



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 05:42 PM UTC

PDB ID : 4P4K / pdb_00004p4k
Title : Structural Basis of Chronic Beryllium Disease: Bridging the Gap Between allergic hypersensitivity and auto immunity
Authors : Clayton, G.M.; Crawford, F.; Kappler, J.W.
Deposited on : 2014-03-12
Resolution : 2.80 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:

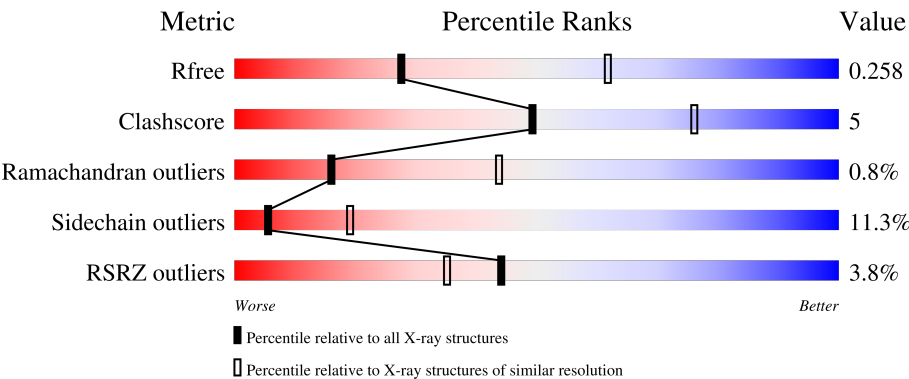
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	183	
1	E	183	
2	B	212	
2	F	212	
3	C	209	

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Mol	Chain	Length	Quality of chain
3	G	209	9% 72% 21% ...
4	D	242	1% 81% 16% .
4	H	242	2% 74% 21% ...

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13276 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 II histocompatibility antigen, DP alpha 1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1449	936	234	274	5			
1	E	181	Total	C	N	O	S	0	0	0
			1470	951	238	276	5			

- Molecule 2 is a protein called mim2 peptide,HLA class II histocompatibility antigen, DP beta 1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	199	Total	C	N	O	S	0	0	0
			1596	1006	275	307	8			
2	F	199	Total	C	N	O	S	0	0	0
			1622	1022	283	309	8			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	GLY	-	linker	UNP P04440
B	-13	GLY	-	linker	UNP P04440
B	-12	GLY	-	linker	UNP P04440
B	-11	SER	-	linker	UNP P04440
B	-10	LEU	-	linker	UNP P04440
B	-9	VAL	-	linker	UNP P04440
B	-8	PRO	-	linker	UNP P04440
B	-7	ARG	-	linker	UNP P04440
B	-6	GLY	-	linker	UNP P04440
B	-5	SER	-	linker	UNP P04440
B	-4	GLY	-	linker	UNP P04440
B	-3	GLY	-	linker	UNP P04440
B	-2	GLY	-	linker	UNP P04440
B	-1	GLY	-	linker	UNP P04440
B	3	SER	THR	variant	UNP P04440
B	36	VAL	ALA	variant	UNP P04440

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Chain	Residue	Modelled	Actual	Comment	Reference
B	55	ASP	ALA	variant	UNP P04440
B	56	GLU	ALA	variant	UNP P04440
B	69	GLU	LYS	variant	UNP P04440
F	-14	GLY	-	linker	UNP P04440
F	-13	GLY	-	linker	UNP P04440
F	-12	GLY	-	linker	UNP P04440
F	-11	SER	-	linker	UNP P04440
F	-10	LEU	-	linker	UNP P04440
F	-9	VAL	-	linker	UNP P04440
F	-8	PRO	-	linker	UNP P04440
F	-7	ARG	-	linker	UNP P04440
F	-6	GLY	-	linker	UNP P04440
F	-5	SER	-	linker	UNP P04440
F	-4	GLY	-	linker	UNP P04440
F	-3	GLY	-	linker	UNP P04440
F	-2	GLY	-	linker	UNP P04440
F	-1	GLY	-	linker	UNP P04440
F	3	SER	THR	variant	UNP P04440
F	36	VAL	ALA	variant	UNP P04440
F	55	ASP	ALA	variant	UNP P04440
F	56	GLU	ALA	variant	UNP P04440
F	69	GLU	LYS	variant	UNP P04440

- Molecule 3 is a protein called hTCRav22 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	204	Total	C	N	O	S	0	0	0
			1522	967	236	311	8			
3	G	203	Total	C	N	O	S	0	0	0
			1496	947	233	308	8			

- Molecule 4 is a protein called hTCRav22 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1871	1178	330	357	6			
4	H	239	Total	C	N	O	S	0	0	0
			1846	1166	319	355	6			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Na	0	0
			1	1		
6	F	1	Total	Na	0	0
			1	1		

- Molecule 7 is BERYLLIUM (CCD ID: 0BE) (formula: Be).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Be	0	0
			1	1		
7	F	1	Total	Be	0	0
			1	1		

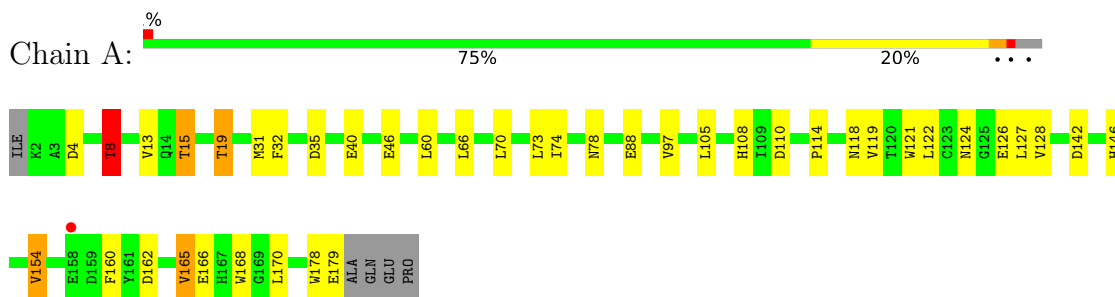
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	33	Total 33	O 33	0	0
8	B	44	Total 44	O 44	0	0
8	C	22	Total 22	O 22	0	0
8	D	41	Total 41	O 41	0	0
8	E	55	Total 55	O 55	0	0
8	F	55	Total 55	O 55	0	0
8	G	19	Total 19	O 19	0	0
8	H	61	Total 61	O 61	0	0

