



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 10:24 AM BST

PDB ID : 1TKK
Title : The Structure of a Substrate-Liganded Complex of the L-Ala-D/L-Glu Epimerase from *Bacillus subtilis*
Authors : Klenchin, V.A.; Schmidt, D.M.; Gerlt, J.A.; Rayment, I.
Deposited on : 2004-06-08
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.4.dev1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

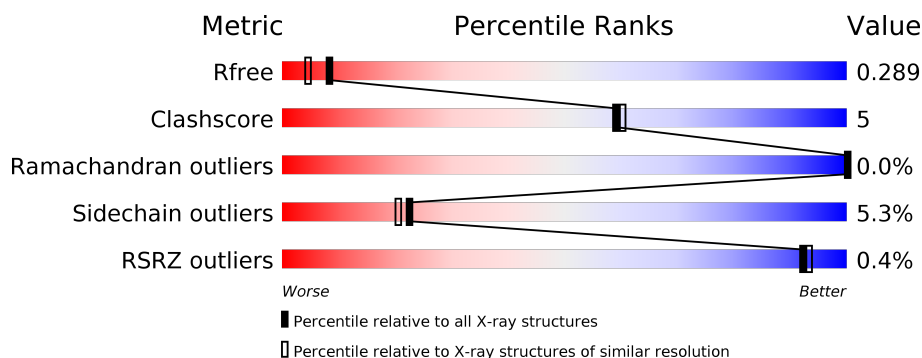
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	366	
1	B	366	
1	C	366	
1	D	366	
1	E	366	
1	F	366	

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Mol	Chain	Length	Quality of chain
1	G	366	<div><div>%</div><div><div></div></div><div>83%14%..</div></div>
1	H	366	<div><div></div><div>84%13%..</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23267 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 similar to chloromuconate cycloisomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2706	1710	461	517	18			
1	B	358	Total	C	N	O	S	0	0	0
			2697	1704	459	516	18			
1	C	359	Total	C	N	O	S	0	0	0
			2705	1710	460	517	18			
1	D	359	Total	C	N	O	S	0	0	0
			2705	1710	460	517	18			
1	E	359	Total	C	N	O	S	0	0	0
			2705	1710	460	517	18			
1	F	358	Total	C	N	O	S	0	0	0
			2697	1704	459	516	18			
1	G	359	Total	C	N	O	S	0	0	0
			2706	1710	461	517	18			
1	H	359	Total	C	N	O	S	0	0	0
			2705	1710	460	517	18			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

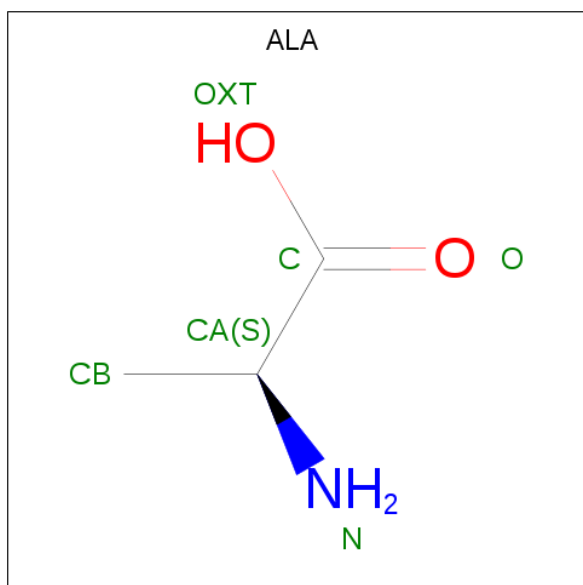
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	H	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

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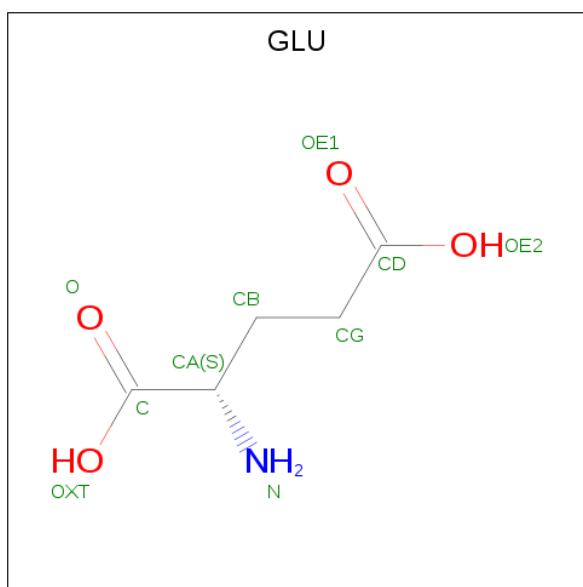
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ALANINE (three-letter code: ALA) (formula: $C_3H_7NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			5	3	1	1		
3	B	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		
3	D	1	Total	C	N	O	0	0
			5	3	1	1		
3	E	1	Total	C	N	O	0	0
			5	3	1	1		
3	F	1	Total	C	N	O	0	0
			5	3	1	1		
3	G	1	Total	C	N	O	0	0
			5	3	1	1		
3	H	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 4 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			9	5	1	3		
4	B	1	Total	C	N	O	0	0
			9	5	1	3		
4	C	1	Total	C	N	O	0	0
			9	5	1	3		
4	D	1	Total	C	N	O	0	0
			9	5	1	3		
4	E	1	Total	C	N	O	0	0
			9	5	1	3		
4	F	1	Total	C	N	O	0	0
			9	5	1	3		
4	G	1	Total	C	N	O	0	0
			9	5	1	3		
4	H	1	Total	C	N	O	0	0
			9	5	1	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	183	Total	O	0	0
			183	183		
5	B	174	Total	O	0	0
			174	174		
5	C	200	Total	O	0	0
			200	200		
5	D	194	Total	O	0	0
			194	194		

