



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2026 – 04:08 PM EDT

PDB ID : 9Z50 / pdb_00009z50
Title : Q61H_Sahin-1 TCR in complex with HLA-A*01:01 presenting KRAS Q61H
10mer peptide (55-ILDTAGHEEY-64)
Authors : Miller, H.A.; Palowitch, G.M.; Dulberger, C.L.
Deposited on : 2025-11-11
Resolution : 2.90 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

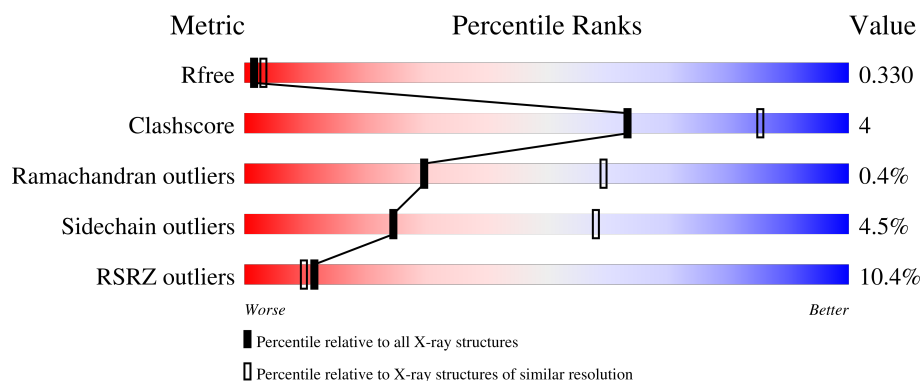
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	E	10	90%10%
1	P	10	80%20%
2	C	303	5% 83%13%
2	F	303	7% 75%6%18%
3	D	100	11% 85%12%..

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Mol	Chain	Length	Quality of chain
3	G	100	
4	A	218	
4	H	218	
5	B	253	
5	I	253	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11560 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 GTPase KRas.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	P	10	Total	C	N	O	0	0	0
			81	50	12	19			
1	E	10	Total	C	N	O	0	0	0
			81	50	12	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	7	HIS	GLN	engineered mutation	UNP P01116
E	7	HIS	GLN	engineered mutation	UNP P01116

- Molecule 2 is a protein called MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	264	Total	C	N	O	S	0	0	0
			1931	1220	337	364	10			
2	F	247	Total	C	N	O	S	0	0	0
			1815	1146	314	346	9			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	initiating methionine	UNP A0A678ZVJ3
C	277	GLY	-	expression tag	UNP A0A678ZVJ3
C	278	SER	-	expression tag	UNP A0A678ZVJ3
C	279	GLY	-	expression tag	UNP A0A678ZVJ3
C	280	GLY	-	expression tag	UNP A0A678ZVJ3
C	281	SER	-	expression tag	UNP A0A678ZVJ3
C	282	GLY	-	expression tag	UNP A0A678ZVJ3
C	283	GLY	-	expression tag	UNP A0A678ZVJ3
C	284	SER	-	expression tag	UNP A0A678ZVJ3
C	285	ALA	-	expression tag	UNP A0A678ZVJ3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	286	GLY	-	expression tag	UNP A0A678ZVJ3
C	287	GLY	-	expression tag	UNP A0A678ZVJ3
C	288	GLY	-	expression tag	UNP A0A678ZVJ3
C	289	LEU	-	expression tag	UNP A0A678ZVJ3
C	290	ASN	-	expression tag	UNP A0A678ZVJ3
C	291	ASP	-	expression tag	UNP A0A678ZVJ3
C	292	ILE	-	expression tag	UNP A0A678ZVJ3
C	293	PHE	-	expression tag	UNP A0A678ZVJ3
C	294	GLU	-	expression tag	UNP A0A678ZVJ3
C	295	ALA	-	expression tag	UNP A0A678ZVJ3
C	296	GLN	-	expression tag	UNP A0A678ZVJ3
C	297	LYS	-	expression tag	UNP A0A678ZVJ3
C	298	ILE	-	expression tag	UNP A0A678ZVJ3
C	299	GLU	-	expression tag	UNP A0A678ZVJ3
C	300	TRP	-	expression tag	UNP A0A678ZVJ3
C	301	HIS	-	expression tag	UNP A0A678ZVJ3
C	302	GLU	-	expression tag	UNP A0A678ZVJ3
F	0	MET	-	initiating methionine	UNP A0A678ZVJ3
F	277	GLY	-	expression tag	UNP A0A678ZVJ3
F	278	SER	-	expression tag	UNP A0A678ZVJ3
F	279	GLY	-	expression tag	UNP A0A678ZVJ3
F	280	GLY	-	expression tag	UNP A0A678ZVJ3
F	281	SER	-	expression tag	UNP A0A678ZVJ3
F	282	GLY	-	expression tag	UNP A0A678ZVJ3
F	283	GLY	-	expression tag	UNP A0A678ZVJ3
F	284	SER	-	expression tag	UNP A0A678ZVJ3
F	285	ALA	-	expression tag	UNP A0A678ZVJ3
F	286	GLY	-	expression tag	UNP A0A678ZVJ3
F	287	GLY	-	expression tag	UNP A0A678ZVJ3
F	288	GLY	-	expression tag	UNP A0A678ZVJ3
F	289	LEU	-	expression tag	UNP A0A678ZVJ3
F	290	ASN	-	expression tag	UNP A0A678ZVJ3
F	291	ASP	-	expression tag	UNP A0A678ZVJ3
F	292	ILE	-	expression tag	UNP A0A678ZVJ3
F	293	PHE	-	expression tag	UNP A0A678ZVJ3
F	294	GLU	-	expression tag	UNP A0A678ZVJ3
F	295	ALA	-	expression tag	UNP A0A678ZVJ3
F	296	GLN	-	expression tag	UNP A0A678ZVJ3
F	297	LYS	-	expression tag	UNP A0A678ZVJ3
F	298	ILE	-	expression tag	UNP A0A678ZVJ3
F	299	GLU	-	expression tag	UNP A0A678ZVJ3
F	300	TRP	-	expression tag	UNP A0A678ZVJ3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	301	HIS	-	expression tag	UNP A0A678ZVJ3
F	302	GLU	-	expression tag	UNP A0A678ZVJ3