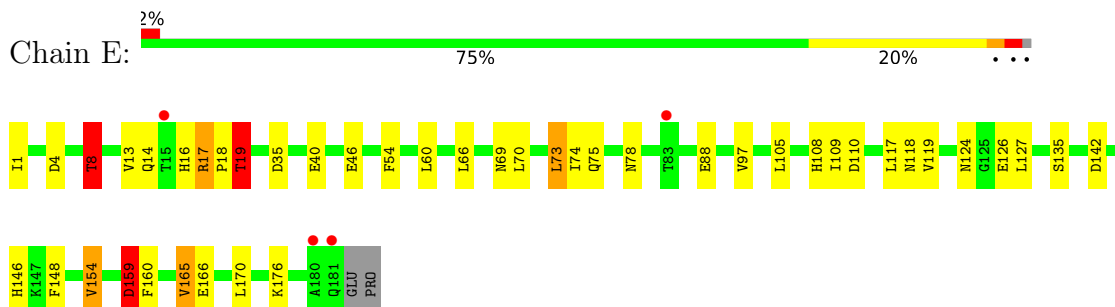
3 Residue-property plots [i](#)

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.

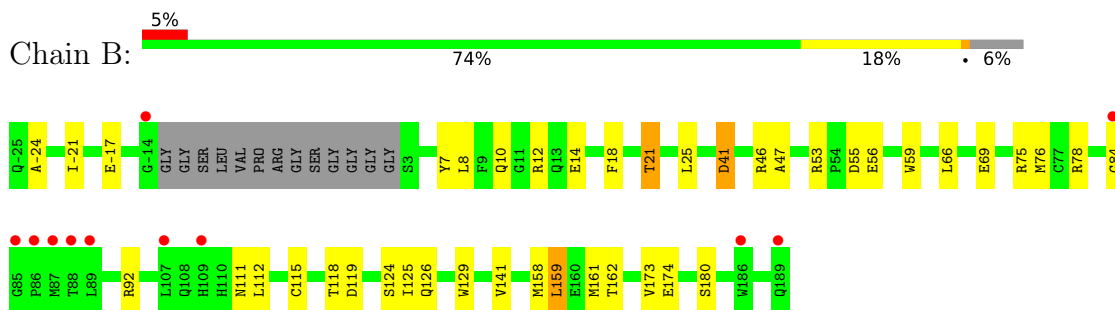
- Molecule 1: HLA class II histocompatibility antigen, DP alpha 1 chain



- Molecule 1: HLA class II histocompatibility antigen, DP alpha 1 chain

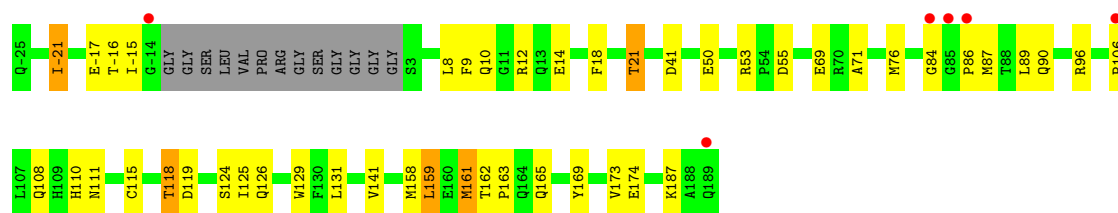


- Molecule 2: mim2 peptide,HLA class II histocompatibility antigen, DP beta 1 chain

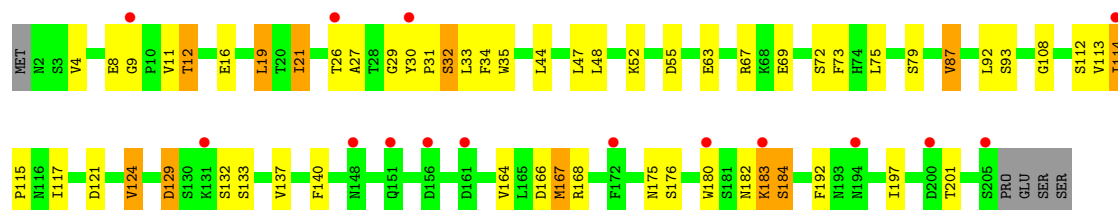


- Molecule 2: mim2 peptide,HLA class II histocompatibility antigen, DP beta 1 chain

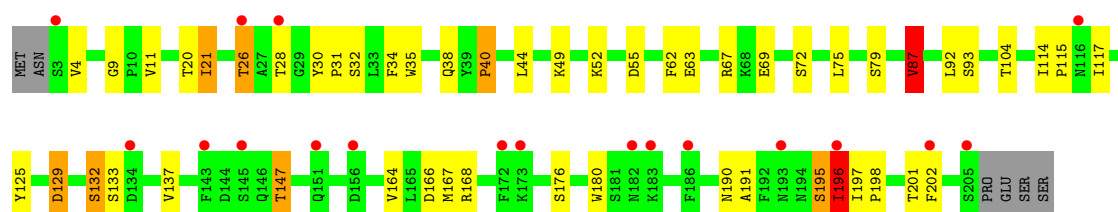
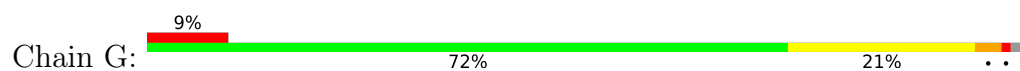




