270:VAL:HG12	1:A:272:LEU:CD2	2.45	0.46
1:A:258:THR:OG1	1:A:260:HIS:HE1	1.99	0.46
2:B:37:VAL:HG22	2:B:82:VAL:HG22	1.97	0.46
1:C:105:PRO:C	1:C:107:ARG:H	2.23	0.46
2:D:4:THR:HG23	2:D:5:PRO:HD2	1.98	0.46
2:B:45:ARG:NH1	2:B:47:GLU:OE2	2.48	0.45
1:C:105:PRO:C	1:C:107:ARG:N	2.75	0.45
1:A:54:GLN:NE2	1:A:55:GLU:OE1	2.45	0.45
2:B:7:ILE:HD11	2:B:82:VAL:HB	1.99	0.45
1:C:48:ARG:NH1	2:D:53:ASP:CG	2.71	0.45
2:B:9:VAL:HG21	2:B:93:VAL:HG22	1.98	0.45
1:C:52:MET:HE1	1:C:174:LYS:HD2	1.98	0.45
2:B:4:THR:HG23	2:B:5:PRO:HD2	1.97	0.45
2:B:22:PHE:CE1	2:B:69:GLU:HG2	2.51	0.45
3:P:3:ALA:HA	3:P:4:PRO:HD3	1.80	0.45
1:C:2:SER:O	1:C:3:HIS:CG	2.70	0.45
1:A:274:TRP:O	1:A:276:PRO:HD3	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:41:LYS:HG3	2:D:78:TYR:CE1	2.52	0.44
1:A:1:GLY:HA2	1:A:105:PRO:HA	1.99	0.44
2:D:89:GLN:HB2	2:D:90:PRO:HD2	1.99	0.44
1:A:125:THR:OG1	1:A:136:VAL:HG21	2.17	0.44
1:C:255:GLN:OE1	1:C:273:ARG:HD3	2.17	0.44
1:A:172:LEU:HD23	1:A:179:LEU:HD23	2.00	0.44
1:A:234:ARG:HD3	2:B:10:TYR:CE1	2.53	0.44
1:C:202:ARG:HD2	1:C:244:TRP:CE3	2.51	0.44
2:D:45:ARG:NH1	2:D:47:GLU:OE1	2.51	0.44
1:C:35:ARG:HG2	1:C:48:ARG:HD3	2.00	0.43
1:C:263:HIS:HD2	1:C:265:GLY:H	1.61	0.43
2:B:3:ARG:HB2	2:B:3:ARG:NH1	2.34	0.43
1:A:187:THR:HA	1:A:204:TRP:O	2.18	0.43
1:A:35:ARG:HD2	1:A:35:ARG:C	2.43	0.43
1:A:74:PHE:CD2	1:A:95:LEU:HD23	2.53	0.43
1:C:1:GLY:CA	4:C:397:HOH:O	2.66	0.43
1:C:259:CYS:HB3	1:C:272:LEU:HB2	2.00	0.43
2:D:23:LEU:O	2:D:67:TYR:HA	2.18	0.43
1:A:2:SER:O	1:A:3:HIS:CG	2.71	0.43
2:B:84:HIS:CE1	2:B:86:THR:HG23	2.53	0.43
1:C:1:GLY:N	4:C:397:HOH:O	2.50	0.43
1:A:35:ARG:HG2	1:A:48:ARG:HD3	2.00	0.43
2:B:3:ARG:HD2	4:B:111:HOH:O	2.18	0.43
1:C:177:GLU:OE1	1:C:178:THR:HG23	2.19	0.43
1:A:129:ASP:CG	4:A:353:HOH:O	2.61	0.42
1:A:172:LEU:HA	1:A:179:LEU:HD23	2.01	0.42
1:A:259:CYS:HB3	1:A:272:LEU:HB2	2.02	0.42
1:A:158:ALA:O	1:A:162:ASP:HB2	2.19	0.42
1:A:202:ARG:HD2	1:A:244:TRP:CE3	2.52	0.42
1:C:125:THR:OG1	1:C:136:VAL:HG21	2.19	0.42
1:C:165:VAL:O	1:C:166:GLU:C	2.59	0.42
1:A:82:ARG:HA	1:A:87:GLN:HE21	1.84	0.42
2:B:16:GLU:OE2	2:B:19:LYS:HG3	2.20	0.42
1:A:222:GLU:O	1:A:223:GLY:C	2.63	0.42
1:C:33:PHE:CD2	1:C:34:VAL:HG13	2.54	0.42
1:A:152:GLU:HB3	3:P:7:LEU:HD21	2.02	0.42
1:A:1:GLY:H1	1:A:107:ARG:HE	1.67	0.42
1:C:51:TRP:CE3	1:C:52:MET:HG2	2.54	0.41
1:A:176:LYS:O	1:A:177:GLU:C	2.62	0.41
1:C:235:PRO:HG2	2:D:65:LEU:HD22	2.01	0.41
1:C:1:GLY:HA2	1:C:105:PRO:HA	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:LYS:HG3	1:C:177:GLU:H	1.86	0.41
1:C:202:ARG:HD3	1:C:244:TRP:CE3	2.55	0.41
1:C:249:VAL:HA	1:C:250:PRO:HD3	1.82	0.41
1:A:51:TRP:CE3	1:A:52:MET:HG2	2.56	0.41
1:C:81:LEU:O	1:C:85:TYR:HD1	2.03	0.41
2:D:88:SER:OG	2:D:89:GLN:HG2	2.20	0.41
1:A:7:TYR:HB2	1:A:99:HIS:CE1	2.55	0.41
1:A:234:ARG:HD3	2:B:10:TYR:CD2	2.56	0.41
1:C:145:GLN:NE2	1:C:146:LYS:HB2	2.35	0.41
1:C:220:ASP:OD2	1:C:256:ARG:HG2	2.21	0.41
1:A:28:VAL:O	1:A:29:ASP:HB2	2.20	0.41
1:A:135:ALA:HB1	1:A:140:ALA:HB3	2.02	0.41
1:A:8:PHE:HD2	2:B:56:PHE:CE1	2.38	0.40
1:A:13:SER:HB3	1:A:78:LEU:HD13	2.03	0.40
1:A:54:GLN:O	1:A:55:GLU:C	2.61	0.40
1:C:228:THR:HG22	4:C:415:HOH:O	1.92	0.40
2:D:50:GLU:HG2	4:D:102:HOH:O	2.22	0.40
1:A:73:ILE:HG21	3:P:6:ALA:O	2.21	0.40
1:A:230:LEU:CD1	1:A:245:ALA:HB2	2.51	0.40
2:B:73:THR:HG22	2:B:75:LYS:H	1.86	0.40
2:B:73:THR:HG21	2:B:75:LYS:HZ2	1.85	0.40
1:C:183:GLU:HA	1:C:184:PRO:HD2	1.97	0.40
1:A:234:ARG:HB2	2:B:10:TYR:OH	2.21	0.40
1:C:110:LEU:HD12	1:C:110:LEU:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	274/276 (99%)	259 (94%)	14 (5%)	1 (0%)	30 49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	274/276 (99%)	254 (93%)	17 (6%)	3 (1%)	11	22
2	B	95/97 (98%)	91 (96%)	4 (4%)	0	100	100
2	D	95/97 (98%)	89 (94%)	6 (6%)	0	100	100
3	P	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	Q	7/9 (78%)	7 (100%)	0	0	100	100
All	All	752/764 (98%)	706 (94%)	42 (6%)	4 (0%)	24	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	137	ASP
1	A	177	GLU
1	C	29	ASP
1	C	55	GLU