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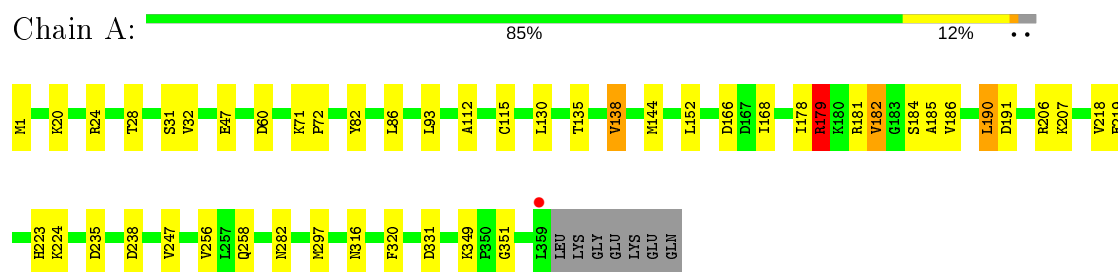
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	214	Total 214	O 214	0	0
5	F	180	Total 180	O 180	0	0
5	G	168	Total 168	O 168	0	0
5	H	208	Total 208	O 208	0	0

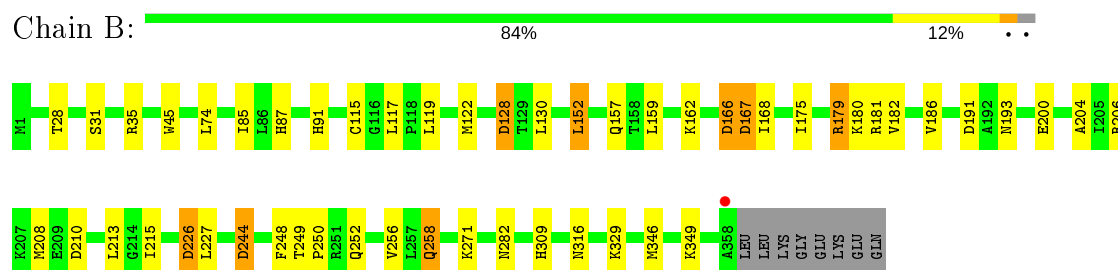
3 Residue-property plots

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.

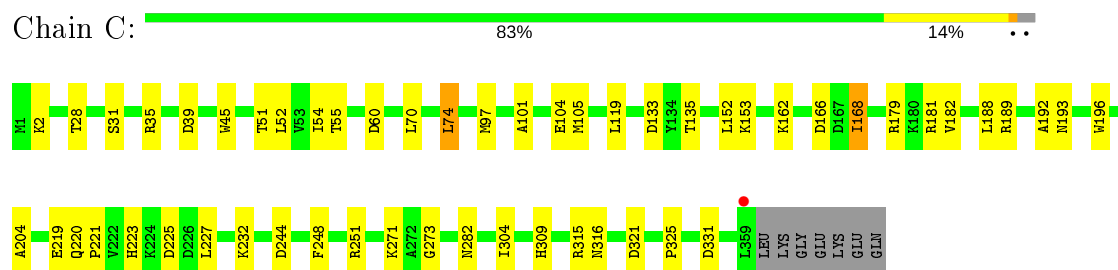
- Molecule 1: similar to chloromuconate cycloisomerase



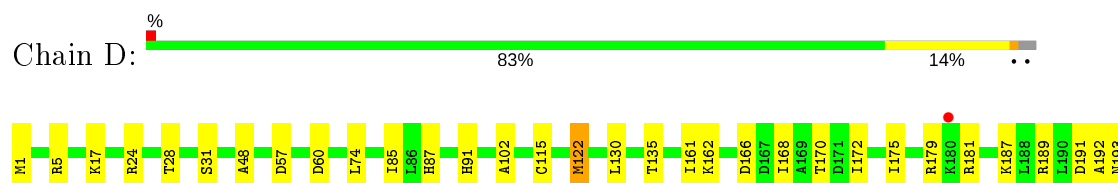
- Molecule 1: similar to chloromuconate cycloisomerase



- Molecule 1: similar to chloromuconate cycloisomerase

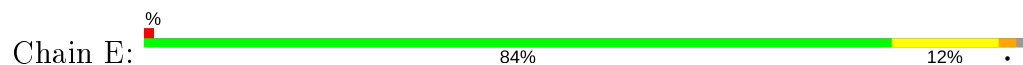


- Molecule 1: similar to chloromuconate cycloisomerase

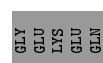




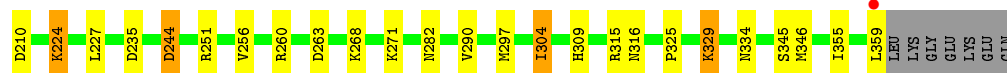
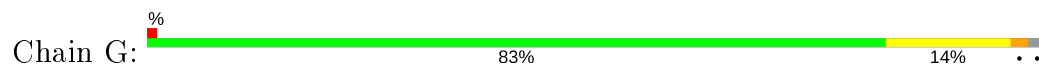
- Molecule 1: similar to chloromuconate cycloisomerase



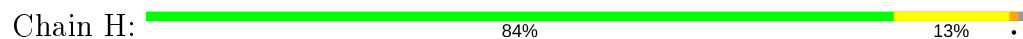
- Molecule 1: similar to chloromuconate cycloisomerase



- Molecule 1: similar to chloromuconate cycloisomerase



- Molecule 1: similar to chloromuconate cycloisomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.40 Å 134.60 Å 194.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 48.73 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.5 (30.00-2.10) 96.5 (48.73-2.10)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.10 Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.219 , 0.285 0.228 , 0.289	Depositor DCC
R_{free} test set	8685 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtrriage
Anisotropy	0.529	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23267	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 81.23 % 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 3.7285e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: MG

