



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:16 PM UTC

PDB ID : 5J84 / pdb_00005j84
Title : Crystal structure of L-arabinonate dehydratase in holo-form
Authors : Rahman, M.M.; Rouvinen, J.; Hakulinen, N.
Deposited on : 2016-04-07
Resolution : 2.40 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

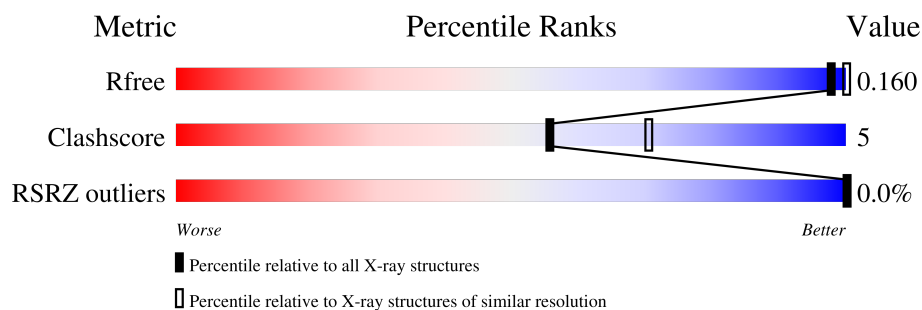
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	588	
1	B	588	
1	C	588	
1	D	588	
1	E	588	
1	F	588	
1	G	588	

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Mol	Chain	Length	Quality of chain
1	H	588	 88%9%•

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36603 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 Dihydroxy-acid dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	575	Total	C	N	O	S	0	0	0
			4349	2724	766	825	34			
1	B	575	Total	C	N	O	S	0	0	0
			4349	2724	766	825	34			
1	C	575	Total	C	N	O	S	0	0	0
			4349	2724	766	825	34			
1	D	575	Total	C	N	O	S	0	0	0
			4349	2724	766	825	34			
1	E	575	Total	C	N	O	S	0	0	0
			4349	2724	766	825	34			
1	F	575	Total	C	N	O	S	0	0	0
			4349	2724	766	825	34			
1	G	575	Total	C	N	O	S	0	0	0
			4349	2724	766	825	34			
1	H	575	Total	C	N	O	S	0	0	0
			4349	2724	766	825	34			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	initiating methionine	UNP B5ZZ34
A	-7	ASP	-	expression tag	UNP B5ZZ34
A	-6	TRP	-	expression tag	UNP B5ZZ34
A	-5	SER	-	expression tag	UNP B5ZZ34
A	-4	HIS	-	expression tag	UNP B5ZZ34
A	-3	PRO	-	expression tag	UNP B5ZZ34
A	-2	GLN	-	expression tag	UNP B5ZZ34
A	-1	PHE	-	expression tag	UNP B5ZZ34
A	0	GLU	-	expression tag	UNP B5ZZ34
A	1	LYS	-	expression tag	UNP B5ZZ34
B	-8	MET	-	initiating methionine	UNP B5ZZ34
B	-7	ASP	-	expression tag	UNP B5ZZ34
B	-6	TRP	-	expression tag	UNP B5ZZ34

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	SER	-	expression tag	UNP B5ZZ34
B	-4	HIS	-	expression tag	UNP B5ZZ34
B	-3	PRO	-	expression tag	UNP B5ZZ34
B	-2	GLN	-	expression tag	UNP B5ZZ34
B	-1	PHE	-	expression tag	UNP B5ZZ34
B	0	GLU	-	expression tag	UNP B5ZZ34
B	1	LYS	-	expression tag	UNP B5ZZ34
C	-8	MET	-	initiating methionine	UNP B5ZZ34
C	-7	ASP	-	expression tag	UNP B5ZZ34
C	-6	TRP	-	expression tag	UNP B5ZZ34
C	-5	SER	-	expression tag	UNP B5ZZ34
C	-4	HIS	-	expression tag	UNP B5ZZ34
C	-3	PRO	-	expression tag	UNP B5ZZ34
C	-2	GLN	-	expression tag	UNP B5ZZ34
C	-1	PHE	-	expression tag	UNP B5ZZ34
C	0	GLU	-	expression tag	UNP B5ZZ34
C	1	LYS	-	expression tag	UNP B5ZZ34
D	-8	MET	-	initiating methionine	UNP B5ZZ34
D	-7	ASP	-	expression tag	UNP B5ZZ34
D	-6	TRP	-	expression tag	UNP B5ZZ34
D	-5	SER	-	expression tag	UNP B5ZZ34
D	-4	HIS	-	expression tag	UNP B5ZZ34
D	-3	PRO	-	expression tag	UNP B5ZZ34
D	-2	GLN	-	expression tag	UNP B5ZZ34
D	-1	PHE	-	expression tag	UNP B5ZZ34
D	0	GLU	-	expression tag	UNP B5ZZ34
D	1	LYS	-	expression tag	UNP B5ZZ34
E	-8	MET	-	initiating methionine	UNP B5ZZ34
E	-7	ASP	-	expression tag	UNP B5ZZ34
E	-6	TRP	-	expression tag	UNP B5ZZ34
E	-5	SER	-	expression tag	UNP B5ZZ34
E	-4	HIS	-	expression tag	UNP B5ZZ34
E	-3	PRO	-	expression tag	UNP B5ZZ34
E	-2	GLN	-	expression tag	UNP B5ZZ34
E	-1	PHE	-	expression tag	UNP B5ZZ34
E	0	GLU	-	expression tag	UNP B5ZZ34
E	1	LYS	-	expression tag	UNP B5ZZ34
F	-8	MET	-	initiating methionine	UNP B5ZZ34
F	-7	ASP	-	expression tag	UNP B5ZZ34
F	-6	TRP	-	expression tag	UNP B5ZZ34
F	-5	SER	-	expression tag	UNP B5ZZ34
F	-4	HIS	-	expression tag	UNP B5ZZ34

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-3	PRO	-	expression tag	UNP B5ZZ34
F	-2	GLN	-	expression tag	UNP B5ZZ34
F	-1	PHE	-	expression tag	UNP B5ZZ34
F	0	GLU	-	expression tag	UNP B5ZZ34
F	1	LYS	-	expression tag	UNP B5ZZ34
G	-8	MET	-	initiating methionine	UNP B5ZZ34
G	-7	ASP	-	expression tag	UNP B5ZZ34
G	-6	TRP	-	expression tag	UNP B5ZZ34
G	-5	SER	-	expression tag	UNP B5ZZ34
G	-4	HIS	-	expression tag	UNP B5ZZ34
G	-3	PRO	-	expression tag	UNP B5ZZ34
G	-2	GLN	-	expression tag	UNP B5ZZ34
G	-1	PHE	-	expression tag	UNP B5ZZ34
G	0	GLU	-	expression tag	UNP B5ZZ34
G	1	LYS	-	expression tag	UNP B5ZZ34
H	-8	MET	-	initiating methionine	UNP B5ZZ34
H	-7	ASP	-	expression tag	UNP B5ZZ34
H	-6	TRP	-	expression tag	UNP B5ZZ34
H	-5	SER	-	expression tag	UNP B5ZZ34
H	-4	HIS	-	expression tag	UNP B5ZZ34
H	-3	PRO	-	expression tag	UNP B5ZZ34
H	-2	GLN	-	expression tag	UNP B5ZZ34
H	-1	PHE	-	expression tag	UNP B5ZZ34
H	0	GLU	-	expression tag	UNP B5ZZ34
H	1	LYS	-	expression tag	UNP B5ZZ34