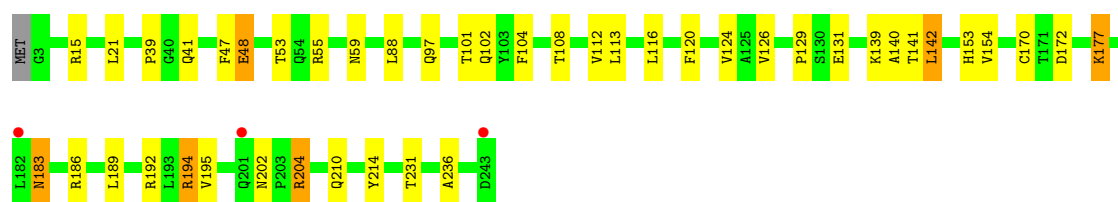
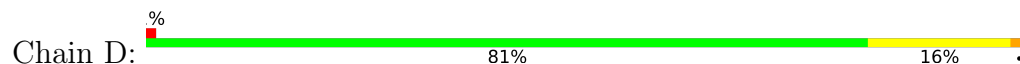
• Molecule 3: hTCRav22 alpha chain



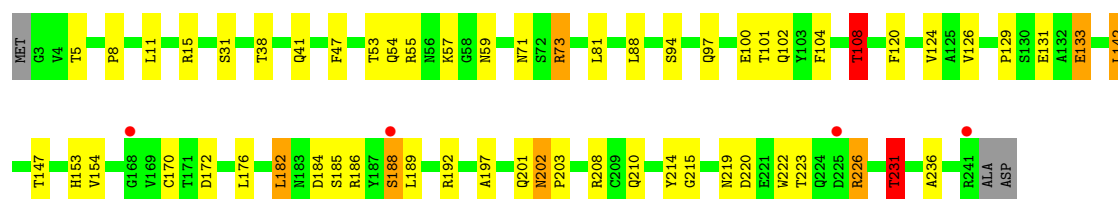
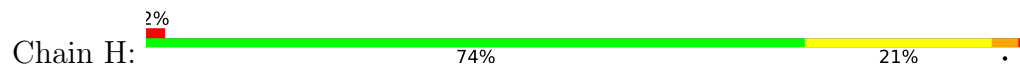
• Molecule 3: hTCRav22 alpha chain



• Molecule 4: hTCRav22 beta chain



• Molecule 4: hTCRav22 beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.40Å 137.24Å 213.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.70 – 2.80 39.70 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.70-2.80) 99.9 (39.70-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.204 , 0.252 0.211 , 0.258	Depositor DCC
R_{free} test set	2949 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	58.9	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13276	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6495e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.80	0/1497	1.46	15/2045 (0.7%)
1	E	0.83	0/1518	1.42	13/2074 (0.6%)
2	B	0.84	1/1637 (0.1%)	1.36	5/2230 (0.2%)
2	F	0.84	0/1664	1.36	8/2263 (0.4%)
3	C	0.89	0/1557	1.52	25/2122 (1.2%)
3	G	0.89	1/1530 (0.1%)	1.50	21/2090 (1.0%)
4	D	0.84	0/1922	1.33	7/2619 (0.3%)
4	H	0.83	0/1897	1.37	11/2589 (0.4%)
All	All	0.85	2/13222 (0.0%)	1.41	105/18032 (0.6%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	30	TYR	CA-C	6.01	1.59	1.52
2	B	180	SER	CA-C	5.24	1.57	1.52