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	0.43	0/2748	0.76	5/3716 (0.1%)
1	B	0.46	0/2739	0.77	7/3703 (0.2%)
1	C	0.46	0/2747	0.78	6/3714 (0.2%)
1	D	0.44	0/2747	0.76	4/3714 (0.1%)
1	E	0.47	0/2747	0.76	9/3714 (0.2%)
1	F	0.44	0/2739	0.77	10/3703 (0.3%)
1	G	0.44	0/2748	0.76	8/3716 (0.2%)
1	H	0.44	0/2747	0.75	4/3714 (0.1%)
All	All	0.45	0/21962	0.76	53/29694 (0.2%)

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	166	ASP	CB-CG-OD2	6.37	124.03	118.30
1	B	226	ASP	CB-CG-OD2	6.33	123.99	118.30
1	G	191	ASP	CB-CG-OD2	6.29	123.96	118.30
1	E	321	ASP	CB-CG-OD2	6.20	123.88	118.30
1	D	60	ASP	CB-CG-OD2	6.07	123.76	118.30
1	H	128	ASP	CB-CG-OD2	6.01	123.71	118.30
1	E	166	ASP	CB-CG-OD2	6.00	123.70	118.30
1	B	191	ASP	CB-CG-OD2	5.89	123.60	118.30
1	G	167	ASP	CB-CG-OD2	5.86	123.57	118.30
1	F	166	ASP	CB-CG-OD2	5.78	123.50	118.30
1	D	57	ASP	CB-CG-OD2	5.67	123.40	118.30
1	D	263	ASP	CB-CG-OD2	5.65	123.39	118.30
1	H	244	ASP	CB-CG-OD2	5.65	123.39	118.30
1	C	321	ASP	CB-CG-OD2	5.62	123.36	118.30
1	C	331	ASP	CB-CG-OD2	5.61	123.35	118.30
1	G	210	ASP	CB-CG-OD2	5.60	123.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	244	ASP	CB-CG-OD2	5.55	123.30	118.30
1	A	235	ASP	CB-CG-OD2	5.53	123.28	118.30
1	F	57	ASP	CB-CG-OD2	5.52	123.27	118.30
1	C	133	ASP	CB-CG-OD2	5.50	123.25	118.30
1	H	226	ASP	CB-CG-OD2	5.47	123.22	118.30
1	F	39	ASP	CB-CG-OD2	5.47	123.22	118.30
1	E	191	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	238	ASP	CB-CG-OD2	5.44	123.19	118.30
1	B	244	ASP	CB-CG-OD2	5.41	123.17	118.30
1	G	244	ASP	CB-CG-OD2	5.41	123.17	118.30
1	F	109	ASP	CB-CG-OD2	5.41	123.16	118.30
1	C	39	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	179	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	331	ASP	CB-CG-OD2	5.35	123.12	118.30
1	E	226	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	128	ASP	CB-CG-OD2	5.31	123.08	118.30
1	H	179	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	F	60	ASP	CB-CG-OD2	5.29	123.06	118.30
1	F	235	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	166	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	60	ASP	CB-CG-OD2	5.21	122.99	118.30
1	G	133	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	167	ASP	CB-CG-OD2	5.20	122.98	118.30
1	E	39	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	210	ASP	CB-CG-OD2	5.16	122.94	118.30
1	E	133	ASP	CB-CG-OD2	5.14	122.93	118.30
1	F	225	ASP	CB-CG-OD2	5.13	122.92	118.30
1	C	244	ASP	CB-CG-OD2	5.13	122.92	118.30
1	F	260	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	E	210	ASP	CB-CG-OD2	5.10	122.89	118.30
1	F	210	ASP	CB-CG-OD2	5.09	122.88	118.30
1	D	191	ASP	CB-CG-OD2	5.09	122.88	118.30
1	E	263	ASP	CB-CG-OD2	5.06	122.85	118.30
1	G	235	ASP	CB-CG-OD2	5.05	122.85	118.30
1	G	171	ASP	CB-CG-OD2	5.03	122.83	118.30
1	C	60	ASP	CB-CG-OD2	5.02	122.82	118.30
1	F	238	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