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

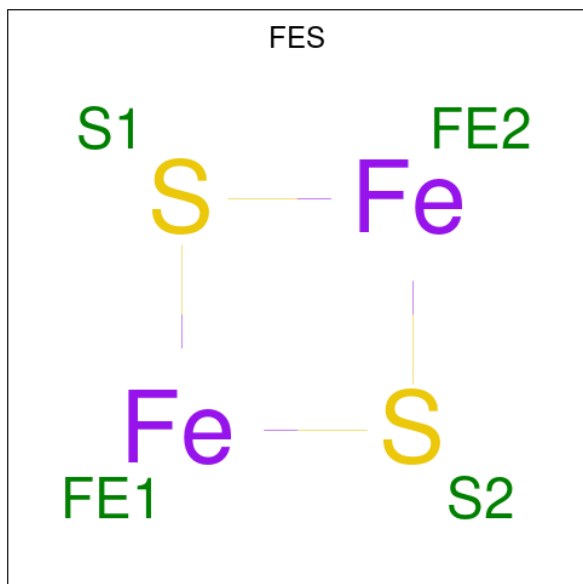
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	1	Total	Mg	0	0
			1	1		

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	B	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	D	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	F	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		
3	H	1	Total	Fe	S	0	0
			4	2	2		

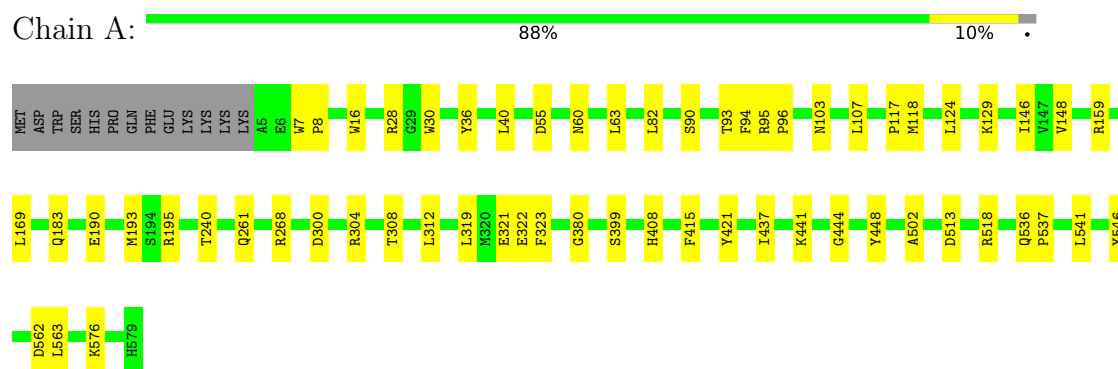
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	234	Total 234	O 234	0	0
4	B	213	Total 213	O 213	0	0
4	C	245	Total 245	O 245	0	0
4	D	209	Total 209	O 209	0	0
4	E	219	Total 219	O 219	0	0
4	F	209	Total 209	O 209	0	0
4	G	208	Total 208	O 208	0	0
4	H	234	Total 234	O 234	0	0

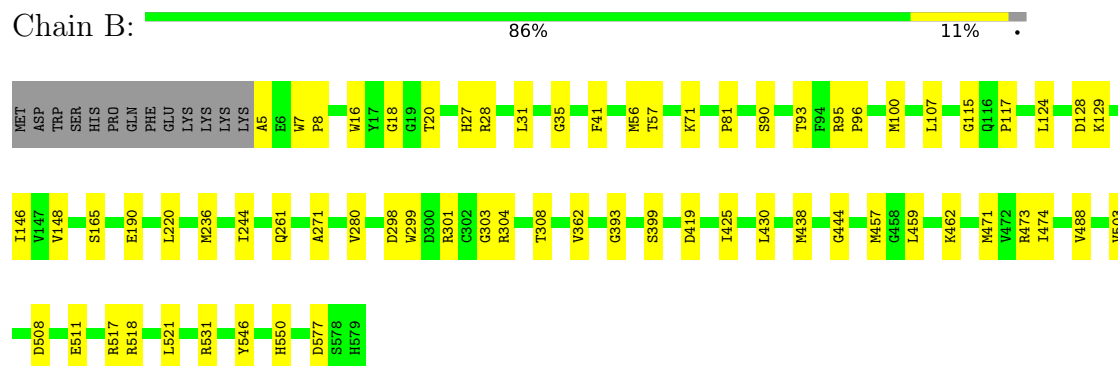
3 Residue-property plots

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.

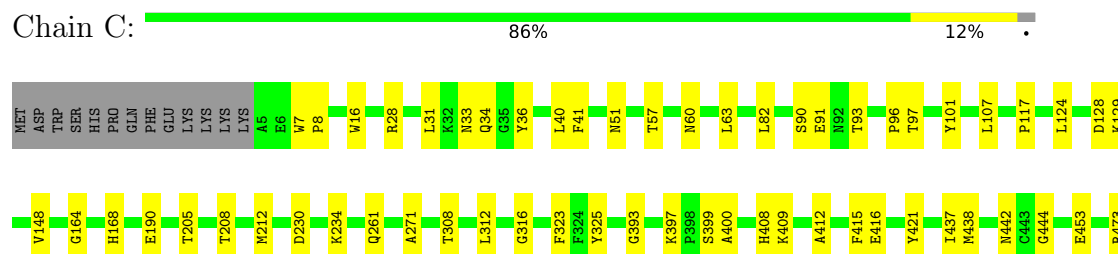
• Molecule 1: Dihydroxy-acid dehydratase



• Molecule 1: Dihydroxy-acid dehydratase



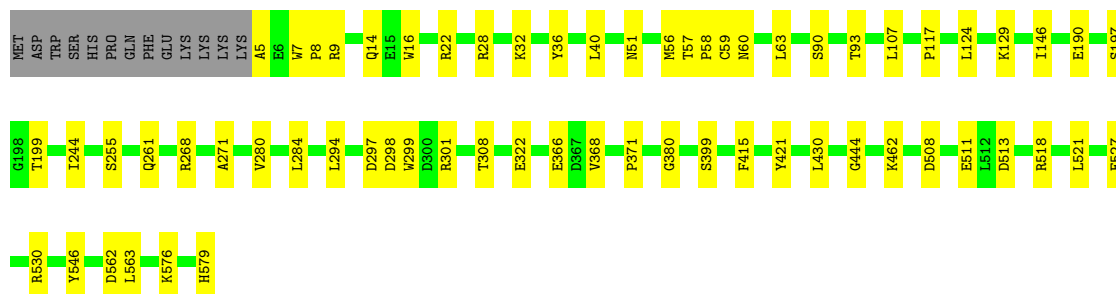
• Molecule 1: Dihydroxy-acid dehydratase