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	98	Total	C	N	O	S	0	0	0
			751	481	128	139	3			
3	G	98	Total	C	N	O	S	0	0	0
			755	483	132	137	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	initiating methionine	UNP P61769
G	0	MET	-	initiating methionine	UNP P61769

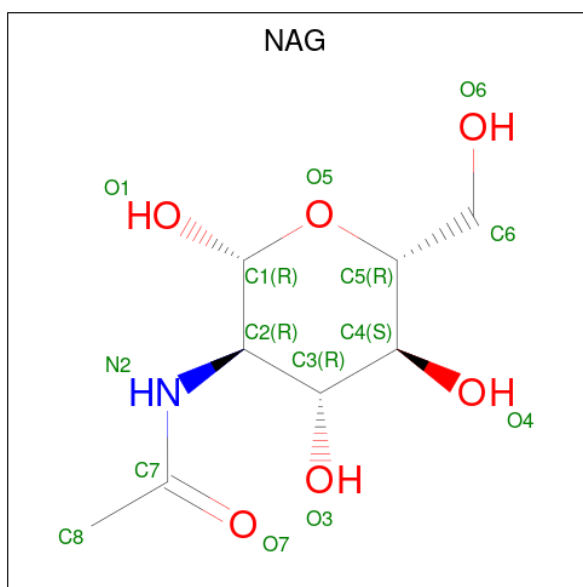
- Molecule 4 is a protein called Q61H_Sahin-1 alpha chain (TRAV14/DV4).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	204	Total	C	N	O	S	0	0	0
			1442	917	234	282	9			
4	H	200	Total	C	N	O	S	0	0	0
			1388	883	225	270	10			

- Molecule 5 is a protein called Q61H_Sahin-1 beta chain (TRBV9).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	236	Total	C	N	O	S	0	0	0
			1706	1100	285	316	5			
5	I	225	Total	C	N	O	S	0	1	0
			1594	1031	261	297	5			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	2	Total	O	0	0
			2	2		

3 Residue-property plots [i](#)

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

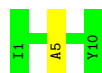
- Molecule 1: GTPase KRas

Chain P: 