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	124	VAL	N-CA-CB	8.30	122.22	112.35
3	G	195	SER	CA-C-N	7.47	135.41	121.97
3	G	195	SER	C-N-CA	7.47	135.41	121.97
1	E	159	ASP	CA-CB-CG	7.19	119.79	112.60
1	A	178	TRP	CA-C-N	6.90	134.12	121.70
1	A	178	TRP	C-N-CA	6.90	134.12	121.70
3	C	114	ILE	CB-CA-C	6.85	118.03	110.71
1	A	74	ILE	N-CA-C	-6.73	103.96	110.42
1	E	154	VAL	CB-CA-C	6.72	118.91	111.18
1	E	74	ILE	N-CA-C	-6.60	104.08	110.42
2	F	119	ASP	N-CA-C	6.50	120.56	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	41	ASP	CA-CB-CG	6.47	119.07	112.60
2	B	119	ASP	N-CA-C	6.45	120.50	112.24
3	C	19	LEU	CD1-CG-CD2	6.44	124.98	110.80
2	B	41	ASP	CA-CB-CG	6.43	119.03	112.60
1	A	154	VAL	CB-CA-C	6.38	118.52	111.18
3	C	133	SER	CA-C-N	6.31	129.03	120.38
3	C	133	SER	C-N-CA	6.31	129.03	120.38
3	C	129	ASP	CA-CB-CG	6.25	118.84	112.60
3	G	196	ILE	N-CA-C	6.24	122.31	109.34
3	C	26	THR	CB-CA-C	6.21	119.56	111.42
3	G	133	SER	CA-C-N	6.14	128.79	120.38
3	G	133	SER	C-N-CA	6.14	128.79	120.38
1	A	110	ASP	CA-CB-CG	6.11	118.71	112.60
3	C	124	VAL	CB-CA-C	6.05	117.81	111.09
4	H	222	TRP	N-CA-C	6.03	118.26	108.26
3	G	129	ASP	CA-CB-CG	6.01	118.61	112.60
3	C	87	VAL	CB-CA-C	6.00	119.28	110.77
2	B	162	THR	CB-CA-C	5.92	122.14	111.12
1	E	142	ASP	CA-CB-CG	5.92	118.52	112.60
3	C	113	VAL	CA-C-N	5.92	126.85	122.59
3	C	113	VAL	C-N-CA	5.92	126.85	122.59
1	A	142	ASP	CA-CB-CG	5.90	118.50	112.60
1	A	35	ASP	N-CA-C	-5.77	99.72	108.67
4	H	108	THR	CB-CA-C	5.74	120.15	110.79
3	G	28	THR	N-CA-C	-5.73	103.54	110.88
3	C	21	ILE	N-CA-CB	5.70	119.08	111.90
3	G	40	PRO	N-CA-C	5.65	124.11	112.47
3	C	55	ASP	CA-CB-CG	5.65	118.25	112.60
2	F	110	HIS	N-CA-C	5.64	118.41	110.23
1	E	4	ASP	CA-CB-CG	5.61	118.21	112.60
3	G	190	ASN	CA-CB-CG	5.60	118.20	112.60
2	F	162	THR	CB-CA-C	5.58	121.99	111.29
1	E	35	ASP	N-CA-C	-5.55	100.06	108.67
4	H	131	GLU	CA-C-N	5.52	127.62	120.44
4	H	131	GLU	C-N-CA	5.52	127.62	120.44
3	G	62	PHE	CA-CB-CG	5.49	119.29	113.80
4	D	131	GLU	CA-C-N	5.49	127.58	120.44
4	D	131	GLU	C-N-CA	5.49	127.58	120.44
3	C	166	ASP	CA-CB-CG	5.49	118.09	112.60
4	H	202	ASN	N-CA-C	5.48	117.56	109.50
4	D	183	ASN	CA-CB-CG	5.48	118.08	112.60
2	F	159	LEU	N-CA-CB	5.48	119.51	110.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	117	ILE	CB-CA-C	5.46	118.19	111.25
1	A	97	VAL	N-CA-CB	5.46	116.88	110.82
3	G	21	ILE	N-CA-CB	5.44	118.76	111.90
3	G	166	ASP	CA-CB-CG	5.43	118.03	112.60
4	H	231	THR	N-CA-C	-5.42	101.82	109.96
1	A	88	GLU	N-CA-C	-5.42	99.90	108.73
1	A	154	VAL	N-CA-CB	5.41	118.60	111.40
2	B	159	LEU	N-CA-CB	5.41	119.40	110.69
4	D	231	THR	N-CA-C	-5.41	101.85	109.96
3	G	87	VAL	CB-CA-C	5.40	118.44	110.77
3	C	114	ILE	N-CA-C	5.39	113.20	107.76
1	E	78	ASN	CA-CB-CG	5.38	117.98	112.60
3	C	72	SER	N-CA-C	5.37	117.35	109.24
1	E	154	VAL	N-CA-CB	5.37	118.54	111.40
1	A	78	ASN	CA-CB-CG	5.33	117.93	112.60
1	E	97	VAL	N-CA-CB	5.31	116.72	110.82
1	A	8	THR	N-CA-C	5.31	118.10	109.24
4	D	39	PRO	CA-C-N	5.30	125.72	119.94
4	D	39	PRO	C-N-CA	5.30	125.72	119.94
3	G	55	ASP	CA-CB-CG	5.27	117.87	112.60
4	H	133	GLU	CA-C-N	5.24	127.16	120.56
4	H	133	GLU	C-N-CA	5.24	127.16	120.56
1	A	4	ASP	CA-CB-CG	5.24	117.84	112.60
3	C	167	MET	CA-C-N	5.23	131.52	121.54
3	C	167	MET	C-N-CA	5.23	131.52	121.54
4	H	185	SER	N-CA-C	5.20	117.57	110.24
1	E	88	GLU	N-CA-C	-5.19	100.84	109.46
3	C	175	ASN	CA-CB-CG	5.18	117.78	112.60
4	H	184	ASP	CA-CB-CG	5.18	117.78	112.60
3	G	167	MET	CA-C-N	5.17	131.41	121.54
3	G	167	MET	C-N-CA	5.17	131.41	121.54
4	H	102	GLN	N-CA-C	5.16	118.23	109.76
1	E	19	THR	CB-CA-C	5.14	121.16	110.32
1	E	8	THR	N-CA-C	5.13	117.80	109.24
1	E	110	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	19	THR	CB-CA-C	5.10	121.09	110.32
2	F	163	PRO	N-CA-C	5.09	118.48	110.80
3	C	183	LYS	CA-C-N	5.08	130.84	121.70
3	C	183	LYS	C-N-CA	5.08	130.84	121.70
3	C	117	ILE	CB-CA-C	5.08	117.70	111.25
4	D	102	GLN	N-CA-C	5.05	118.03	109.76
3	C	184	SER	CA-C-N	5.04	129.15	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	184	SER	C-N-CA	5.04	129.15	120.72
1	A	4	ASP	N-CA-C	-5.04	105.49	111.69
3	G	72	SER	N-CA-C	5.04	116.72	109.07
2	F	71	ALA	CA-C-N	5.03	125.26	120.43
2	F	71	ALA	C-N-CA	5.03	125.26	120.43
3	G	202	PHE	CA-CB-CG	5.03	118.83	113.80
3	G	26	THR	CA-C-N	5.02	128.34	120.75
3	G	26	THR	C-N-CA	5.02	128.34	120.75
3	C	32	SER	N-CA-C	-5.02	102.09	110.17
2	B	-24	ALA	N-CA-C	5.01	118.37	109.96

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1449	0	1330	18	0
1	E	1470	0	1362	19	0
2	B	1596	0	1450	13	0
2	F	1622	0	1499	17	0
3	C	1522	0	1400	23	0
3	G	1496	0	1352	19	0
4	D	1871	0	1740	17	0
4	H	1846	0	1712	21	0
5	A	28	0	26	1	0
5	B	14	0	13	0	0
5	E	28	0	26	0	0
6	B	1	0	0	0	0
6	F	1	0	0	0	0
7	B	1	0	0	0	0
7	F	1	0	0	0	0
8	A	33	0	0	0	0
8	B	44	0	0	6	0
8	C	22	0	0	0	0
8	D	41	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	E	55	0	0	2	0
8	F	55	0	0	0	0
8	G	19	0	0	1	0
8	H	61	0	0	2	0
All	All	13276	0	11910	133	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 5.