- Molecule 1: Dihydroxy-acid dehydratase

Chain D: 87% 11%



- Molecule 1: Dihydroxy-acid dehydratase

Chain E: 87% 11%



- Molecule 1: Dihydroxy-acid dehydratase

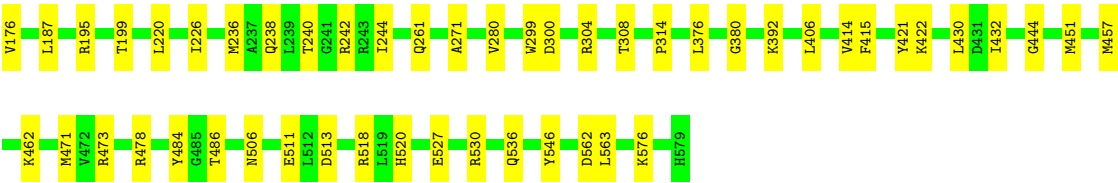
Chain F: 86% 11%



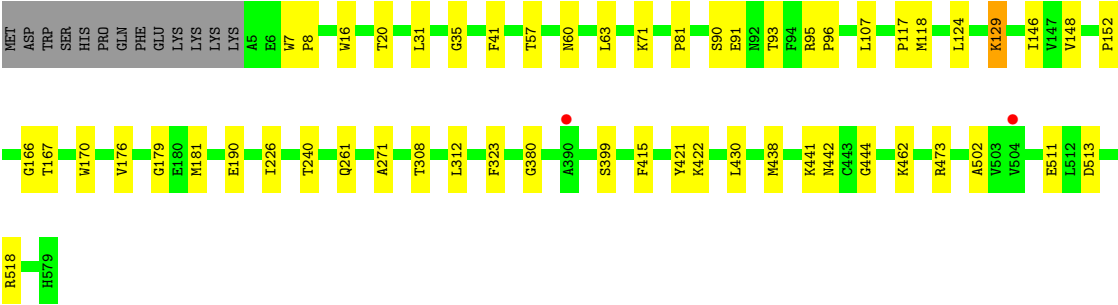
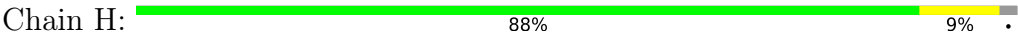
- Molecule 1: Dihydroxy-acid dehydratase

Chain G: 85% 13%





• Molecule 1: Dihydroxy-acid dehydratase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.07Å 208.61Å 147.09Å 90.00° 90.43° 90.00°	Depositor
Resolution (Å)	39.89 – 2.40 39.89 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.89-2.40) 97.1 (39.89-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.156 , 0.185 (Not available) , 0.160	Depositor DCC
R_{free} test set	12347 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.398 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	36603	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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: KCX, FES, 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	0.31	0/4422	0.76	4/5988 (0.1%)
1	B	0.31	0/4422	0.77	4/5988 (0.1%)
1	C	0.31	0/4422	0.75	3/5988 (0.1%)
1	D	0.31	0/4422	0.75	4/5988 (0.1%)
1	E	0.31	0/4422	0.75	2/5988 (0.0%)
1	F	0.30	0/4422	0.74	2/5988 (0.0%)
1	G	0.31	0/4422	0.75	2/5988 (0.0%)
1	H	0.31	0/4422	0.75	2/5988 (0.0%)
All	All	0.31	0/35376	0.75	23/47904 (0.0%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	541	LEU	CA-C-N	7.90	127.83	119.85
1	E	541	LEU	C-N-CA	7.90	127.83	119.85
1	B	393	GLY	N-CA-C	7.07	118.67	111.95
1	H	444	GLY	CA-C-N	6.85	126.36	119.24
1	H	444	GLY	C-N-CA	6.85	126.36	119.24
1	B	425	ILE	N-CA-C	6.33	117.08	110.62
1	C	444	GLY	CA-C-N	6.27	125.76	119.24
1	C	444	GLY	C-N-CA	6.27	125.76	119.24
1	B	444	GLY	CA-C-N	6.23	125.72	119.24
1	B	444	GLY	C-N-CA	6.23	125.72	119.24
1	C	393	GLY	N-CA-C	6.13	117.77	111.95
1	A	541	LEU	CA-C-N	6.08	125.99	119.85
1	A	541	LEU	C-N-CA	6.08	125.99	119.85
1	D	444	GLY	CA-C-N	6.03	125.51	119.24
1	D	444	GLY	C-N-CA	6.03	125.51	119.24
1	F	444	GLY	CA-C-N	5.64	125.10	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	444	GLY	C-N-CA	5.64	125.10	119.24
1	A	444	GLY	CA-C-N	5.32	124.77	119.24
1	A	444	GLY	C-N-CA	5.32	124.77	119.24
1	G	444	GLY	CA-C-N	5.01	124.45	119.24
1	G	444	GLY	C-N-CA	5.01	124.45	119.24
1	D	57	THR	CA-C-N	5.00	124.66	119.56
1	D	57	THR	C-N-CA	5.00	124.66	119.56