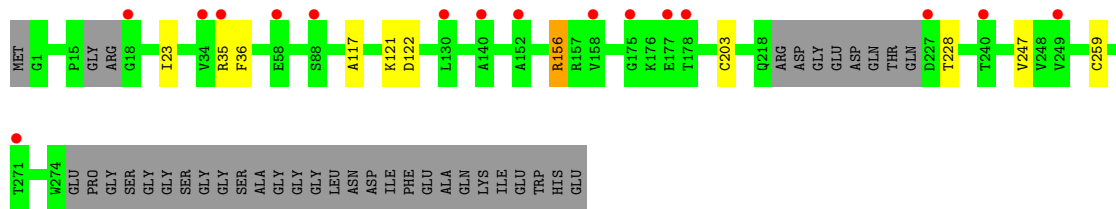
- Molecule 1: GTPase KRas

Chain E: 



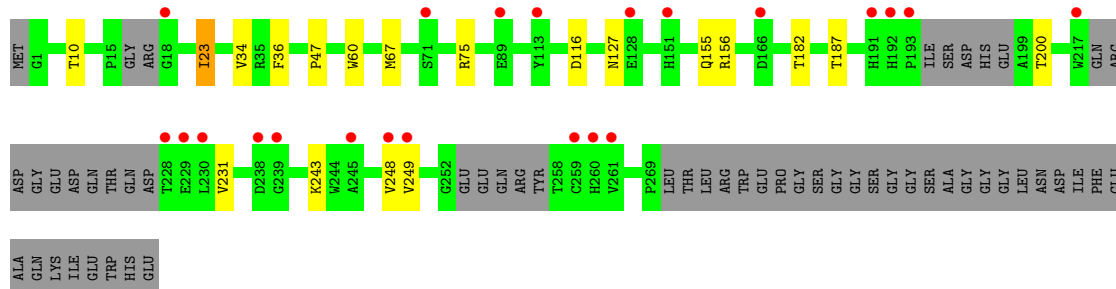
- Molecule 2: MHC class I antigen

Chain C: 

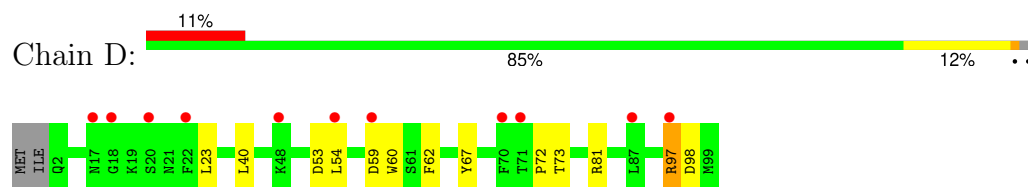


- Molecule 2: MHC class I antigen

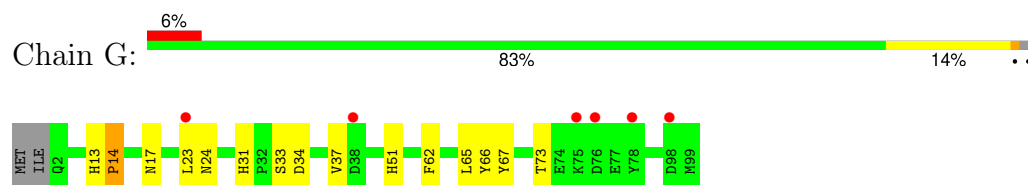
Chain F: 