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	2706	0	2773	22	0
1	B	2697	0	2758	27	0
1	C	2705	0	2769	24	0
1	D	2705	0	2769	27	0
1	E	2705	0	2769	24	0
1	F	2697	0	2758	34	0
1	G	2706	0	2773	30	0
1	H	2705	0	2769	27	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	5	0	4	1	0
3	B	5	0	4	0	0
3	C	5	0	4	1	0
3	D	5	0	4	1	0
3	E	5	0	4	0	0
3	F	5	0	4	1	0
3	G	5	0	4	0	0
3	H	5	0	4	1	0
4	A	9	0	6	1	0
4	B	9	0	6	0	0
4	C	9	0	6	0	0
4	D	9	0	6	1	0
4	E	9	0	6	0	0
4	F	9	0	6	2	0
4	G	9	0	6	3	0
4	H	9	0	6	0	0
5	A	183	0	0	5	0
5	B	174	0	0	2	0
5	C	200	0	0	3	0
5	D	194	0	0	3	0
5	E	214	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	180	0	0	6	0
5	G	168	0	0	7	0
5	H	208	0	0	5	0
All	All	23267	0	22218	206	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 (206) 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:E:189:ARG:HA	5:E:2692:HOH:O	1.66	0.95
1:G:162:LYS:NZ	1:G:193:ASN:HD21	1.83	0.77
1:D:1:MET:CA	5:D:2645:HOH:O	2.37	0.72
1:E:87:HIS:CD2	1:E:91:HIS:CD2	2.80	0.70
1:D:334:ASN:HB2	5:D:2508:HOH:O	1.91	0.69
1:C:223:HIS:HD2	1:C:225:ASP:H	1.43	0.67
1:E:5:ARG:HD2	5:E:2567:HOH:O	1.94	0.66
1:F:152:LEU:HD22	1:F:182:VAL:HG22	1.77	0.66
1:F:135:THR:HG1	3:F:2480:ALA:N	1.94	0.66
1:G:74:LEU:HD22	1:G:85:ILE:HG23	1.76	0.66
1:D:74:LEU:HD22	1:D:85:ILE:HG23	1.78	0.65
1:H:282:ASN:HD21	1:H:316:ASN:HB3	1.62	0.64
1:F:1:MET:CA	5:F:2660:HOH:O	2.46	0.63
1:G:162:LYS:HZ2	1:G:193:ASN:HD21	1.47	0.63
1:H:162:LYS:NZ	1:H:193:ASN:HD21	1.97	0.63
1:D:168:ILE:HD12	1:D:204:ALA:HB2	1.82	0.61
1:E:152:LEU:HD13	1:E:159:LEU:HD21	1.82	0.61
1:C:162:LYS:NZ	1:C:193:ASN:HD21	1.98	0.61
1:F:87:HIS:CD2	1:F:91:HIS:CD2	2.89	0.60
1:F:162:LYS:NZ	1:F:193:ASN:HD21	2.00	0.60
1:D:162:LYS:NZ	1:D:193:ASN:HD21	2.00	0.60
1:A:115:CYS:SG	1:B:115:CYS:HB3	2.42	0.59
1:H:223:HIS:HD2	1:H:225:ASP:H	1.51	0.58
1:B:87:HIS:CD2	1:B:91:HIS:CD2	2.93	0.56
1:E:74:LEU:HD22	1:E:85:ILE:HG23	1.87	0.56
1:H:268:LYS:NZ	5:H:2635:HOH:O	2.31	0.56
1:E:315:ARG:CZ	1:F:87:HIS:CE1	2.89	0.56
1:B:74:LEU:HD22	1:B:85:ILE:HG23	1.87	0.55
1:B:282:ASN:ND2	1:B:316:ASN:HD22	2.04	0.55
1:B:168:ILE:HD12	1:B:204:ALA:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:260:ARG:HD2	5:F:2577:HOH:O	2.07	0.55
1:G:224:LYS:O	5:G:2644:HOH:O	2.18	0.55
1:C:135:THR:HG1	3:C:2474:ALA:N	2.05	0.55
1:D:162:LYS:HZ2	1:D:193:ASN:HD21	1.55	0.54
1:C:168:ILE:HD11	1:C:196:TRP:CE2	2.43	0.54
1:B:227:LEU:HD11	1:B:256:VAL:HG22	1.90	0.53
1:D:263:ASP:O	1:D:290:VAL:HG13	2.08	0.53
1:H:135:THR:HG1	3:H:2484:ALA:N	2.05	0.53
1:D:135:THR:HG1	3:D:2476:ALA:N	2.06	0.53
1:E:217:LEU:HG	5:E:2692:HOH:O	2.08	0.53
1:F:179:ARG:NH1	1:F:213:LEU:O	2.38	0.52
1:G:263:ASP:O	1:G:290:VAL:HG13	2.10	0.52
1:D:87:HIS:CD2	1:D:91:HIS:CD2	2.97	0.52
1:G:162:LYS:HZ3	1:G:193:ASN:HD21	1.57	0.52
1:B:179:ARG:NH2	1:B:186:VAL:O	2.42	0.52
1:F:36:ILE:HD12	1:F:106:ALA:HB3	1.91	0.52
1:A:112:ALA:HB3	1:A:351:GLY:HA2	1.92	0.52
1:B:309:HIS:CD2	1:B:346:MET:CE	2.93	0.52
1:C:162:LYS:HZ2	1:C:193:ASN:HD21	1.57	0.52
1:E:309:HIS:CD2	1:E:346:MET:CE	2.93	0.52
1:C:54:ILE:O	1:H:94:THR:HG21	2.10	0.51
1:A:185:ALA:HB3	5:A:2591:HOH:O	2.11	0.51
1:H:162:LYS:HZ2	1:H:193:ASN:HD21	1.56	0.51
1:G:168:ILE:HG21	5:G:2523:HOH:O	2.11	0.51
1:B:244:ASP:OD1	1:B:271:LYS:NZ	2.31	0.51
1:F:179:ARG:NH2	1:F:186:VAL:O	2.44	0.51
1:H:172:ILE:O	1:H:176:GLN:HG3	2.11	0.50
1:B:117:LEU:HD12	1:B:122:MET:SD	2.51	0.50
1:G:64:SER:OG	1:G:68:HIS:HD2	1.95	0.50
1:D:334:ASN:HD22	1:D:355:ILE:CD1	2.25	0.50
1:A:135:THR:HG1	3:A:2470:ALA:N	2.10	0.50