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	4349	0	4320	43	0
1	B	4349	0	4320	46	0
1	C	4349	0	4320	52	0
1	D	4349	0	4320	43	0
1	E	4349	0	4320	45	0
1	F	4349	0	4320	45	0
1	G	4349	0	4320	54	0
1	H	4349	0	4320	36	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	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
3	E	4	0	0	0	0
3	F	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	4	0	0	0	0
3	H	4	0	0	0	0
4	A	234	0	0	8	0
4	B	213	0	0	8	0
4	C	245	0	0	6	0
4	D	209	0	0	7	0
4	E	219	0	0	10	0
4	F	209	0	0	12	0
4	G	208	0	0	14	0
4	H	234	0	0	4	0
All	All	36603	0	34560	326	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 (326) 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:G:406:LEU:O	4:G:701:HOH:O	2.05	0.75
1:B:90:SER:OG	1:B:93:THR:OG1	2.09	0.70
1:H:422:LYS:NZ	4:H:705:HOH:O	2.23	0.70
1:G:91:GLU:OE2	1:G:129:KCX:OQ1	2.09	0.70
1:F:289:ARG:NH2	4:F:705:HOH:O	2.24	0.70
1:F:162:ARG:NH1	4:F:710:HOH:O	2.25	0.69
1:C:91:GLU:OE1	1:C:453:GLU:OE2	2.11	0.68
1:H:430:LEU:O	1:H:462:LYS:NZ	2.24	0.67
1:A:195:ARG:NH2	1:C:325:TYR:OH	2.28	0.67
1:D:90:SER:OG	1:D:93:THR:OG1	2.11	0.67
1:B:577:ASP:OD1	4:B:701:HOH:O	2.12	0.67
1:A:322:GLU:OE2	4:A:701:HOH:O	2.12	0.67
1:G:5:ALA:N	4:G:711:HOH:O	2.26	0.66
1:E:511:GLU:OE1	1:E:518:ARG:NH1	2.27	0.66
1:B:128:ASP:OD1	4:B:702:HOH:O	2.13	0.66
1:G:457:MET:O	1:G:473:ARG:NH1	2.28	0.65
1:G:76:GLU:OE1	4:G:702:HOH:O	2.14	0.65
1:G:314:PRO:HB2	1:G:484:TYR:HB3	1.79	0.64
1:B:438:MET:HB2	1:B:473:ARG:HG2	1.79	0.64
1:C:33:ASN:O	4:C:702:HOH:O	2.15	0.64
1:C:505:LYS:O	4:C:701:HOH:O	2.13	0.64
1:G:10:LYS:NZ	4:G:716:HOH:O	2.29	0.64
1:E:60:ASN:HB3	1:E:63:LEU:HD22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:90:SER:OG	1:H:93:THR:OG1	2.15	0.62
1:F:298:ASP:OD1	1:F:301:ARG:NH2	2.32	0.62
1:F:90:SER:OG	1:F:93:THR:OG1	2.19	0.61
1:A:118:MET:HB3	1:B:56:MET:HE1	1.83	0.61
1:C:442:ASN:ND2	4:C:714:HOH:O	2.33	0.61
1:G:57:THR:HG23	1:G:90:SER:HB3	1.83	0.61
1:H:513:ASP:HB3	1:H:518:ARG:HG2	1.83	0.61
1:G:513:ASP:HB3	1:G:518:ARG:HG2	1.81	0.61
1:H:442:ASN:ND2	4:H:725:HOH:O	2.33	0.60
1:G:91:GLU:HG3	1:G:128:ASP:HB2	1.83	0.60
1:E:90:SER:OG	1:E:93:THR:OG1	2.19	0.60
1:D:60:ASN:HB3	1:D:63:LEU:HD22	1.84	0.60
1:A:90:SER:OG	1:A:93:THR:OG1	2.18	0.59
1:E:20:THR:O	1:F:183:GLN:NE2	2.35	0.59
1:F:60:ASN:HB3	1:F:63:LEU:HD22	1.84	0.59
1:F:7:TRP:CD2	1:F:8:PRO:HA	2.38	0.59
1:H:308:THR:HG21	1:H:399:SER:HB3	1.85	0.59
1:B:18:GLY:O	4:B:703:HOH:O	2.16	0.58
1:A:308:THR:HG21	1:A:399:SER:HB3	1.86	0.58
1:E:334:LYS:NZ	4:E:726:HOH:O	2.35	0.58
1:E:391:PRO:O	4:E:701:HOH:O	2.17	0.58
1:A:159:ARG:NH1	4:A:717:HOH:O	2.36	0.57
1:G:60:ASN:HB3	1:G:63:LEU:HD22	1.86	0.57
1:B:5:ALA:N	4:B:721:HOH:O	2.37	0.57
1:E:308:THR:HG23	1:E:380:GLY:HA3	1.87	0.57
1:F:293:ASP:OD1	4:F:701:HOH:O	2.18	0.57
1:G:238:GLN:NE2	4:G:702:HOH:O	2.37	0.56
1:B:27:HIS:NE2	4:B:701:HOH:O	2.32	0.56
1:B:457:MET:O	1:B:473:ARG:NH1	2.35	0.56
1:D:430:LEU:O	1:D:462:LYS:NZ	2.31	0.56
1:C:308:THR:HG21	1:C:399:SER:HB3	1.87	0.56
1:G:300:ASP:OD2	1:G:304:ARG:NH2	2.39	0.56
1:G:511:GLU:OE1	1:G:518:ARG:NH1	2.39	0.55
1:D:298:ASP:OD1	1:D:301:ARG:NH2	2.34	0.55
1:D:255:SER:O	4:D:701:HOH:O	2.18	0.55
1:A:513:ASP:HB3	1:A:518:ARG:HG2	1.86	0.55
1:C:91:GLU:CD	1:C:128:ASP:OD2	2.49	0.55
1:E:166:GLY:N	4:E:739:HOH:O	2.40	0.55
1:G:536:GLN:NE2	4:G:709:HOH:O	2.25	0.55
1:G:195:ARG:NH2	4:G:703:HOH:O	2.20	0.55
1:A:16:TRP:CD2	1:A:117:PRO:HB3	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:LYS:HE3	1:C:400:ALA:HB3	1.88	0.54
1:G:155:ASN:O	1:G:195:ARG:NH1	2.38	0.54
1:H:124:LEU:HD23	1:H:148:VAL:HB	1.89	0.54
1:B:7:TRP:CD2	1:B:8:PRO:HA	2.42	0.54
1:H:7:TRP:CD2	1:H:8:PRO:HA	2.42	0.54
1:A:441:LYS:NZ	1:A:502:ALA:O	2.34	0.54
1:G:62:HIS:O	1:G:65:GLU:HG2	2.07	0.54
1:D:308:THR:HG23	1:D:380:GLY:HA3	1.90	0.54
1:G:392:LYS:NZ	4:G:735:HOH:O	2.40	0.53
1:G:546:TYR:HB2	1:H:107:LEU:HD21	1.89	0.53
1:C:164:GLY:H	1:C:168:HIS:CD2	2.27	0.53
1:A:169:LEU:HG	1:A:193:MET:HE1	1.90	0.53
1:H:312:LEU:HD11	1:H:323:PHE:HB2	1.91	0.53
1:G:422:LYS:NZ	4:G:738:HOH:O	2.41	0.53
1:D:7:TRP:CD2	1:D:8:PRO:HA	2.44	0.53
1:H:511:GLU:OE1	1:H:518:ARG:NH1	2.41	0.53
1:G:90:SER:OG	1:G:93:THR:OG1	2.26	0.53
1:A:107:LEU:HD21	1:B:546:TYR:HB2	1.90	0.52
1:E:312:LEU:HD11	1:E:323:PHE:HB2	1.91	0.52
1:A:576:LYS:O	1:B:96:PRO:HA	2.09	0.52
1:D:5:ALA:N	4:D:735:HOH:O	2.43	0.52
1:E:129:KCX:OQ1	1:E:282:HIS:NE2	2.36	0.52
1:D:513:ASP:HB3	1:D:518:ARG:HG2	1.91	0.52
1:E:7:TRP:CD2	1:E:8:PRO:HA	2.45	0.52
1:E:146:ILE:HG22	1:E:244:ILE:HD13	1.92	0.52
1:B:16:TRP:CD2	1:B:117:PRO:HB3	2.44	0.51
1:C:511:GLU:OE1	1:C:518:ARG:NH1	2.39	0.51
1:C:190:GLU:OE1	1:D:28:ARG:NH1	2.43	0.51
1:F:531:ARG:NH2	4:F:735:HOH:O	2.43	0.51
1:F:312:LEU:HD11	1:F:323:PHE:HB2	1.92	0.51
1:F:415:PHE:CD1	1:F:421:TYR:HA	2.46	0.51
1:F:529:ALA:O	4:F:702:HOH:O	2.19	0.51
1:E:61:GLY:O	4:E:702:HOH:O	2.19	0.51
1:G:7:TRP:CD2	1:G:8:PRO:HA	2.45	0.51
1:D:297:ASP:OD2	4:D:702:HOH:O	2.19	0.51
1:A:319:LEU:N	4:A:701:HOH:O	2.44	0.51
1:C:107:LEU:HD21	1:D:546:TYR:HB2	1.92	0.51
1:C:409:LYS:HG2	1:C:509:MET:HE3	1.93	0.51
1:E:441:LYS:NZ	1:E:502:ALA:O	2.37	0.50
1:H:146:ILE:HD13	1:H:240:THR:HG23	1.93	0.50
1:A:546:TYR:HB2	1:B:107:LEU:HD21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:28:ARG:HD2	1:H:190:GLU:OE2	2.11	0.50
1:G:146:ILE:HG22	1:G:244:ILE:HD13	1.94	0.50
1:E:546:TYR:HB2	1:F:107:LEU:HD21	1.93	0.50
1:F:16:TRP:CD2	1:F:117:PRO:HB3	2.47	0.50
1:G:430:LEU:O	1:G:462:LYS:NZ	2.33	0.50
1:H:16:TRP:CD2	1:H:117:PRO:HB3	2.46	0.50
1:C:16:TRP:CD2	1:C:117:PRO:HB3	2.46	0.50
1:C:513:ASP:HB3	1:C:518:ARG:HG2	1.92	0.50
1:D:9:ARG:NH2	4:D:707:HOH:O	2.44	0.50
1:B:146:ILE:HG22	1:B:244:ILE:HD13	1.94	0.50
1:D:511:GLU:OE1	1:D:518:ARG:NH1	2.41	0.50
1:F:164:GLY:H	1:F:168:HIS:CD2	2.29	0.50
1:H:31:LEU:HD23	1:H:41:PHE:HE2	1.77	0.49
1:C:416:GLU:O	1:C:442:ASN:ND2	2.44	0.49
1:B:35:GLY:HA3	1:C:234:LYS:HB2	1.93	0.49
1:D:280:VAL:HA	1:D:299:TRP:CZ2	2.47	0.49
1:A:7:TRP:CD2	1:A:8:PRO:HA	2.48	0.49
1:E:271:ALA:O	1:E:308:THR:HG22	2.12	0.49
1:H:91:GLU:OE1	1:H:129:KCX:OQ1	2.30	0.49
1:B:362:VAL:O	4:B:704:HOH:O	2.20	0.49
1:F:124:LEU:HD23	1:F:148:VAL:HB	1.94	0.49
1:H:166:GLY:N	4:H:729:HOH:O	2.37	0.49
1:A:28:ARG:NH1	1:B:190:GLU:OE1	2.45	0.49
1:A:36:TYR:HB3	1:A:40:LEU:HD12	1.95	0.49
1:C:7:TRP:CD2	1:C:8:PRO:HA	2.47	0.49
1:C:409:LYS:HD2	1:C:511:GLU:HG2	1.93	0.49
1:G:16:TRP:CD2	1:G:117:PRO:HB3	2.48	0.48
1:G:17:TYR:HB3	1:G:41:PHE:HB3	1.95	0.48
1:B:31:LEU:HD23	1:B:41:PHE:HE1	1.78	0.48
1:F:562:ASP:OD1	4:F:705:HOH:O	2.20	0.48
1:B:508:ASP:HB3	1:B:521:LEU:HD11	1.95	0.48
1:C:97:THR:N	4:C:731:HOH:O	2.41	0.48
1:G:473:ARG:NH2	4:G:715:HOH:O	2.28	0.48
1:C:312:LEU:HD11	1:C:323:PHE:HB2	1.95	0.48
1:D:22:ARG:NH2	1:D:579:HIS:OXT	2.46	0.48
1:B:298:ASP:OD1	1:B:301:ARG:NH2	2.40	0.48
1:F:83:GLU:OE2	4:F:704:HOH:O	2.20	0.48
1:B:511:GLU:OE1	1:B:518:ARG:NH1	2.46	0.48
1:E:435:ASN:ND2	4:E:740:HOH:O	2.41	0.48
1:A:268:ARG:NH1	4:A:714:HOH:O	2.35	0.48
1:C:438:MET:HB2	1:C:473:ARG:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:TYR:HB3	1:D:40:LEU:HD12	1.96	0.48
1:E:435:ASN:OD1	4:E:703:HOH:O	2.20	0.48
1:G:85:PRO:O	4:G:704:HOH:O	2.20	0.48
1:C:34:GLN:NE2	1:D:58:PRO:O	2.47	0.47
1:F:23:ASP:OD2	4:F:703:HOH:O	2.19	0.47
1:H:415:PHE:CD1	1:H:421:TYR:HA	2.49	0.47
1:A:190:GLU:OE2	1:B:28:ARG:HD2	2.14	0.47
1:A:261:GLN:OE1	1:A:261:GLN:N	2.46	0.47
1:C:271:ALA:O	1:C:308:THR:HG22	2.14	0.47
1:H:152:PRO:HD2	1:H:226:ILE:O	2.14	0.47
1:C:36:TYR:HB3	1:C:40:LEU:HD12	1.96	0.47
1:E:107:LEU:HD21	1:F:546:TYR:HB2	1.95	0.47
1:C:164:GLY:H	1:C:168:HIS:HD2	1.62	0.47
1:D:366:GLU:HB3	1:D:371:PRO:HD3	1.96	0.47
1:G:56:MET:HE1	1:H:118:MET:HB3	1.97	0.47
1:A:183:GLN:NE2	1:B:20:THR:O	2.46	0.47
1:A:321:GLU:OE1	4:A:702:HOH:O	2.21	0.47
1:A:408:HIS:HD2	1:A:437:ILE:HD11	1.80	0.47
1:E:110:GLU:OE1	4:E:704:HOH:O	2.20	0.47
1:E:190:GLU:OE1	1:F:28:ARG:NH1	2.48	0.47
1:C:408:HIS:HD2	1:C:437:ILE:HD11	1.79	0.47
1:H:57:THR:HG23	1:H:90:SER:HB3	1.97	0.47
1:B:124:LEU:HD23	1:B:148:VAL:HB	1.96	0.46
1:D:146:ILE:HG22	1:D:244:ILE:HD13	1.97	0.46
1:C:28:ARG:HD2	1:D:190:GLU:OE2	2.15	0.46
1:E:226:ILE:O	1:E:233:ARG:NH2	2.44	0.46
1:G:451:MET:HG2	1:G:478:ARG:HG3	1.96	0.46
1:B:95:ARG:HA	1:B:96:PRO:C	2.41	0.46
1:B:304:ARG:HH22	1:B:517:ARG:HG3	1.81	0.46
1:H:179:GLY:O	4:H:701:HOH:O	2.20	0.46
1:H:95:ARG:HA	1:H:96:PRO:C	2.40	0.46
1:B:261:GLN:OE1	1:B:261:GLN:N	2.45	0.46
1:H:271:ALA:O	1:H:308:THR:HG22	2.16	0.46
1:C:57:THR:HG23	1:C:90:SER:HB3	1.98	0.46
1:D:415:PHE:CD1	1:D:421:TYR:HA	2.51	0.46
1:E:62:HIS:O	1:E:65:GLU:HG2	2.16	0.46
1:H:308:THR:HG23	1:H:380:GLY:HA3	1.98	0.46
1:C:539:HIS:O	1:C:541:LEU:HD12	2.15	0.46
1:G:271:ALA:O	1:G:308:THR:HG22	2.15	0.46
1:A:448:TYR:OH	1:B:577:ASP:O	2.29	0.46
1:C:128:ASP:CG	1:C:205:THR:HB	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:513:ASP:HB3	1:F:518:ARG:HG2	1.98	0.46
1:C:51:ASN:HA	1:C:124:LEU:HB2	1.97	0.45
1:D:261:GLN:OE1	1:D:261:GLN:N	2.44	0.45
1:D:508:ASP:HB3	1:D:521:LEU:HD11	1.98	0.45
1:F:59:CYS:HB3	1:F:199:THR:HG22	1.98	0.45
1:H:441:LYS:NZ	1:H:502:ALA:O	2.34	0.45
1:E:308:THR:HG21	1:E:399:SER:HB3	1.99	0.45
1:C:28:ARG:NH1	1:D:190:GLU:OE1	2.49	0.45
1:C:96:PRO:HA	1:D:576:LYS:O	2.17	0.45
1:F:128:ASP:HB2	4:F:835:HOH:O	2.16	0.45
1:F:146:ILE:HD13	1:F:240:THR:HG23	1.98	0.45
1:G:187:LEU:HD11	1:H:20:THR:HB	1.98	0.45
1:H:60:ASN:HB3	1:H:63:LEU:HD22	1.98	0.45
1:D:308:THR:HG21	1:D:399:SER:HB3	1.99	0.45
1:E:261:GLN:OE1	1:E:261:GLN:N	2.46	0.45
1:G:280:VAL:HA	1:G:299:TRP:CZ2	2.52	0.45
1:G:242:ARG:NH2	4:G:702:HOH:O	2.49	0.45
1:G:415:PHE:CD1	1:G:421:TYR:HA	2.51	0.45
1:E:513:ASP:HB3	1:E:518:ARG:HG2	1.97	0.45
1:A:300:ASP:OD2	1:A:304:ARG:NH2	2.49	0.45
1:E:523:ILE:HD11	1:E:528:LEU:HG	1.97	0.45
1:F:164:GLY:H	1:F:168:HIS:HD2	1.64	0.45
1:H:31:LEU:HD23	1:H:41:PHE:CE2	2.51	0.45
1:B:503:VAL:HB	1:B:531:ARG:HB3	1.99	0.45
1:D:51:ASN:HA	1:D:124:LEU:HB2	1.99	0.45
1:A:415:PHE:CD1	1:A:421:TYR:HA	2.52	0.44
1:A:562:ASP:OD1	1:A:563:LEU:N	2.49	0.44
1:F:562:ASP:OD1	1:F:563:LEU:N	2.50	0.44
1:A:82:LEU:HD12	1:B:56:MET:HE2	1.99	0.44
1:B:303:GLY:HA3	4:B:811:HOH:O	2.16	0.44
1:B:474:ILE:HG12	1:B:488:VAL:HB	1.98	0.44
1:E:478:ARG:NH2	4:E:707:HOH:O	2.34	0.44
1:A:536:GLN:HA	1:A:537:PRO:HD3	1.75	0.44
1:E:190:GLU:OE2	1:F:28:ARG:HD2	2.17	0.44
1:A:304:ARG:NH1	4:A:749:HOH:O	2.50	0.44
1:B:419:ASP:O	4:B:705:HOH:O	2.21	0.44
1:C:60:ASN:HB3	1:C:63:LEU:HD22	1.99	0.44
1:F:308:THR:HG23	1:F:380:GLY:HA3	2.00	0.44
1:C:261:GLN:OE1	1:C:261:GLN:N	2.46	0.44
1:C:31:LEU:HD23	1:C:41:PHE:HE1	1.83	0.44
1:G:486:THR:N	4:G:715:HOH:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ILE:HD13	1:A:240:THR:HG23	1.99	0.43
1:B:57:THR:HG23	1:B:90:SER:HB3	1.99	0.43
1:G:527:GLU:OE1	1:G:530:ARG:NH1	2.51	0.43
1:B:430:LEU:O	1:B:462:LYS:NZ	2.37	0.43
1:A:60:ASN:HB3	1:A:63:LEU:HD22	2.00	0.43
1:C:124:LEU:HD23	1:C:148:VAL:HB	2.00	0.43
1:D:284:LEU:HD23	1:D:294:LEU:HD23	1.99	0.43
1:D:14:GLN:NE2	4:D:727:HOH:O	2.38	0.43
1:E:280:VAL:HA	1:E:299:TRP:CZ2	2.53	0.43
1:F:91:GLU:HA	1:F:98:ALA:HB2	1.99	0.43
1:F:478:ARG:HG2	1:F:490:HIS:CE1	2.54	0.43
1:G:576:LYS:O	1:H:96:PRO:HA	2.19	0.43
1:B:220:LEU:HB2	1:B:236:MET:SD	2.59	0.43
1:F:481:GLY:O	4:F:706:HOH:O	2.22	0.43
1:G:220:LEU:HB2	1:G:236:MET:SD	2.59	0.43
1:G:308:THR:HG23	1:G:380:GLY:HA3	2.01	0.43
1:F:530:ARG:O	1:F:534:GLU:HG2	2.19	0.43
1:H:71:LYS:HG2	1:H:81:PRO:HB2	2.00	0.43
1:H:261:GLN:OE1	1:H:261:GLN:N	2.49	0.43
1:A:408:HIS:CD2	1:A:437:ILE:HD11	2.54	0.43
1:F:152:PRO:HD2	1:F:226:ILE:O	2.19	0.43
1:E:187:LEU:HD11	1:F:20:THR:HB	2.00	0.43
1:G:546:TYR:N	4:G:740:HOH:O	2.41	0.43
1:A:28:ARG:HD2	1:B:190:GLU:OE2	2.19	0.42
1:B:271:ALA:O	1:B:308:THR:HG22	2.18	0.42
1:A:55:ASP:O	4:A:703:HOH:O	2.21	0.42
1:C:190:GLU:OE2	1:D:28:ARG:HD2	2.18	0.42
1:C:415:PHE:CD1	1:C:421:TYR:HA	2.54	0.42
1:C:503:VAL:HB	1:C:531:ARG:HB3	2.01	0.42
1:G:59:CYS:HB3	1:G:199:THR:HG22	2.00	0.42
1:G:308:THR:OG1	1:G:376:LEU:HB2	2.19	0.42
1:B:71:LYS:HG2	1:B:81:PRO:HB2	2.02	0.42
1:C:101:TYR:HE2	4:C:731:HOH:O	2.02	0.42
1:D:268:ARG:NH1	4:D:724:HOH:O	2.37	0.42
1:D:308:THR:CG2	1:D:380:GLY:HA3	2.49	0.42
1:H:438:MET:HB2	1:H:473:ARG:HG2	2.01	0.42
1:B:308:THR:HG21	1:B:399:SER:HB3	2.00	0.42
1:G:152:PRO:HD2	1:G:226:ILE:O	2.20	0.42
1:D:322:GLU:HB3	1:D:368:VAL:HG21	2.01	0.42
1:F:175:MET:HE2	1:F:181:MET:HB2	2.02	0.42
1:G:432:ILE:HD11	1:G:471:MET:HE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:SER:OG	1:C:93:THR:OG1	2.33	0.42
1:C:190:GLU:OE2	1:D:32:LYS:NZ	2.44	0.42
1:F:417:ASP:OD1	1:F:420:ASP:N	2.40	0.42
1:H:176:VAL:HA	1:H:181:MET:O	2.20	0.42
1:D:16:TRP:CD2	1:D:117:PRO:HB3	2.55	0.42
1:F:432:ILE:HD11	1:F:471:MET:HE1	2.02	0.42
1:G:172:PHE:O	1:G:176:VAL:HG23	2.20	0.42
1:A:312:LEU:HD11	1:A:323:PHE:HB2	2.00	0.41
1:F:509:MET:HB2	1:F:522:ASP:HB3	2.02	0.41
1:C:546:TYR:HB2	1:D:107:LEU:HD21	2.02	0.41
1:E:176:VAL:HA	1:E:181:MET:O	2.20	0.41
1:E:265:ASN:HD21	1:E:343:HIS:HB2	1.85	0.41
1:F:57:THR:HG23	1:F:90:SER:HB3	2.01	0.41
1:F:271:ALA:O	1:F:308:THR:HG22	2.20	0.41
1:A:195:ARG:NH1	1:C:230:ASP:OD2	2.53	0.41
1:G:511:GLU:HB2	1:G:520:HIS:HB3	2.00	0.41
1:E:57:THR:HG23	1:E:90:SER:HB3	2.03	0.41
1:E:527:GLU:HA	1:E:530:ARG:HG2	2.03	0.41
1:G:414:VAL:N	1:G:506:ASN:OD1	2.43	0.41
1:D:197:SER:OG	4:D:703:HOH:O	2.22	0.41
1:F:283:LEU:HD12	1:F:299:TRP:CZ2	2.56	0.41
1:G:261:GLN:OE1	1:G:261:GLN:N	2.47	0.41
1:B:459:LEU:HD22	1:B:471:MET:HB2	2.03	0.41
1:D:59:CYS:HB3	1:D:199:THR:HG22	2.01	0.41
1:A:94:PHE:HA	1:B:115:GLY:O	2.21	0.41
1:C:541:LEU:HD23	1:C:551:GLN:HG2	2.03	0.41
1:H:167:THR:HA	1:H:170:TRP:CD1	2.55	0.41
1:E:16:TRP:CD2	1:E:117:PRO:HB3	2.55	0.41
1:G:146:ILE:HD13	1:G:240:THR:HG23	2.03	0.41
1:A:95:ARG:HA	1:A:96:PRO:C	2.45	0.41
1:A:124:LEU:HD23	1:A:148:VAL:HB	2.02	0.41
1:C:312:LEU:O	1:C:316:GLY:N	2.37	0.41
1:C:412:ALA:HB3	4:C:701:HOH:O	2.21	0.41
1:E:195:ARG:NH1	4:E:771:HOH:O	2.54	0.41
1:E:267:ILE:HD13	1:E:299:TRP:HA	2.03	0.41
1:A:308:THR:HG23	1:A:380:GLY:HA3	2.03	0.41
1:A:30:TRP:HZ2	1:B:165:SER:HB3	1.84	0.40
1:B:280:VAL:HA	1:B:299:TRP:CZ2	2.56	0.40
1:E:28:ARG:HD2	1:F:190:GLU:OE2	2.20	0.40
1:E:415:PHE:CD1	1:E:421:TYR:HA	2.56	0.40
1:G:562:ASP:OD1	1:G:563:LEU:N	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:562:ASP:OD1	1:C:563:LEU:N	2.51	0.40
1:D:527:GLU:HA	1:D:530:ARG:HG2	2.04	0.40
1:E:356:ASP:O	4:E:705:HOH:O	2.22	0.40
1:E:478:ARG:HG2	1:E:490:HIS:CE1	2.56	0.40
1:B:100:MET:HE3	1:B:550:HIS:CD2	2.56	0.40
1:C:208:THR:O	1:C:212:MET:HG2	2.21	0.40
1:E:284:LEU:HD23	1:E:294:LEU:HD23	2.03	0.40
1:F:501:LEU:O	4:F:707:HOH:O	2.22	0.40
1:G:28:ARG:HG3	1:G:41:PHE:CG	2.57	0.40
1:A:103:ASN:ND2	4:A:753:HOH:O	2.53	0.40
1:C:82:LEU:HD12	1:D:56:MET:HE2	2.04	0.40
1:D:562:ASP:OD1	1:D:563:LEU:N	2.53	0.40
1:F:97:THR:N	4:F:718:HOH:O	2.38	0.40
1:D:271:ALA:O	1:D:308:THR:HG22	2.21	0.40
1:E:31:LEU:HD23	1:E:41:PHE:HE2	1.86	0.40
1:E:234:LYS:HB2	1:H:35:GLY:HA3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are 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
1	KCX	F	129	1,2	10,11,12	1.70	2 (20%)	6,12,14	3.49	2 (33%)
1	KCX	B	129	1,2	10,11,12	1.80	3 (30%)	6,12,14	3.31	2 (33%)
1	KCX	H	129	1,2	10,11,12	1.76	3 (30%)	6,12,14	3.67	2 (33%)
1	KCX	G	129	1,2	10,11,12	1.85	3 (30%)	6,12,14	3.39	2 (33%)
1	KCX	E	129	1,2	10,11,12	1.68	2 (20%)	6,12,14	3.19	2 (33%)
1	KCX	C	129	1,2	10,11,12	1.67	2 (20%)	6,12,14	3.52	2 (33%)
1	KCX	A	129	1,2	10,11,12	1.73	2 (20%)	6,12,14	3.24	2 (33%)
1	KCX	D	129	1,2	10,11,12	1.65	1 (10%)	6,12,14	3.50	2 (33%)