All (133) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:183:LYS:HB3	3:C:184:SER:HA	1.54	0.90
1:E:108:HIS:HE1	1:E:146:HIS:HD2	1.24	0.84
1:A:114:PRO:HG3	8:B:339:HOH:O	1.81	0.80
4:H:8:PRO:O	4:H:108:THR:HB	1.84	0.78
1:A:108:HIS:HE1	1:A:146:HIS:CD2	2.03	0.75
1:A:114:PRO:HB3	8:B:339:HOH:O	1.87	0.74
1:A:108:HIS:HE1	1:A:146:HIS:HD2	1.31	0.74
1:E:108:HIS:HE1	1:E:146:HIS:CD2	2.04	0.74
4:D:21:LEU:HD22	4:D:108:THR:HG21	1.70	0.73
1:E:124:ASN:HD21	1:E:159:ASP:HB3	1.54	0.72
2:B:78:ARG:HD2	3:C:30:TYR:HE1	1.56	0.71
3:C:34:PHE:HE2	3:C:93:SER:HB2	1.56	0.70
3:G:115:PRO:HG3	3:G:164:VAL:HG21	1.74	0.69
3:G:34:PHE:HE2	3:G:93:SER:HB2	1.57	0.69
1:A:114:PRO:CB	8:B:339:HOH:O	2.39	0.69
4:D:120:PHE:CD1	4:D:186:ARG:HD3	2.28	0.68
4:D:139:LYS:HB3	4:D:194:ARG:HD3	1.77	0.66
1:A:114:PRO:CG	8:B:339:HOH:O	2.43	0.66
1:E:108:HIS:CE1	1:E:146:HIS:HD2	2.11	0.65
4:D:177:LYS:HD3	4:D:177:LYS:H	1.62	0.65
2:F:-17:GLU:OE1	2:F:69:GLU:OE2	2.15	0.64
3:G:34:PHE:CE2	3:G:93:SER:HB2	2.33	0.63
2:F:86:PRO:HA	2:F:90:GLN:HB2	1.79	0.63
3:C:34:PHE:CE2	3:C:93:SER:HB2	2.33	0.63
1:A:15:THR:HG23	2:B:7:TYR:H	1.61	0.63
3:C:183:LYS:HB3	3:C:184:SER:CA	2.29	0.62
3:G:4:VAL:CG2	3:G:92:LEU:HG	2.30	0.62
2:B:18:PHE:O	2:B:21:THR:HG22	2.00	0.62
1:A:118:ASN:HB2	1:A:166:GLU:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:THR:HG21	8:E:351:HOH:O	2.00	0.61
2:F:18:PHE:O	2:F:21:THR:HG22	2.00	0.60
2:B:53:ARG:HD3	2:F:53:ARG:NH2	2.17	0.59
2:B:47:ALA:O	8:B:327:HOH:O	2.17	0.59
1:E:17:ARG:HA	1:E:18:PRO:C	2.28	0.59
1:A:108:HIS:CE1	1:A:146:HIS:HD2	2.17	0.58
2:B:8:LEU:HD21	2:B:10:GLN:HG3	1.85	0.58
4:D:202:ASN:HD21	4:D:204:ARG:HB2	1.68	0.58
1:E:118:ASN:HB2	1:E:166:GLU:HB2	1.84	0.58
2:F:8:LEU:HD21	2:F:10:GLN:HG3	1.86	0.58
4:D:177:LYS:H	4:D:177:LYS:CD	2.17	0.57
3:G:4:VAL:HG22	3:G:92:LEU:HG	1.86	0.57
4:D:55:ARG:NH2	4:D:97:GLN:O	2.35	0.57
2:F:111:ASN:HB3	2:F:161:MET:HE3	1.87	0.56
2:B:-17:GLU:OE1	2:B:69:GLU:OE2	2.23	0.56
4:H:197:ALA:O	4:H:201:GLN:HG2	2.06	0.55
1:E:69:ASN:HD21	2:F:-16:THR:HA	1.72	0.55
1:E:146:HIS:HE1	8:E:317:HOH:O	1.90	0.54
1:E:14:GLN:NE2	1:E:16:HIS:O	2.40	0.54
1:E:69:ASN:ND2	2:F:-15:ILE:H	2.05	0.54
3:C:47:LEU:HG	3:C:48:LEU:HD13	1.89	0.53
2:F:126:GLN:HB2	2:F:174:GLU:HB2	1.91	0.53
3:G:147:THR:HG21	3:G:198:PRO:HG3	1.91	0.52
3:G:137:VAL:HG12	3:G:180:TRP:HB3	1.91	0.52
3:C:115:PRO:HG3	3:C:164:VAL:HG21	1.92	0.52
1:E:17:ARG:HA	1:E:19:THR:N	2.25	0.51
2:F:50:GLU:HG2	2:F:53:ARG:NH2	2.25	0.51
2:F:96:ARG:HB2	2:F:118:THR:HG22	1.93	0.50
1:A:122:LEU:HB2	1:A:162:ASP:HB2	1.93	0.50
3:C:129:ASP:HB3	3:C:132:SER:O	2.12	0.50
4:D:48:GLU:OE2	4:D:55:ARG:NH1	2.44	0.50
4:H:31:SER:HB3	4:H:94:SER:HB3	1.94	0.50
8:B:327:HOH:O	2:F:50:GLU:HG3	2.12	0.49
3:G:44:LEU:O	4:H:104:PHE:HB2	2.13	0.49
3:C:33:LEU:HD23	3:C:73:PHE:HB2	1.95	0.49
3:G:38:GLN:HB3	3:G:87:VAL:HG13	1.94	0.49
3:G:129:ASP:HB3	3:G:132:SER:O	2.13	0.49
4:H:226:ARG:HH11	4:H:226:ARG:HB3	1.78	0.49
4:D:129:PRO:HD3	4:D:142:LEU:HG	1.95	0.49
1:E:109:ILE:HG21	1:E:117:LEU:HD21	1.93	0.49
4:H:71:ASN:OD1	4:H:73:ARG:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:12:THR:HG23	3:C:112:SER:HB2	1.94	0.48
4:D:172:ASP:HB2	4:D:189:LEU:HD12	1.95	0.48