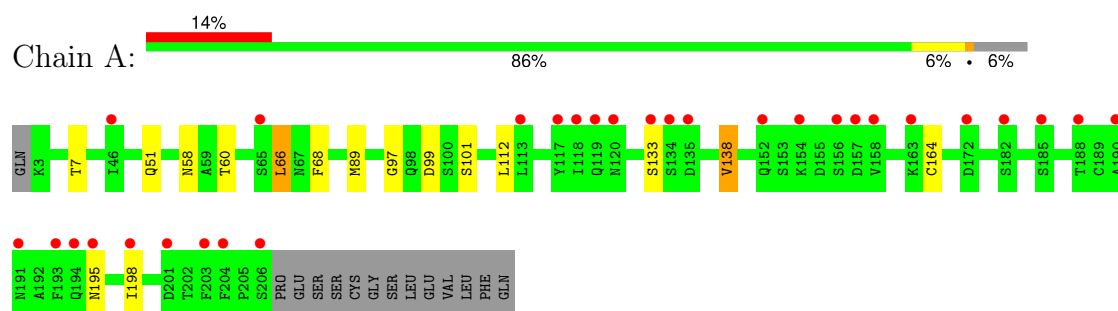
- Molecule 3: Beta-2-microglobulin



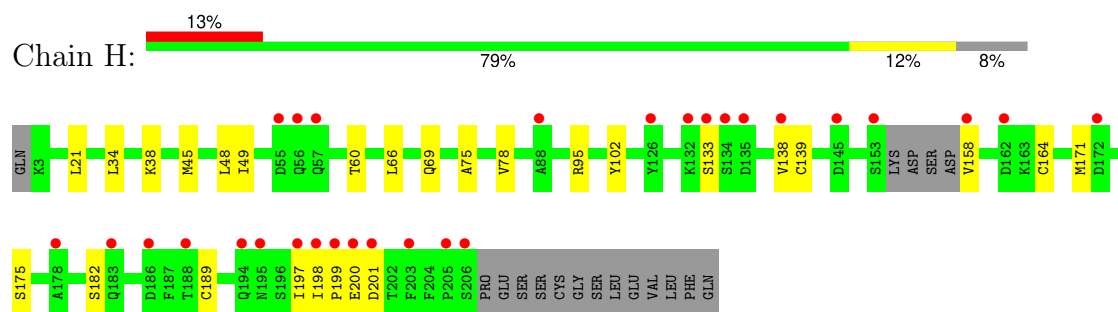
- Molecule 3: Beta-2-microglobulin



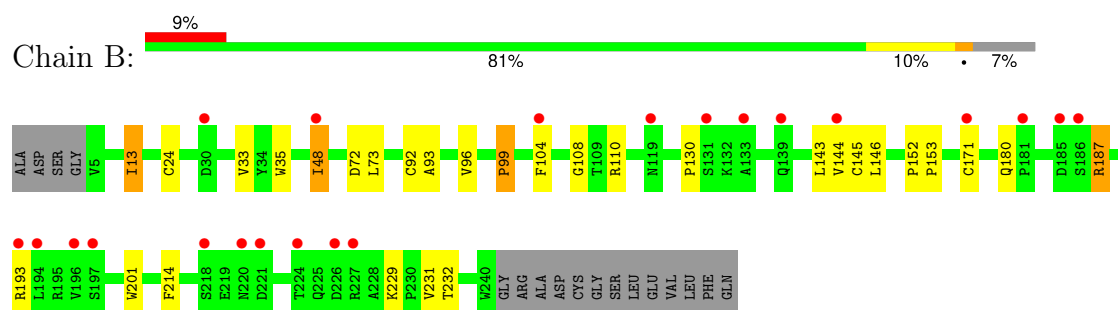
- Molecule 4: Q61H_Sahin-1 alpha chain (TRAV14/DV4)



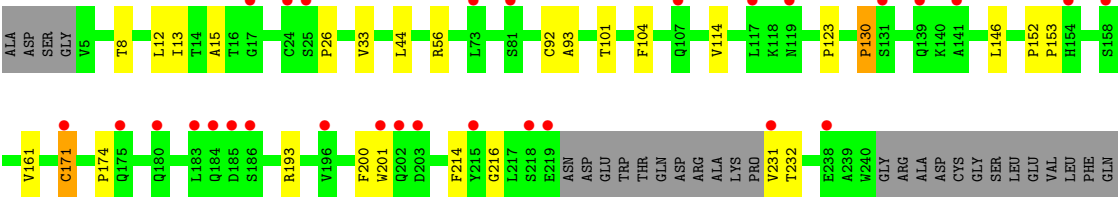
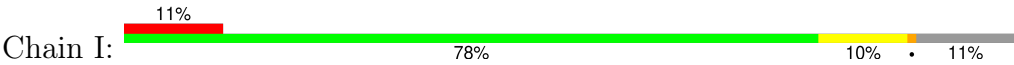
- Molecule 4: Q61H_Sahin-1 alpha chain (TRAV14/DV4)



- Molecule 5: Q61H_Sahin-1 beta chain (TRBV9)



- Molecule 5: Q61H_Sahin-1 beta chain (TRBV9)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.89Å 119.93Å 229.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.77 – 2.90 44.77 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (44.77-2.90) 98.5 (44.77-2.90)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.286 , 0.332 0.287 , 0.330	Depositor DCC
R_{free} test set	2480 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	43.8	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	11560	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 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	E	0.49	0/82	0.97	0/109
1	P	0.50	0/82	0.88	1/109 (0.9%)
2	C	0.47	0/1988	0.86	0/2726
2	F	0.48	0/1865	0.87	0/2554
3	D	0.46	0/774	0.77	0/1060
3	G	0.46	0/778	0.75	0/1065
4	A	0.47	0/1477	0.79	0/2023
4	H	0.48	0/1420	0.82	0/1946
5	B	0.47	0/1756	0.78	0/2419
5	I	0.48	0/1642	0.78	0/2265
All	All	0.47	0/11864	0.81	1/16276 (0.0%)