1:C:179:ARG:NH1	1:C:188:LEU:HD12	2.26	0.50
1:H:168:ILE:HD11	1:H:196:TRP:CE2	2.46	0.50
1:G:5:ARG:CD	5:G:2508:HOH:O	2.60	0.50
1:E:244:ASP:O	1:E:271:LYS:NZ	2.45	0.50
1:E:324:ALA:HB3	1:E:325:PRO:HD3	1.93	0.49
1:G:244:ASP:OD1	1:G:271:LYS:NZ	2.34	0.49
1:G:309:HIS:CD2	1:G:346:MET:HE1	2.47	0.49
1:A:224:LYS:NZ	5:A:2654:HOH:O	2.45	0.49
1:C:315:ARG:CZ	1:D:87:HIS:CE1	2.95	0.49
1:F:171:ASP:O	1:F:175:ILE:HG12	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:162:LYS:HZ2	1:F:193:ASN:HD21	1.60	0.49
1:C:119:LEU:HB3	1:C:309:HIS:ND1	2.28	0.49
1:F:175:ILE:HG21	1:F:215:ILE:HD11	1.95	0.49
1:G:1:MET:HG3	1:G:114:MET:HB2	1.94	0.49
1:G:309:HIS:CD2	1:G:346:MET:CE	2.96	0.49
1:C:104:GLU:OE2	5:C:2672:HOH:O	2.19	0.49
1:A:179:ARG:HD2	5:A:2507:HOH:O	2.13	0.49
1:D:332:VAL:HA	1:D:358:ALA:HB2	1.94	0.49
1:C:97:MET:O	1:C:273:GLY:HA2	2.13	0.48
1:C:51:THR:HG1	1:C:55:THR:HG1	1.61	0.48
1:D:24:ARG:HD3	4:D:2477:GLU:OE1	2.13	0.48
1:B:119:LEU:HB3	1:B:309:HIS:ND1	2.28	0.48
1:E:282:ASN:HD21	1:E:316:ASN:HB3	1.78	0.48
1:H:17:LYS:NZ	5:H:2541:HOH:O	2.46	0.48
1:D:334:ASN:HD22	1:D:355:ILE:HD13	1.78	0.48
1:G:11:ILE:HG13	5:G:2646:HOH:O	2.13	0.48
1:B:152:LEU:HD13	1:B:159:LEU:HD21	1.94	0.47
1:G:282:ASN:HD21	1:G:316:ASN:HB3	1.79	0.47
1:H:223:HIS:CD2	1:H:225:ASP:H	2.32	0.47
1:G:304:ILE:HG12	1:G:325:PRO:CG	2.44	0.47
1:G:334:ASN:ND2	1:G:355:ILE:HD13	2.30	0.47
1:F:297:MET:HA	4:F:2481:GLU:HG2	1.94	0.47
1:B:162:LYS:NZ	1:B:193:ASN:HD21	2.13	0.47
1:A:20:LYS:O	1:A:138:VAL:HG22	2.14	0.47
1:A:297:MET:HA	4:A:2471:GLU:HG2	1.96	0.47
1:C:304:ILE:HG13	1:C:325:PRO:CG	2.44	0.47
1:A:82:TYR:O	1:A:86:LEU:HG	2.15	0.47
1:H:8:THR:HG22	1:H:34:VAL:HG22	1.96	0.47
1:C:153:LYS:HD2	5:C:2626:HOH:O	2.14	0.47
1:F:179:ARG:HD2	5:F:2630:HOH:O	2.13	0.47
1:F:282:ASN:HD21	1:F:316:ASN:HB3	1.80	0.47
1:A:71:LYS:HB3	1:A:72:PRO:HD3	1.95	0.46
1:B:175:ILE:HG21	1:B:215:ILE:HD11	1.97	0.46
1:B:309:HIS:CD2	1:B:346:MET:HE3	2.51	0.46
1:B:226:ASP:OD1	1:H:260:ARG:NH2	2.42	0.46
1:G:260:ARG:HD2	5:G:2642:HOH:O	2.14	0.46
1:G:57:ASP:OD1	1:G:96:ASN:HA	2.15	0.46
1:B:309:HIS:CD2	1:B:346:MET:HE1	2.51	0.46
1:F:130:LEU:HD13	1:F:320:PHE:CG	2.50	0.46
1:D:309:HIS:CD2	1:D:346:MET:CE	2.99	0.46
1:F:71:LYS:HB3	1:F:72:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:LYS:HE3	1:D:335:GLY:O	2.16	0.45
1:E:152:LEU:CD1	1:E:159:LEU:HD21	2.44	0.45
1:G:227:LEU:HD11	1:G:256:VAL:HG22	1.99	0.45
1:H:192:ALA:HB3	1:H:221:PRO:HA	1.98	0.45
1:A:282:ASN:HD21	1:A:316:ASN:HB3	1.81	0.45
1:D:248:PHE:HB2	1:D:252:GLN:OE1	2.16	0.45
1:C:101:ALA:O	1:C:105:MET:HG3	2.17	0.45
1:H:35:ARG:HD3	1:H:45:TRP:CH2	2.52	0.45
1:B:248:PHE:HB2	1:B:252:GLN:OE1	2.17	0.45
1:B:309:HIS:HA	1:B:346:MET:HE1	1.99	0.45
1:E:112:ALA:HB3	1:E:351:GLY:HA2	1.99	0.45
1:E:248:PHE:HB2	1:E:252:GLN:OE1	2.17	0.45
1:D:309:HIS:CD2	1:D:346:MET:HE1	2.52	0.45
1:C:70:LEU:O	1:C:74:LEU:HG	2.17	0.45
1:D:324:ALA:HB3	1:D:325:PRO:HD3	1.99	0.44
1:C:192:ALA:HB3	1:C:221:PRO:HA	1.99	0.44
1:F:119:LEU:HB3	1:F:309:HIS:ND1	2.31	0.44
5:A:2506:HOH:O	1:F:52:LEU:HD11	2.17	0.44
1:B:167:ASP:HA	5:B:2560:HOH:O	2.17	0.44
1:H:219:GLU:O	1:H:220:GLN:C	2.56	0.44
1:A:190:LEU:HB2	1:A:218:VAL:HG22	1.99	0.44
1:B:282:ASN:HD21	1:B:316:ASN:HB3	1.82	0.44
1:F:111:TRP:CZ3	1:F:122:MET:HG3	2.53	0.44
1:D:48:ALA:HB2	1:D:102:ALA:HB2	1.99	0.44
1:G:11:ILE:HG12	1:G:33:ILE:CD1	2.48	0.44
1:G:297:MET:HA	4:G:2483:GLU:HG2	2.00	0.44
1:D:122:MET:HA	1:D:122:MET:CE	2.48	0.44