4:D:126:VAL:HG23	4:D:236:ALA:HB3	1.94	0.48
4:H:126:VAL:HG23	4:H:236:ALA:HB3	1.95	0.48
2:B:46:ARG:HA	2:B:56:GLU:HG3	1.95	0.47
4:D:202:ASN:ND2	4:D:204:ARG:HB2	2.28	0.47
1:E:135:SER:HB2	1:E:148:PHE:H	1.79	0.47
4:H:129:PRO:HD3	4:H:142:LEU:HG	1.96	0.47
4:H:55:ARG:NH2	4:H:97:GLN:O	2.41	0.47
1:A:124:ASN:HA	1:A:160:PHE:CE1	2.50	0.46
4:H:172:ASP:HB2	4:H:189:LEU:HD12	1.97	0.46
4:D:141:THR:OG1	4:D:194:ARG:HG3	2.15	0.46
1:E:124:ASN:HA	1:E:160:PHE:CE2	2.51	0.46
3:G:21:ILE:HD12	3:G:75:LEU:HD23	1.98	0.45
2:F:115:CYS:HB2	2:F:129:TRP:CZ2	2.51	0.45
3:G:34:PHE:HE2	3:G:93:SER:CB	2.28	0.45
1:A:121:TRP:CB	1:A:128:VAL:HG22	2.46	0.45
3:C:137:VAL:HG12	3:C:180:TRP:HB3	1.98	0.45
2:B:115:CYS:HB2	2:B:129:TRP:CZ2	2.52	0.44
3:C:183:LYS:CB	3:C:184:SER:HA	2.34	0.44
4:D:129:PRO:HG3	4:D:140:ALA:HB1	2.00	0.44
3:G:49:LYS:NZ	8:G:311:HOH:O	2.41	0.44
4:H:120:PHE:CD2	4:H:186:ARG:HD3	2.53	0.44
2:F:131:LEU:HD13	2:F:169:TYR:CE1	2.52	0.44
2:B:126:GLN:HB2	2:B:174:GLU:HB2	2.00	0.44
4:H:54:GLN:NE2	4:H:57:LYS:HB2	2.33	0.44
3:C:34:PHE:HE2	3:C:93:SER:CB	2.28	0.43
3:G:93:SER:OG	4:H:100:GLU:HG2	2.18	0.43
1:E:54:PHE:HE1	2:F:-21:ILE:HG23	1.83	0.43
3:C:44:LEU:O	4:D:104:PHE:HB2	2.18	0.43
3:G:32:SER:HB2	3:G:93:SER:HB3	2.00	0.43
3:C:4:VAL:HG22	3:C:92:LEU:HG	2.00	0.43
3:G:35:TRP:CE2	3:G:75:LEU:HB2	2.54	0.43
3:G:92:LEU:HB2	3:G:104:THR:HB	2.01	0.43
2:B:111:ASN:HB3	2:B:161:MET:HE3	2.01	0.43
3:C:32:SER:HB2	3:C:93:SER:HB3	2.00	0.43
4:H:5:THR:HA	8:H:351:HOH:O	2.18	0.43
3:C:35:TRP:CE2	3:C:75:LEU:HB2	2.54	0.42
1:A:121:TRP:HB2	1:A:128:VAL:HG22	2.01	0.42
1:A:8:THR:HB	2:B:14:GLU:HA	2.01	0.42
3:C:21:ILE:HD12	3:C:75:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:140:PHE:HB2	3:C:192:PHE:CE1	2.55	0.42
4:H:54:GLN:HE22	4:H:57:LYS:HD3	1.85	0.41
4:H:202:ASN:HA	4:H:203:PRO:HD3	1.89	0.41
3:C:4:VAL:CG2	3:C:92:LEU:HG	2.50	0.41
3:G:31:PRO:HB2	3:G:92:LEU:HD22	2.01	0.41
4:D:153:HIS:HB3	4:D:214:TYR:HB2	2.02	0.41
4:H:208:ARG:NH2	8:H:301:HOH:O	2.45	0.41
4:H:215:GLY:H	4:H:231:THR:HG22	1.85	0.41
4:H:147:THR:HG22	4:H:188:SER:HB3	2.03	0.41
3:C:31:PRO:HB2	3:C:92:LEU:HD22	2.03	0.41
4:H:153:HIS:HB3	4:H:214:TYR:HB2	2.02	0.41
2:B:-17:GLU:HB2	2:B:59:TRP:CZ2	2.56	0.41
3:C:167:MET:SD	4:D:194:ARG:HD2	2.61	0.41
1:E:73:LEU:HD13	2:F:9:PHE:HE2	1.86	0.41
3:G:125:TYR:CE1	4:H:133:GLU:HG3	2.56	0.41
1:A:119:VAL:HG22	1:A:165:VAL:HB	2.03	0.40
1:A:31:MET:HG2	1:A:32:PHE:HD2	1.86	0.40
1:A:105:LEU:HD23	1:A:105:LEU:HA	1.96	0.40
1:E:8:THR:HB	2:F:14:GLU:HA	2.03	0.40
3:C:27:ALA:HB3	3:C:31:PRO:HG3	2.02	0.40
1:E:119:VAL:HG22	1:E:165:VAL:HB	2.04	0.40
1:A:168:TRP:CD1	5:A:202:NAG:H82	2.57	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	176/183 (96%)	173 (98%)	3 (2%)	0	100	100
1	E	179/183 (98%)	174 (97%)	5 (3%)	0	100	100
2	B	195/212 (92%)	183 (94%)	11 (6%)	1 (0%)	24	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	195/212 (92%)	184 (94%)	9 (5%)	2 (1%)	12	38
3	C	202/209 (97%)	178 (88%)	20 (10%)	4 (2%)	6	21
3	G	201/209 (96%)	182 (90%)	14 (7%)	5 (2%)	4	16
4	D	239/242 (99%)	231 (97%)	8 (3%)	0	100	100
4	H	237/242 (98%)	225 (95%)	11 (5%)	1 (0%)	30	60
All	All	1624/1692 (96%)	1530 (94%)	81 (5%)	13 (1%)	16	44