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
1	KCX	F	129	1,2	-	7/9/10/12	-
1	KCX	B	129	1,2	-	6/9/10/12	-
1	KCX	H	129	1,2	-	4/9/10/12	-
1	KCX	G	129	1,2	-	4/9/10/12	-
1	KCX	E	129	1,2	-	0/9/10/12	-
1	KCX	C	129	1,2	-	5/9/10/12	-
1	KCX	A	129	1,2	-	4/9/10/12	-
1	KCX	D	129	1,2	-	5/9/10/12	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	129	KCX	CX-NZ	3.72	1.41	1.35
1	G	129	KCX	CX-NZ	3.57	1.41	1.35
1	B	129	KCX	CX-NZ	3.53	1.41	1.35
1	E	129	KCX	CX-NZ	3.51	1.41	1.35
1	F	129	KCX	CX-NZ	3.48	1.41	1.35
1	H	129	KCX	CX-NZ	3.41	1.41	1.35
1	C	129	KCX	CX-NZ	3.36	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	129	KCX	CX-NZ	3.32	1.41	1.35
1	G	129	KCX	OQ1-CX	2.78	1.26	1.21
1	H	129	KCX	OQ1-CX	2.65	1.26	1.21
1	B	129	KCX	OQ1-CX	2.59	1.26	1.21
1	A	129	KCX	OQ1-CX	2.18	1.25	1.21
1	B	129	KCX	O-C	2.10	1.27	1.20
1	E	129	KCX	O-C	2.08	1.27	1.20
1	F	129	KCX	O-C	2.06	1.27	1.20
1	H	129	KCX	O-C	2.05	1.27	1.20
1	C	129	KCX	OQ1-CX	2.01	1.25	1.21
1	G	129	KCX	O-C	2.01	1.27	1.20