1:G:329:LYS:HG3	5:G:2643:HOH:O	2.17	0.44
1:C:152:LEU:HD22	1:C:182:VAL:HG22	1.99	0.43
1:C:248:PHE:HA	1:C:271:LYS:HB3	1.99	0.43
1:F:138:VAL:HG13	1:F:162:LYS:O	2.17	0.43
1:D:115:CYS:HB2	1:D:122:MET:SD	2.58	0.43
1:F:314:LYS:HB2	1:F:317:ILE:HD12	2.00	0.43
1:F:268:LYS:NZ	5:F:2581:HOH:O	2.39	0.43
1:H:179:ARG:HD2	1:H:213:LEU:O	2.19	0.43
1:F:309:HIS:CD2	1:F:346:MET:CE	3.02	0.43
1:D:192:ALA:HB3	1:D:221:PRO:HA	1.99	0.43
1:F:162:LYS:NZ	1:F:191:ASP:OD2	2.50	0.43
1:A:130:LEU:HD13	1:A:320:PHE:CG	2.54	0.43
1:F:168:ILE:HD12	1:F:204:ALA:HB2	2.00	0.43
5:B:2526:HOH:O	1:G:251:ARG:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:232:LYS:NZ	5:H:2620:HOH:O	2.50	0.43
1:E:162:LYS:NZ	1:E:191:ASP:OD2	2.50	0.43
1:E:131:GLU:HG2	5:E:2513:HOH:O	2.18	0.43
1:B:168:ILE:HD11	1:B:200:GLU:HG2	2.00	0.43
1:H:35:ARG:HD2	5:H:2507:HOH:O	2.18	0.43
1:E:119:LEU:HB3	1:E:309:HIS:ND1	2.34	0.42
1:H:74:LEU:HD22	1:H:85:ILE:HG23	2.00	0.42
1:H:185:ALA:HB3	5:H:2607:HOH:O	2.18	0.42
1:C:251:ARG:CZ	5:C:2492:HOH:O	2.67	0.42
1:C:35:ARG:HD3	1:C:45:TRP:CH2	2.54	0.42
1:G:87:HIS:CD2	1:G:91:HIS:CD2	3.07	0.42
1:B:208:MET:HG2	1:B:213:LEU:HD12	2.01	0.42
1:C:282:ASN:HD21	1:C:316:ASN:HB3	1.85	0.42
1:D:347:PRO:HG2	5:D:2514:HOH:O	2.19	0.42
1:E:11:ILE:CD1	1:E:300:THR:HG21	2.50	0.42
1:F:51:THR:HB	1:F:54:ILE:HB	2.02	0.42
1:B:227:LEU:HD11	1:B:256:VAL:CG2	2.51	0.41
1:C:219:GLU:O	1:C:220:GLN:C	2.57	0.41
1:C:168:ILE:HD12	1:C:204:ALA:HB1	2.02	0.41
1:A:144:MET:HB3	1:A:178:ILE:HD11	2.03	0.41
1:A:191:ASP:HA	1:A:219:GLU:HB2	2.02	0.41
1:F:248:PHE:HA	1:F:271:LYS:HB3	2.01	0.41
1:F:36:ILE:HD12	1:F:106:ALA:CB	2.50	0.41
1:G:74:LEU:CD2	1:G:85:ILE:HG23	2.46	0.41
1:A:224:LYS:HE3	5:F:2536:HOH:O	2.20	0.41
1:G:268:LYS:HE2	4:G:2483:GLU:HA	2.03	0.41
1:A:223:HIS:HE1	5:A:2579:HOH:O	2.02	0.41
1:G:189:ARG:HB3	5:G:2498:HOH:O	2.21	0.41
1:H:42:ALA:HB1	1:H:113:GLN:OE1	2.20	0.41
1:H:203:THR:HG22	1:H:207:LYS:HE3	2.01	0.41
1:E:309:HIS:CD2	1:E:346:MET:HE1	2.56	0.41
1:E:282:ASN:ND2	1:E:316:ASN:HD22	2.18	0.41
1:E:87:HIS:CE1	1:F:315:ARG:HD3	2.55	0.41
1:H:278:ALA:HB1	1:H:310:PHE:CE2	2.55	0.41
1:B:35:ARG:HD3	1:B:45:TRP:CH2	2.56	0.41
1:H:93:LEU:HD23	1:H:93:LEU:N	2.36	0.41
1:A:224:LYS:HD3	5:F:2536:HOH:O	2.21	0.40
1:A:258:GLN:CG	1:B:258:GLN:HE21	2.34	0.40
1:A:32:VAL:O	1:A:47:GLU:HA	2.20	0.40
1:E:87:HIS:ND1	1:F:315:ARG:CD	2.85	0.40
1:H:8:THR:HA	1:H:33:ILE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:VAL:CG2	1:A:256:VAL:HG21	2.51	0.40
1:H:293:MET:HB2	1:H:319:ARG:HB2	2.03	0.40
1:D:282:ASN:ND2	1:D:316:ASN:HD22	2.19	0.40
1:F:24:ARG:NH1	4:F:2481:GLU:OE2	2.54	0.40
1:A:152:LEU:HD22	1:A:182:VAL:HG22	2.02	0.40
1:G:116:GLY:O	1:G:117:LEU:HD23	2.22	0.40
1:G:24:ARG:HD3	4:G:2483:GLU:OE1	2.22	0.40
1:B:249:THR:HB	1:B:250:PRO:HD2	2.04	0.40
1:D:161:ILE:HG21	1:D:175:ILE:CD1	2.51	0.40
1:D:189:ARG:HG2	1:D:217:LEU:HD11	2.03	0.40
1:E:168:ILE:HG23	1:E:204:ALA:HB2	2.04	0.40
1:E:87:HIS:CE1	1:F:315:ARG:CD	3.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	357/366 (98%)	342 (96%)	15 (4%)	0	100	100
1	B	356/366 (97%)	341 (96%)	15 (4%)	0	100	100
1	C	357/366 (98%)	346 (97%)	11 (3%)	0	100	100
1	D	357/366 (98%)	342 (96%)	15 (4%)	0	100	100
1	E	357/366 (98%)	346 (97%)	11 (3%)	0	100	100
1	F	356/366 (97%)	342 (96%)	14 (4%)	0	100	100
1	G	357/366 (98%)	339 (95%)	17 (5%)	1 (0%)	41	41
1	H	357/366 (98%)	342 (96%)	15 (4%)	0	100	100
All	All	2854/2928 (98%)	2740 (96%)	113 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	166	ASP