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	238/238 (100%)	225 (94%)	13 (6%)	19	40
1	C	238/238 (100%)	223 (94%)	15 (6%)	16	34
2	B	92/92 (100%)	87 (95%)	5 (5%)	20	41
2	D	92/92 (100%)	85 (92%)	7 (8%)	12	26
3	P	7/7 (100%)	7 (100%)	0	100	100
3	Q	7/7 (100%)	7 (100%)	0	100	100
All	All	674/674 (100%)	634 (94%)	40 (6%)	18	37

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	21	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	35	ARG
1	A	53	GLU
1	A	82	ARG
1	A	115	GLN
1	A	136	VAL
1	A	138	THR
1	A	177	GLU
1	A	179	LEU
1	A	234	ARG
1	A	268	GLU
1	A	276	PRO
2	B	3	ARG
2	B	12	ARG
2	B	83	ASN
2	B	89	GLN
2	B	93	VAL
1	C	14	ARG
1	C	21	ARG
1	C	35	ARG
1	C	92	SER
1	C	108	ARG
1	C	115	GLN
1	C	136	VAL
1	C	138	THR
1	C	177	GLU
1	C	179	LEU
1	C	225	THR
1	C	228	THR
1	C	234	ARG
1	C	253	GLU
1	C	268	GLU
2	D	3	ARG
2	D	4	THR
2	D	12	ARG
2	D	36	GLU
2	D	48	LYS
2	D	83	ASN
2	D	93	VAL

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

Mol	Chain	Res	Type
1	A	72	GLN
1	A	87	GLN
1	A	115	GLN
1	A	127	ASN
1	A	145	GLN
1	A	155	HIS
1	A	156	GLN
1	A	169	HIS
1	A	218	GLN
1	A	219	GLN
1	A	224	HIS
1	A	260	HIS
1	A	262	GLN
1	A	263	HIS
2	B	42	ASN
2	B	83	ASN
1	C	72	GLN
1	C	87	GLN
1	C	115	GLN
1	C	127	ASN
1	C	145	GLN
1	C	155	HIS
1	C	218	GLN
1	C	219	GLN
1	C	224	HIS
1	C	260	HIS
1	C	263	HIS
2	D	42	ASN
2	D	83	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	276/276 (100%)	-0.23	5 (1%) 67 64	21, 32, 50, 66	0
1	C	276/276 (100%)	-0.13	8 (2%) 53 49	23, 33, 52, 63	0
2	B	97/97 (100%)	-0.16	0 100 100	24, 34, 51, 60	0
2	D	97/97 (100%)	-0.02	1 (1%) 79 76	24, 38, 53, 64	0
3	P	9/9 (100%)	-0.49	0 100 100	21, 27, 33, 35	0
3	Q	9/9 (100%)	-0.37	0 100 100	26, 29, 32, 33	0
All	All	764/764 (100%)	-0.16	14 (1%) 67 64	21, 33, 52, 66	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	137	ASP	6.1
1	A	275	LYS	5.1
1	C	136	VAL	3.7
1	A	276	PRO	2.8
1	C	275	LYS	2.8
1	C	276	PRO	2.8
1	A	107	ARG	2.4
1	A	177	GLU	2.4
1	C	177	GLU	2.4
1	C	1	GLY	2.3
1	C	226	GLN	2.2
2	D	48	LYS	2.2
1	A	136	VAL	2.0
1	C	2	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.