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	29	GLY
3	C	168	ARG
2	F	84	GLY
3	G	40	PRO
3	G	168	ARG
3	C	9	GLY
2	F	106	PRO
2	B	84	GLY
4	H	182	LEU
3	G	191	ALA
3	G	196	ILE
3	C	108	GLY
3	G	9	GLY

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	157/164 (96%)	141 (90%)	16 (10%)	7	23
1	E	159/164 (97%)	139 (87%)	20 (13%)	4	15
2	B	168/186 (90%)	150 (89%)	18 (11%)	6	21
2	F	174/186 (94%)	156 (90%)	18 (10%)	7	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	164/184 (89%)	146 (89%)	18 (11%)	6	20
3	G	159/184 (86%)	142 (89%)	17 (11%)	6	21
4	D	198/211 (94%)	176 (89%)	22 (11%)	6	20
4	H	197/211 (93%)	171 (87%)	26 (13%)	4	14
All	All	1376/1490 (92%)	1221 (89%)	155 (11%)	5	19

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	13	VAL
1	A	15	THR
1	A	19	THR
1	A	40	GLU
1	A	46	GLU
1	A	60	LEU
1	A	66	LEU
1	A	70	LEU
1	A	73	LEU
1	A	126	GLU
1	A	127	LEU
1	A	154	VAL
1	A	165	VAL
1	A	170	LEU
1	A	179	GLU
2	B	-21	ILE
2	B	12	ARG
2	B	21	THR
2	B	25	LEU
2	B	41	ASP
2	B	55	ASP
2	B	66	LEU
2	B	75	ARG
2	B	76	MET
2	B	92	ARG
2	B	112	LEU
2	B	118	THR
2	B	124	SER
2	B	125	ILE
2	B	141	VAL
2	B	158	MET

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Mol	Chain	Res	Type
2	B	159	LEU
2	B	173	VAL
3	C	8	GLU
3	C	11	VAL
3	C	12	THR
3	C	16	GLU
3	C	19	LEU
3	C	52	LYS
3	C	63	GLU
3	C	67	ARG
3	C	69	GLU
3	C	79	SER
3	C	87	VAL
3	C	114	ILE
3	C	121	ASP
3	C	124	VAL
3	C	176	SER
3	C	182	ASN
3	C	197	ILE
3	C	201	THR
4	D	15	ARG
4	D	41	GLN
4	D	47	PHE
4	D	48	GLU
4	D	53	THR
4	D	59	ASN
4	D	88	LEU
4	D	101	THR
4	D	112	VAL
4	D	113	LEU
4	D	116	LEU
4	D	124	VAL
4	D	142	LEU
4	D	154	VAL
4	D	170	CYS
4	D	177	LYS
4	D	183	ASN
4	D	192	ARG
4	D	194	ARG
4	D	195	VAL
4	D	204	ARG
4	D	210	GLN

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Mol	Chain	Res	Type
1	E	1	ILE
1	E	8	THR
1	E	13	VAL
1	E	17	ARG
1	E	19	THR
1	E	40	GLU
1	E	46	GLU
1	E	60	LEU
1	E	66	LEU
1	E	70	LEU
1	E	73	LEU
1	E	75	GLN
1	E	105	LEU
1	E	126	GLU
1	E	127	LEU
1	E	154	VAL
1	E	159	ASP
1	E	165	VAL
1	E	170	LEU
1	E	176	LYS
2	F	-21	ILE
2	F	12	ARG
2	F	21	THR
2	F	55	ASP
2	F	76	MET
2	F	87	MET
2	F	89	LEU
2	F	108	GLN
2	F	118	THR
2	F	124	SER
2	F	125	ILE
2	F	141	VAL
2	F	158	MET
2	F	159	LEU
2	F	161	MET
2	F	165	GLN
2	F	173	VAL
2	F	187	LYS
3	G	11	VAL
3	G	20	THR
3	G	26	THR
3	G	52	LYS