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
2	C	0	1
5	I	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	3	ASP	CA-CB-CG	5.07	117.67	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	156	ARG	Sidechain
5	I	193	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	E	81	0	71	1	0
1	P	81	0	71	1	0
2	C	1931	0	1643	6	0
2	F	1815	0	1565	6	0
3	D	751	0	655	9	0
3	G	755	0	669	8	0
4	A	1442	0	1197	9	0
4	H	1388	0	1134	11	0
5	B	1706	0	1493	17	0
5	I	1594	0	1375	17	0
6	A	14	0	13	4	0
7	C	2	0	0	0	0
All	All	11560	0	9886	73	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 4.

All (73) 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)
4:A:58:ASN:HD21	6:A:301:NAG:C1	1.76	0.99
4:A:58:ASN:ND2	6:A:301:NAG:C1	2.32	0.92
4:H:164:CYS:HG	5:I:171:CYS:HG	1.19	0.81
4:H:164:CYS:CB	5:I:171:CYS:HG	2.04	0.69
5:B:187:ARG:HH21	5:B:187:ARG:HG2	1.66	0.60
4:A:138:VAL:HG11	5:B:144:VAL:HG11	1.85	0.58
4:H:45:MET:HE3	5:I:44:LEU:HD11	1.87	0.56
4:H:34:LEU:HD13	4:H:75:ALA:HB2	1.87	0.56
3:D:73:THR:O	3:D:97:ARG:NH1	2.39	0.55
3:G:24:ASN:HB3	3:G:65:LEU:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:51:GLN:HB2	4:A:66:LEU:HD13	1.90	0.53
4:H:164:CYS:HG	5:I:171:CYS:CB	2.21	0.53
3:D:72:PRO:HB2	3:D:97:ARG:HH11	1.73	0.52
4:H:164:CYS:HB3	5:I:171:CYS:HG	1.76	0.51
4:A:99:ASP:C	4:A:101:SER:H	2.18	0.51
5:I:93:ALA:HA	5:I:104:PHE:O	2.11	0.51
3:G:23:LEU:O	3:G:67:TYR:HA	2.11	0.50
5:B:35:TRP:HB2	5:B:48:ILE:HD12	1.92	0.50
1:E:5:ALA:HB1	2:F:155:GLN:HB3	1.94	0.50
4:A:164:CYS:CB	5:B:171:CYS:HG	2.23	0.49
2:F:10:THR:HB	2:F:23:ILE:HG23	1.95	0.49
4:H:139:CYS:SG	4:H:189:CYS:HA	2.52	0.49
5:I:152:PRO:HB2	5:I:153:PRO:HD2	1.94	0.49
5:I:13:ILE:HD11	5:I:152:PRO:HG3	1.93	0.48
5:I:171:CYS:SG	5:I:171:CYS:O	2.70	0.48
5:I:13:ILE:CD1	5:I:152:PRO:HG3	2.44	0.48
3:D:54:LEU:HD11	3:D:62:PHE:HB3	1.95	0.47
2:F:231:VAL:O	2:F:243:LYS:NZ	2.47	0.47
3:G:33:SER:O	3:G:34:ASP:C	2.57	0.47
2:F:23:ILE:HD12	2:F:36:PHE:O	2.14	0.47
4:A:97:GLY:HA2	5:B:99:PRO:HG3	1.95	0.47
4:H:199:PRO:O	4:H:201:ASP:N	2.48	0.47
5:B:145:CYS:SG	5:B:146:LEU:N	2.89	0.46
4:H:95:ARG:NE	4:H:102:TYR:O	2.48	0.46
5:I:123:PRO:HD3	5:I:214:PHE:CG	2.51	0.46
5:B:13:ILE:HD12	5:B:152:PRO:HG3	1.96	0.46
5:B:24:CYS:SG	5:B:92:CYS:CB	3.05	0.45
3:D:59:ASP:O	3:D:60:TRP:HB2	2.17	0.45
5:B:72:ASP:O	5:B:73:LEU:HB2	2.15	0.45
4:H:38:LYS:HB2	4:H:48:LEU:HD11	1.98	0.44
2:C:203:CYS:CB	2:C:259:CYS:HG	2.25	0.44
2:C:121:LYS:O	2:C:122:ASP:C	2.60	0.44
3:D:40:LEU:HD11	3:D:81:ARG:HB2	2.00	0.44
3:G:17:ASN:ND2	3:G:73:THR:O	2.51	0.44