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	286/292 (98%)	269 (94%)	17 (6%)	19	17
1	B	284/292 (97%)	269 (95%)	15 (5%)	22	20
1	C	285/292 (98%)	274 (96%)	11 (4%)	32	33
1	D	285/292 (98%)	270 (95%)	15 (5%)	22	20
1	E	285/292 (98%)	267 (94%)	18 (6%)	18	15
1	F	284/292 (97%)	266 (94%)	18 (6%)	18	15
1	G	286/292 (98%)	273 (96%)	13 (4%)	27	27
1	H	285/292 (98%)	271 (95%)	14 (5%)	25	23
All	All	2280/2336 (98%)	2159 (95%)	121 (5%)	22	20

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	24	ARG
1	A	28	THR
1	A	31	SER
1	A	93	LEU
1	A	138	VAL
1	A	166	ASP
1	A	168	ILE
1	A	179	ARG
1	A	181	ARG
1	A	182	VAL
1	A	184	SER
1	A	186	VAL
1	A	190	LEU
1	A	206	ARG

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Mol	Chain	Res	Type
1	A	207	LYS
1	A	349	LYS
1	B	28	THR
1	B	31	SER
1	B	128	ASP
1	B	130	LEU
1	B	152	LEU
1	B	157	GLN
1	B	166	ASP
1	B	179	ARG
1	B	180	LYS
1	B	181	ARG
1	B	182	VAL
1	B	206	ARG
1	B	258	GLN
1	B	329	LYS
1	B	349	LYS
1	C	2	LYS
1	C	28	THR
1	C	31	SER
1	C	52	LEU
1	C	74	LEU
1	C	166	ASP
1	C	168	ILE
1	C	181	ARG
1	C	189	ARG
1	C	227	LEU
1	C	232	LYS
1	D	5	ARG
1	D	17	LYS
1	D	28	THR
1	D	31	SER
1	D	122	MET
1	D	130	LEU
1	D	166	ASP
1	D	170	THR
1	D	172	ILE
1	D	179	ARG
1	D	181	ARG
1	D	187	LYS
1	D	246	SER
1	D	255	GLU

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Mol	Chain	Res	Type
1	D	359	LEU
1	E	28	THR
1	E	31	SER
1	E	74	LEU
1	E	130	LEU
1	E	152	LEU
1	E	166	ASP
1	E	167	ASP
1	E	179	ARG
1	E	180	LYS
1	E	181	ARG
1	E	182	VAL
1	E	186	VAL
1	E	189	ARG
1	E	206	ARG
1	E	210	ASP
1	E	224	LYS
1	E	246	SER
1	E	359	LEU
1	F	2	LYS
1	F	28	THR
1	F	52	LEU
1	F	74	LEU
1	F	88	ASP
1	F	94	THR
1	F	138	VAL
1	F	153	LYS
1	F	166	ASP
1	F	179	ARG
1	F	180	LYS
1	F	181	ARG
1	F	182	VAL
1	F	186	VAL
1	F	187	LYS
1	F	207	LYS
1	F	258	GLN
1	F	329	LYS
1	G	5	ARG
1	G	28	THR
1	G	31	SER
1	G	128	ASP
1	G	179	ARG

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Mol	Chain	Res	Type
1	G	181	ARG
1	G	182	VAL
1	G	224	LYS
1	G	304	ILE
1	G	315	ARG
1	G	329	LYS
1	G	345	SER
1	G	359	LEU
1	H	17	LYS
1	H	28	THR
1	H	31	SER
1	H	52	LEU
1	H	74	LEU
1	H	78	SER
1	H	153	LYS
1	H	166	ASP
1	H	168	ILE
1	H	181	ARG
1	H	189	ARG
1	H	232	LYS
1	H	258	GLN
1	H	304	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	GLN
1	A	193	ASN
1	A	223	HIS
1	A	282	ASN
1	B	87	HIS
1	B	91	HIS
1	B	157	GLN
1	B	193	ASN
1	B	223	HIS
1	B	258	GLN
1	B	282	ASN
1	B	334	ASN
1	C	91	HIS
1	C	193	ASN
1	C	223	HIS
1	C	282	ASN