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Mol	Chain	Res	Type
3	G	63	GLU
3	G	67	ARG
3	G	69	GLU
3	G	79	SER
3	G	87	VAL
3	G	114	ILE
3	G	132	SER
3	G	147	THR
3	G	176	SER
3	G	195	SER
3	G	196	ILE
3	G	197	ILE
3	G	201	THR
4	H	11	LEU
4	H	15	ARG
4	H	38	THR
4	H	41	GLN
4	H	47	PHE
4	H	53	THR
4	H	59	ASN
4	H	73	ARG
4	H	81	LEU
4	H	88	LEU
4	H	101	THR
4	H	108	THR
4	H	124	VAL
4	H	142	LEU
4	H	154	VAL
4	H	170	CYS
4	H	176	LEU
4	H	182	LEU
4	H	188	SER
4	H	192	ARG
4	H	210	GLN
4	H	219	ASN
4	H	220	ASP
4	H	223	THR
4	H	226	ARG
4	H	231	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	75	GLN
1	A	101	GLN
1	A	108	HIS
1	A	146	HIS
2	B	62	GLN
2	B	172	GLN
3	C	38	GLN
3	C	59	ASN
3	C	102	GLN
3	C	126	GLN
4	D	36	GLN
4	D	37	GLN
4	D	118	ASN
4	D	138	GLN
4	D	202	ASN
4	D	232	GLN
1	E	69	ASN
1	E	79	HIS
1	E	101	GLN
1	E	108	HIS
1	E	146	HIS
2	F	6	ASN
2	F	62	GLN
2	F	90	GLN
2	F	172	GLN
3	G	38	GLN
3	G	102	GLN
3	G	119	ASN
4	H	18	GLN
4	H	37	GLN
4	H	44	GLN
4	H	54	GLN
4	H	77	ASN
4	H	102	GLN
4	H	205	ASN
4	H	212	GLN
4	H	232	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	A	202	1	14,14,15	0.40	0	17,19,21	2.83	3 (17%)
5	NAG	E	202	1	14,14,15	0.40	0	17,19,21	1.26	3 (17%)
5	NAG	B	201	2	14,14,15	0.35	0	17,19,21	0.72	1 (5%)
5	NAG	A	201	1	14,14,15	0.36	0	17,19,21	1.07	3 (17%)
5	NAG	E	201	1	14,14,15	0.33	0	17,19,21	1.37	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	202	1	-	4/6/23/26	0/1/1/1
5	NAG	E	202	1	-	0/6/23/26	0/1/1/1
5	NAG	B	201	2	-	0/6/23/26	0/1/1/1
5	NAG	A	201	1	-	0/6/23/26	0/1/1/1
5	NAG	E	201	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	A	202	NAG	C1-C2-N2	10.19	126.49	110.43
5	E	201	NAG	C1-C2-N2	-5.01	102.54	110.43
5	A	202	NAG	C1-O5-C5	4.83	118.66	112.19
5	E	202	NAG	C1-O5-C5	3.23	116.51	112.19
5	E	202	NAG	C1-C2-N2	2.77	114.79	110.43
5	A	202	NAG	C2-N2-C7	2.63	126.42	122.90
5	E	202	NAG	O5-C1-C2	-2.53	107.38	111.29
5	A	201	NAG	C1-O5-C5	2.51	115.55	112.19
5	A	201	NAG	C1-C2-N2	2.51	114.38	110.43
5	B	201	NAG	C1-O5-C5	2.39	115.39	112.19
5	A	201	NAG	O5-C1-C2	-2.26	107.80	111.29

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	202	NAG	C1-C2-N2-C7
5	A	202	NAG	C8-C7-N2-C2
5	A	202	NAG	O7-C7-N2-C2
5	E	201	NAG	O5-C5-C6-O6
5	E	201	NAG	C4-C5-C6-O6
5	A	202	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	202	NAG	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

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	178/183 (97%)	-0.03	1 (0%) 85 80	38, 53, 72, 86	0
1	E	181/183 (98%)	-0.01	4 (2%) 62 52	37, 51, 70, 95	0
2	B	199/212 (93%)	0.21	11 (5%) 30 23	40, 57, 93, 107	0
2	F	199/212 (93%)	0.05	6 (3%) 52 42	35, 50, 89, 106	0
3	C	204/209 (97%)	0.66	15 (7%) 20 15	43, 67, 101, 113	0
3	G	203/209 (97%)	0.72	18 (8%) 15 11	43, 70, 94, 113	0
4	D	241/242 (99%)	0.13	3 (1%) 76 68	39, 56, 86, 110	0
4	H	239/242 (98%)	0.09	4 (1%) 69 60	34, 52, 89, 103	0
All	All	1644/1692 (97%)	0.23	62 (3%) 44 35	34, 57, 92, 113	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	205	SER	5.2
2	B	189	GLN	4.9
2	F	189	GLN	4.8
2	F	84	GLY	4.5
1	E	181	GLN	4.5
4	D	243	ASP	4.4
2	B	86	PRO	3.7
2	B	109	HIS	3.7
3	C	200	ASP	3.6
2	F	-14	GLY	3.5
1	E	15	THR	3.5
4	D	201	GLN	3.3
3	C	156	ASP	3.2
2	B	89	LEU	3.1
2	B	-14	GLY	3.1
3	G	173	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
4	H	225	ASP	3.0
3	G	28	THR	2.9
2	F	86	PRO	2.8
3	G	26	THR	2.8
2	B	107	LEU	2.8
3	C	30	TYR	2.7
2	B	85	GLY	2.7
3	C	131	LYS	2.6
2	F	85	GLY	2.6
3	C	151	GLN	2.6
2	B	84	GLY	2.6
3	G	172	PHE	2.5
3	C	183	LYS	2.5
3	G	202	PHE	2.5
3	G	145	SER	2.4
4	H	241	ARG	2.4
4	D	182	LEU	2.4
3	C	161	ASP	2.4
3	C	26	THR	2.4
3	C	148	ASN	2.3
3	C	194	ASN	2.3
3	C	172	PHE	2.3
4	H	188	SER	2.3
2	B	88	THR	2.3
3	G	3	SER	2.3
2	B	87	MET	2.2
1	A	158	GLU	2.2
3	G	156	ASP	2.2
2	F	106	PRO	2.2
3	G	186	PHE	2.2
3	C	114	ILE	2.2
3	G	196	ILE	2.2
1	E	180	ALA	2.2
3	G	143	PHE	2.1
3	G	151	GLN	2.1
3	G	182	ASN	2.1
3	G	205	SER	2.1
3	G	193	ASN	2.1
2	B	186	TRP	2.1
3	G	183	LYS	2.0
3	G	116	ASN	2.0
3	C	9	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	83	THR	2.0
4	H	168	GLY	2.0
3	G	134	ASP	2.0
3	C	180	TRP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	E	202	14/15	0.60	0.16	102,103,107,108	0
5	NAG	B	201	14/15	0.65	0.15	108,113,114,115	0
5	NAG	A	201	14/15	0.70	0.14	117,120,121,121	0
5	NAG	E	201	14/15	0.78	0.14	72,84,93,96	0
5	NAG	A	202	14/15	0.84	0.12	72,74,78,80	0
6	NA	B	202	1/1	0.84	0.14	63,63,63,63	0
6	NA	F	201	1/1	0.92	0.11	52,52,52,52	0
7	0BE	F	202	1/1	0.93	0.23	18,18,18,18	0
7	0BE	B	203	1/1	0.96	0.10	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.