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	129	KCX	CE-NZ-CX	-8.01	108.39	121.98
1	C	129	KCX	CE-NZ-CX	-7.56	109.16	121.98
1	D	129	KCX	CE-NZ-CX	-7.55	109.17	121.98
1	F	129	KCX	CE-NZ-CX	-7.52	109.23	121.98
1	G	129	KCX	CE-NZ-CX	-7.31	109.57	121.98
1	A	129	KCX	CE-NZ-CX	-7.12	109.91	121.98
1	B	129	KCX	CE-NZ-CX	-7.08	109.96	121.98
1	E	129	KCX	CE-NZ-CX	-6.89	110.28	121.98
1	F	129	KCX	OQ1-CX-NZ	-3.53	119.55	124.92
1	C	129	KCX	OQ1-CX-NZ	-3.48	119.63	124.92
1	D	129	KCX	OQ1-CX-NZ	-3.44	119.70	124.92
1	H	129	KCX	OQ1-CX-NZ	-3.36	119.81	124.92
1	B	129	KCX	OQ1-CX-NZ	-3.35	119.83	124.92
1	E	129	KCX	OQ1-CX-NZ	-3.32	119.88	124.92
1	G	129	KCX	OQ1-CX-NZ	-3.32	119.88	124.92
1	A	129	KCX	OQ1-CX-NZ	-3.00	120.36	124.92