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Mol	Chain	Res	Type
1	D	68	HIS
1	D	87	HIS
1	D	91	HIS
1	D	154	GLN
1	D	193	ASN
1	D	223	HIS
1	D	258	GLN
1	D	282	ASN
1	D	309	HIS
1	D	334	ASN
1	E	87	HIS
1	E	91	HIS
1	E	176	GLN
1	E	193	ASN
1	E	223	HIS
1	E	282	ASN
1	F	87	HIS
1	F	154	GLN
1	F	193	ASN
1	F	223	HIS
1	F	258	GLN
1	F	282	ASN
1	G	68	HIS
1	G	91	HIS
1	G	154	GLN
1	G	157	GLN
1	G	193	ASN
1	G	258	GLN
1	G	282	ASN
1	G	334	ASN
1	H	68	HIS
1	H	87	HIS
1	H	193	ASN
1	H	223	HIS
1	H	258	GLN
1	H	282	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	$\# Z > 2$
3	ALA	E	2478	4	3,4,5	0.57	0	2,4,6	0.65	0
3	ALA	F	2480	4	3,4,5	0.73	0	2,4,6	0.64	0
3	ALA	B	2472	4	3,4,5	0.91	0	2,4,6	0.73	0
3	ALA	H	2484	4	3,4,5	0.55	0	2,4,6	0.85	0
3	ALA	D	2476	4	3,4,5	0.44	0	2,4,6	0.78	0
4	GLU	H	2485	3,2	4,8,9	0.63	0	1,9,11	0.81	0
3	ALA	G	2482	4	3,4,5	0.58	0	2,4,6	0.70	0
4	GLU	B	2473	3,2	4,8,9	0.52	0	1,9,11	0.26	0
4	GLU	F	2481	3,2	4,8,9	0.46	0	1,9,11	0.62	0
4	GLU	G	2483	3,2	4,8,9	0.33	0	1,9,11	0.99	0
4	GLU	A	2471	3,2	4,8,9	0.48	0	1,9,11	0.13	0
4	GLU	D	2477	3,2	4,8,9	0.43	0	1,9,11	0.09	0
4	GLU	C	2475	3,2	4,8,9	0.72	0	1,9,11	0.80	0
3	ALA	A	2470	4	3,4,5	0.62	0	2,4,6	0.64	0
3	ALA	C	2474	4	3,4,5	0.64	0	2,4,6	0.80	0
4	GLU	E	2479	3,2	4,8,9	0.63	0	1,9,11	0.23	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
3	ALA	E	2478	4	-	0/0/2/4	-
3	ALA	F	2480	4	-	0/0/2/4	-
3	ALA	B	2472	4	-	0/0/2/4	-
3	ALA	H	2484	4	-	0/0/2/4	-
3	ALA	D	2476	4	-	0/0/2/4	-
4	GLU	H	2485	3,2	-	2/4/7/9	-
3	ALA	G	2482	4	-	0/0/2/4	-
4	GLU	B	2473	3,2	-	2/4/7/9	-
4	GLU	F	2481	3,2	-	1/4/7/9	-
4	GLU	G	2483	3,2	-	1/4/7/9	-
4	GLU	A	2471	3,2	-	2/4/7/9	-
4	GLU	D	2477	3,2	-	3/4/7/9	-
4	GLU	C	2475	3,2	-	2/4/7/9	-
3	ALA	A	2470	4	-	0/0/2/4	-
3	ALA	C	2474	4	-	0/0/2/4	-
4	GLU	E	2479	3,2	-	1/4/7/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	2483	GLU	O-C-CA-CB
4	F	2481	GLU	O-C-CA-CB
4	B	2473	GLU	O-C-CA-CB
4	D	2477	GLU	O-C-CA-CB
4	C	2475	GLU	O-C-CA-CB
4	C	2475	GLU	CA-CB-CG-CD
4	H	2485	GLU	O-C-CA-CB
4	A	2471	GLU	O-C-CA-CB
4	E	2479	GLU	O-C-CA-CB
4	B	2473	GLU	CA-CB-CG-CD
4	D	2477	GLU	CA-CB-CG-CD
4	H	2485	GLU	CA-CB-CG-CD
4	D	2477	GLU	N-CA-CB-CG
4	A	2471	GLU	N-CA-CB-CG

There are no ring outliers.

9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2480	ALA	1	0
3	H	2484	ALA	1	0
3	D	2476	ALA	1	0
4	F	2481	GLU	2	0
4	G	2483	GLU	3	0
4	A	2471	GLU	1	0
4	D	2477	GLU	1	0
3	A	2470	ALA	1	0
3	C	2474	ALA	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	359/366 (98%)	-0.41	1 (0%) 94 94	14, 28, 45, 77	0
1	B	358/366 (97%)	-0.47	1 (0%) 94 94	14, 26, 41, 66	0
1	C	359/366 (98%)	-0.46	1 (0%) 94 94	13, 25, 41, 58	0
1	D	359/366 (98%)	-0.35	2 (0%) 89 91	9, 25, 49, 67	0
1	E	359/366 (98%)	-0.50	2 (0%) 89 91	13, 24, 38, 70	0
1	F	358/366 (97%)	-0.47	1 (0%) 94 94	15, 27, 42, 61	0
1	G	359/366 (98%)	-0.31	3 (0%) 86 88	14, 27, 48, 69	0
1	H	359/366 (98%)	-0.46	0 100 100	15, 26, 41, 64	0
All	All	2870/2928 (98%)	-0.43	11 (0%) 92 93	9, 26, 43, 77	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	359	LEU	5.8
1	G	359	LEU	5.2
1	D	359	LEU	4.6
1	E	359	LEU	3.2
1	B	358	ALA	2.7
1	C	359	LEU	2.5
1	E	358	ALA	2.3
1	D	180	LYS	2.3
1	F	358	ALA	2.3
1	G	185	ALA	2.2
1	G	182	VAL	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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(\AA^2)	Q<0.9
4	GLU	D	2477	9/10	0.82	0.16	25,27,29,30	0
4	GLU	E	2479	9/10	0.82	0.13	19,25,28,28	0
4	GLU	H	2485	9/10	0.86	0.12	17,26,33,36	0
2	MG	B	1602	1/1	0.88	0.08	25,25,25,25	0
4	GLU	C	2475	9/10	0.88	0.12	22,28,33,34	0
4	GLU	F	2481	9/10	0.89	0.12	24,28,33,34	0
4	GLU	G	2483	9/10	0.89	0.10	21,23,26,28	0
4	GLU	B	2473	9/10	0.91	0.10	21,26,29,29	0
4	GLU	A	2471	9/10	0.93	0.13	23,27,29,34	0
3	ALA	H	2484	5/6	0.94	0.09	20,21,22,22	0
2	MG	C	1603	1/1	0.94	0.06	27,27,27,27	0
3	ALA	B	2472	5/6	0.95	0.09	24,24,26,27	0
3	ALA	A	2470	5/6	0.96	0.10	26,26,27,28	0
3	ALA	C	2474	5/6	0.96	0.08	17,21,22,23	0
2	MG	A	1601	1/1	0.96	0.07	30,30,30,30	0
3	ALA	D	2476	5/6	0.97	0.11	24,25,26,26	0
3	ALA	F	2480	5/6	0.97	0.08	21,26,27,27	0
2	MG	F	1606	1/1	0.97	0.05	37,37,37,37	0
3	ALA	E	2478	5/6	0.97	0.06	20,20,22,24	0
2	MG	E	1605	1/1	0.97	0.07	28,28,28,28	0
2	MG	H	1608	1/1	0.98	0.04	25,25,25,25	0
2	MG	G	1607	1/1	0.98	0.06	22,22,22,22	0
2	MG	D	1604	1/1	0.98	0.05	22,22,22,22	0
3	ALA	G	2482	5/6	0.98	0.10	17,18,19,24	0

6.5 Other polymers ⓘ

There are no such residues in this entry.