2:C:35:ARG:NH1	3:D:53:ASP:OD1	2.51	0.43
5:I:26:PRO:HG3	5:I:33:VAL:CG2	2.48	0.43
1:P:8:GLU:HB3	2:C:156:ARG:HH21	1.83	0.43
3:G:13:HIS:O	3:G:14:PRO:C	2.60	0.43
5:B:229:LYS:HD2	5:B:231:VAL:HG13	2.00	0.42
3:G:37:VAL:HB	3:G:66:TYR:CE2	2.54	0.42
5:I:15:ALA:HA	5:I:114:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:117:ALA:HB2	3:D:60:TRP:CE2	2.54	0.42
3:G:51:HIS:HB3	3:G:66:TYR:CD2	2.54	0.42
2:C:23:ILE:HA	2:C:36:PHE:O	2.19	0.42
5:B:130:PRO:HD2	5:B:201:TRP:CZ2	2.54	0.42
5:I:130:PRO:HD2	5:I:201:TRP:CZ2	2.55	0.42
5:I:161:VAL:HG11	5:I:200:PHE:HE2	1.85	0.42
5:I:33:VAL:HG13	5:I:92:CYS:SG	2.60	0.41
3:D:23:LEU:O	3:D:67:TYR:HA	2.20	0.41
4:A:68:PHE:HB3	6:A:301:NAG:H82	2.02	0.41
5:B:93:ALA:HA	5:B:104:PHE:O	2.19	0.41
5:B:214:PHE:O	5:B:232:THR:HG23	2.20	0.41
5:B:152:PRO:HB2	5:B:153:PRO:HD2	2.03	0.41
3:G:31:HIS:CD2	3:G:62:PHE:CE2	3.09	0.41
4:H:158:VAL:HG22	4:H:182:SER:CB	2.51	0.41
2:F:47:PRO:HB3	2:F:60:TRP:CZ2	2.56	0.41
2:F:36:PHE:CD1	2:F:67:MET:HE2	2.56	0.40
5:I:216:GLY:N	5:I:232:THR:OG1	2.52	0.40
5:B:143:LEU:O	5:B:193:ARG:HA	2.22	0.40
4:A:58:ASN:CG	6:A:301:NAG:C1	2.92	0.40
5:B:108:GLY:O	5:B:110:ARG:NH1	2.55	0.40
5:B:130:PRO:HD2	5:B:201:TRP:CE2	2.57	0.40
3:D:59:ASP:O	3:D:60:TRP:CB	2.70	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	E	8/10 (80%)	8 (100%)	0	0	100	100
1	P	8/10 (80%)	8 (100%)	0	0	100	100
2	C	258/303 (85%)	241 (93%)	17 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	237/303 (78%)	225 (95%)	12 (5%)	0	100	100
3	D	96/100 (96%)	91 (95%)	5 (5%)	0	100	100
3	G	96/100 (96%)	88 (92%)	7 (7%)	1 (1%)	12	39
4	A	202/218 (93%)	183 (91%)	18 (9%)	1 (0%)	24	54
4	H	196/218 (90%)	172 (88%)	22 (11%)	2 (1%)	12	39
5	B	234/253 (92%)	217 (93%)	16 (7%)	1 (0%)	30	59
5	I	222/253 (88%)	207 (93%)	13 (6%)	2 (1%)	14	41
All	All	1557/1768 (88%)	1440 (92%)	110 (7%)	7 (0%)	30	59

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	200	GLU
4	A	133	SER
4	H	133	SER
5	I	174	PRO
5	B	180	GLN
5	I	130	PRO
3	G	14	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	E	8/8 (100%)	8 (100%)	0	100	100
1	P	8/8 (100%)	8 (100%)	0	100	100
2	C	170/250 (68%)	168 (99%)	2 (1%)	63	86
2	F	165/250 (66%)	154 (93%)	11 (7%)	15	43
3	D	75/95 (79%)	73 (97%)	2 (3%)	39	73
3	G	76/95 (80%)	76 (100%)	0	100	100
4	A	129/196 (66%)	121 (94%)	8 (6%)	16	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	120/196 (61%)	109 (91%)	11 (9%)	8	27
5	B	157/219 (72%)	151 (96%)	6 (4%)	29	64
5	I	144/219 (66%)	137 (95%)	7 (5%)	22	54
All	All	1052/1536 (68%)	1005 (96%)	47 (4%)	24	58