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	129	KCX	C-CA-CB-CG
1	B	129	KCX	N-CA-CB-CG
1	B	129	KCX	C-CA-CB-CG
1	B	129	KCX	OQ1-CX-NZ-CE
1	C	129	KCX	C-CA-CB-CG
1	D	129	KCX	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	D	129	KCX	C-CA-CB-CG
1	F	129	KCX	N-CA-CB-CG
1	F	129	KCX	C-CA-CB-CG
1	G	129	KCX	C-CA-CB-CG
1	G	129	KCX	OQ1-CX-NZ-CE
1	H	129	KCX	C-CA-CB-CG
1	H	129	KCX	OQ1-CX-NZ-CE
1	H	129	KCX	OQ2-CX-NZ-CE
1	A	129	KCX	CG-CD-CE-NZ
1	A	129	KCX	CA-CB-CG-CD
1	F	129	KCX	CA-CB-CG-CD
1	F	129	KCX	CE-CD-CG-CB
1	B	129	KCX	CE-CD-CG-CB
1	F	129	KCX	CG-CD-CE-NZ
1	D	129	KCX	CA-CB-CG-CD
1	D	129	KCX	CE-CD-CG-CB
1	B	129	KCX	CA-CB-CG-CD
1	B	129	KCX	OQ2-CX-NZ-CE
1	C	129	KCX	OQ1-CX-NZ-CE
1	C	129	KCX	OQ2-CX-NZ-CE
1	G	129	KCX	OQ2-CX-NZ-CE
1	D	129	KCX	CG-CD-CE-NZ
1	G	129	KCX	CA-CB-CG-CD
1	C	129	KCX	CA-CB-CG-CD
1	F	129	KCX	OQ1-CX-NZ-CE
1	F	129	KCX	OQ2-CX-NZ-CE
1	A	129	KCX	N-CA-CB-CG
1	C	129	KCX	N-CA-CB-CG
1	H	129	KCX	N-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	H	129	KCX	1	0
1	G	129	KCX	1	0
1	E	129	KCX	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	FES	G	602	1	0,4,4	-	-	-		
3	FES	H	602	1	0,4,4	-	-	-		
3	FES	D	602	1	0,4,4	-	-	-		
3	FES	A	602	1	0,4,4	-	-	-		
3	FES	B	602	4,1	0,4,4	-	-	-		
3	FES	F	602	1	0,4,4	-	-	-		
3	FES	C	602	1	0,4,4	-	-	-		
3	FES	E	602	1	0,4,4	-	-	-		