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	228	THR
2	C	247	VAL
3	D	97	ARG
3	D	98	ASP
4	A	7	THR
4	A	60	THR
4	A	66	LEU
4	A	89	MET
4	A	112	LEU
4	A	138	VAL
4	A	195	ASN
4	A	198	ILE
5	B	13	ILE
5	B	33	VAL
5	B	48	ILE
5	B	96	VAL
5	B	99	PRO
5	B	187	ARG
2	F	23	ILE
2	F	34	VAL
2	F	75	ARG
2	F	116	ASP
2	F	127	ASN
2	F	156	ARG
2	F	182	THR
2	F	187	THR
2	F	200	THR
2	F	248	VAL
2	F	249	VAL
4	H	21	LEU
4	H	49	ILE
4	H	60	THR
4	H	66	LEU

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Mol	Chain	Res	Type
4	H	69	GLN
4	H	78	VAL
4	H	138	VAL
4	H	171	MET
4	H	175	SER
4	H	197	ILE
4	H	198	ILE
5	I	8	THR
5	I	12	LEU
5	I	56	ARG
5	I	101	THR
5	I	146	LEU
5	I	171	CYS
5	I	231	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	87	GLN
4	A	67	ASN
4	A	69	GLN
5	B	11	HIS
2	F	87	GLN
4	H	127	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

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
6	NAG	A	301	-	14,14,15	0.34	0	17,19,21	0.55	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
6	NAG	A	301	-	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	301	NAG	O5-C5-C6-O6
6	A	301	NAG	C4-C5-C6-O6
6	A	301	NAG	C8-C7-N2-C2
6	A	301	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	301	NAG	4	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 ⓘ

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	E	10/10 (100%)	0.39	0	100	100	20, 23, 28, 28	0
1	P	10/10 (100%)	0.54	0	100	100	24, 25, 28, 29	0
2	C	264/303 (87%)	0.84	16 (6%)	27	21	27, 33, 48, 57	0
2	F	247/303 (81%)	0.88	22 (8%)	15	13	21, 32, 52, 64	0
3	D	98/100 (98%)	1.03	11 (11%)	10	9	27, 40, 55, 64	0
3	G	98/100 (98%)	0.76	6 (6%)	27	21	24, 33, 53, 59	0
4	A	204/218 (93%)	1.01	30 (14%)	6	4	22, 33, 58, 64	0
4	H	200/218 (91%)	1.11	29 (14%)	6	4	24, 32, 54, 73	0
5	B	236/253 (93%)	0.94	22 (9%)	14	12	21, 34, 52, 60	0
5	I	225/253 (88%)	1.10	29 (12%)	7	6	26, 38, 49, 58	1 (0%)
All	All	1592/1768 (90%)	0.96	165 (10%)	11	10	20, 34, 54, 73	1 (0%)

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	17	ASN	6.6
4	H	133	SER	6.2
4	H	134	SER	5.3
2	F	192	HIS	4.3
5	B	185	ASP	4.1
4	A	119	GLN	4.1
4	A	117	TYR	4.0
4	A	206	SER	4.0
5	I	171	CYS	3.9
2	F	230	LEU	3.9
4	H	198	ILE	3.8
4	H	57	GLN	3.7
5	I	231	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
4	A	185	SER	3.5
5	I	139	GLN	3.5
3	D	70	PHE	3.5
4	H	135	ASP	3.4
5	B	186	SER	3.4
5	B	224	THR	3.4
5	I	201	TRP	3.4
2	F	18	GLY	3.3
4	H	200	GLU	3.3
4	H	153	SER	3.3
5	B	181	PRO	3.3
4	A	190	ALA	3.3
4	H	56	GLN	3.2
5	B	131	SER	3.1
4	A	198	ILE	3.1
2	C	249	VAL	3.1
3	D	71	THR	3.0
2	C	227	ASP	3.0
5	I	185	ASP	3.0
4	H	88	ALA	3.0
4	A	203	PHE	3.0
4	H	203	PHE	3.0
2	F	113	TYR	3.0
5	I	107	GLN	2.9
2	F	191	HIS	2.9
5	I	119	ASN	2.9
2	F	193	PRO	2.9
4	A	158	VAL	2.9
5	B	196	VAL	2.9
3	D	20	SER	2.9
5	B	197	SER	2.8
4	H	194	GLN	2.8
5	I	203	ASP	2.8
5	I	186	SER	2.8
2	F	248	VAL	2.8
4	A	195	ASN	2.8
2	F	238	ASP	2.8
2	F	71	SER	2.8
3	G	38	ASP	2.8
3	D	87	LEU	2.7
4	A	201	ASP	2.7
5	B	30	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
4	A	182	SER	2.7
4	H	158	VAL	2.7
2	C	178	THR	2.7
3	G	98	ASP	2.7
2	C	271	THR	2.6
2	C	34	VAL	2.6
2	F	89	GLU	2.6
4	H	206	SER	2.6
5	B	227	ARG	2.6
2	F	239	GLY	2.6
4	A	172	ASP	2.6
4	H	172	ASP	2.6
2	F	260	HIS	2.6
4	A	157	ASP	2.6
2	F	228	THR	2.6
5	I	184	GLN	2.6
4	A	191	ASN	2.6
4	H	145	ASP	2.6
4	H	188	THR	2.5
5	I	219	GLU	2.5
3	D	59	ASP	2.5
4	A	134	SER	2.5
3	D	54	LEU	2.5
2	C	18	GLY	2.5
4	A	120	ASN	2.5
4	A	118	ILE	2.4
4	H	183	GLN	2.4
4	A	188	THR	2.4
4	H	195	ASN	2.4
3	G	76	ASP	2.4
3	D	22	PHE	2.4
4	A	194	GLN	2.4
3	G	23	LEU	2.4
5	B	119	ASN	2.4
4	A	65	SER	2.4
4	A	156	SER	2.4
5	I	17	GLY	2.4
4	H	186	ASP	2.4
4	H	201	ASP	2.4
5	I	24	CYS	2.4
5	I	73	LEU	2.4
2	F	249	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	259	CYS	2.3
2	F	128	GLU	2.3
2	F	217	TRP	2.3
4	H	197	ILE	2.3
2	C	177	GLU	2.3
4	H	126	TYR	2.3
2	F	261	VAL	2.3
3	D	18	GLY	2.3
2	C	58	GLU	2.2
5	B	220	ASN	2.2
5	B	194	LEU	2.2
5	B	139	GLN	2.2
4	H	55	ASP	2.2
5	I	81	SER	2.2
2	F	166	ASP	2.2
2	C	88	SER	2.2
5	I	25	SER	2.2
4	A	193	PHE	2.2
2	F	229	GLU	2.2
4	A	113	LEU	2.2
5	I	183	LEU	2.2
2	C	35	ARG	2.2
4	H	199	PRO	2.2
5	B	144	VAL	2.2
5	I	196	VAL	2.2
2	C	240	THR	2.2
5	I	238	GLU	2.2
5	B	193	ARG	2.2
5	I	154	HIS	2.2
4	H	132	LYS	2.2
4	A	204	PHE	2.2
5	B	171	CYS	2.2
5	I	117	LEU	2.2
5	I	202	GLN	2.1
2	C	158	VAL	2.1
5	B	226	ASP	2.1
3	D	48	LYS	2.1
5	B	104	PHE	2.1
5	I	215	TYR	2.1
5	B	218	SER	2.1
5	I	141	ALA	2.1
3	G	75	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
5	B	221	ASP	2.1
4	H	178	ALA	2.1
5	B	133	ALA	2.1
4	A	46	ILE	2.1
5	I	218	SER	2.1
4	H	162	ASP	2.1
2	F	245	ALA	2.1
3	G	78	TYR	2.1
5	B	48	ILE	2.1
5	I	158	SER	2.1
4	A	152	GLN	2.1
4	A	154	LYS	2.1
2	C	175	GLY	2.1
2	C	140	ALA	2.1
4	A	133	SER	2.0
5	I	131	SER	2.0
2	F	151	HIS	2.0
5	I	175	GLN	2.0
5	I	180	GLN	2.0
2	C	152	ALA	2.0
4	A	163	LYS	2.0
4	H	205	PRO	2.0
2	C	130	LEU	2.0
3	D	97	ARG	2.0
4	A	135	ASP	2.0
4	H	138	VAL	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
6	NAG	A	301	14/15	0.80	0.16	33,34,35,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.