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	FES	G	602	1	-	-	0/1/1/1
3	FES	H	602	1	-	-	0/1/1/1
3	FES	D	602	1	-	-	0/1/1/1
3	FES	A	602	1	-	-	0/1/1/1
3	FES	B	602	4,1	-	-	0/1/1/1
3	FES	F	602	1	-	-	0/1/1/1
3	FES	C	602	1	-	-	0/1/1/1
3	FES	E	602	1	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	574/588 (97%)	-0.83	0 100 100	22, 37, 58, 93	0
1	B	574/588 (97%)	-0.64	0 100 100	19, 38, 63, 100	0
1	C	574/588 (97%)	-0.76	0 100 100	21, 38, 62, 90	0
1	D	574/588 (97%)	-0.57	0 100 100	22, 37, 59, 92	0
1	E	574/588 (97%)	-0.78	0 100 100	22, 37, 59, 88	0
1	F	574/588 (97%)	-0.65	0 100 100	22, 39, 63, 92	0
1	G	574/588 (97%)	-0.71	0 100 100	20, 38, 64, 97	0
1	H	574/588 (97%)	-0.53	2 (0%) 90 88	22, 37, 59, 94	0
All	All	4592/4704 (97%)	-0.68	2 (0%) 100 100	19, 37, 62, 100	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	504	VAL	2.8
1	H	390	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	KCX	H	129	12/13	0.97	0.08	16,31,58,75	0
1	KCX	C	129	12/13	0.98	0.06	22,34,45,52	0
1	KCX	D	129	12/13	0.98	0.06	17,31,39,41	0
1	KCX	E	129	12/13	0.98	0.06	14,25,37,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	KCX	F	129	12/13	0.98	0.07	23,32,50,55	0
1	KCX	G	129	12/13	0.98	0.06	24,38,72,75	0
1	KCX	B	129	12/13	0.98	0.08	21,44,51,57	0
1	KCX	A	129	12/13	0.99	0.06	13,39,65,66	0

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
2	MG	E	601	1/1	0.96	0.07	33,33,33,33	0
2	MG	C	601	1/1	0.97	0.04	29,29,29,29	0
2	MG	A	601	1/1	0.98	0.03	43,43,43,43	0
3	FES	F	602	4/4	0.98	0.07	51,53,56,110	0
3	FES	G	602	4/4	0.98	0.06	50,62,63,66	0
3	FES	H	602	4/4	0.98	0.04	51,54,72,91	0
2	MG	H	601	1/1	0.99	0.03	37,37,37,37	0
3	FES	A	602	4/4	0.99	0.05	41,61,65,73	0
3	FES	B	602	4/4	0.99	0.04	50,57,58,67	0
3	FES	C	602	4/4	0.99	0.04	47,52,65,66	0
3	FES	D	602	4/4	0.99	0.05	43,47,51,87	0
3	FES	E	602	4/4	0.99	0.04	42,43,45,60	0
2	MG	D	601	1/1	0.99	0.03	45,45,45,45	0
2	MG	B	601	1/1	0.99	0.03	45,45,45,45	0
2	MG	G	601	1/1	0.99	0.04	58,58,58,58	0
2	MG	F	601	1/1	1.00	0.02	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.