



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:25 PM UTC

PDB ID : 3EZQ / pdb_00003ezq
Title : Crystal Structure of the Fas/FADD Death Domain Complex
Authors : Schwarzenbacher, R.; Robinson, H.; Stec, B.; Riedl, S.J.
Deposited on : 2008-10-23
Resolution : 2.73 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

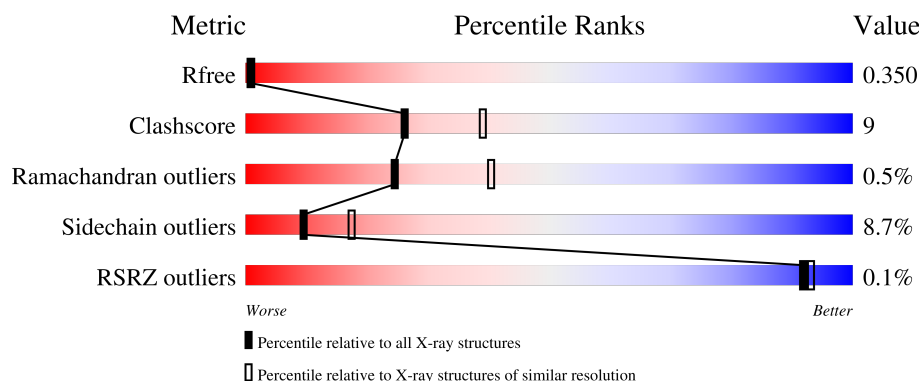
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	115	80% 19% .
1	C	115	80% 17% ..
1	E	115	81% 17% .
1	G	115	84% 14% .
1	I	115	83% 13% .

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Mol	Chain	Length	Quality of chain
1	K	115	
1	M	115	
1	O	115	
2	B	122	
2	D	122	
2	F	122	
2	H	122	
2	J	122	
2	L	122	
2	N	122	
2	P	122	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	K	13	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13933 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 Tumor necrosis factor receptor superfamily member 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	115	Total	C	N	O	S	0	0	0
			916	571	159	184	2			
1	C	115	Total	C	N	O	S	0	0	0
			916	571	159	184	2			
1	E	115	Total	C	N	O	S	0	0	0
			916	571	159	184	2			
1	G	115	Total	C	N	O	S	0	0	0
			916	571	159	184	2			
1	I	115	Total	C	N	O	S	0	0	0
			916	571	159	184	2			
1	K	115	Total	C	N	O	S	0	0	0
			916	571	159	184	2			
1	M	115	Total	C	N	O	S	0	0	0
			916	571	159	184	2			
1	O	115	Total	C	N	O	S	0	0	0
			916	571	159	184	2			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	336	LEU	-	expression tag	UNP P25445
A	337	GLU	-	expression tag	UNP P25445
C	336	LEU	-	expression tag	UNP P25445
C	337	GLU	-	expression tag	UNP P25445
E	336	LEU	-	expression tag	UNP P25445
E	337	GLU	-	expression tag	UNP P25445
G	336	LEU	-	expression tag	UNP P25445
G	337	GLU	-	expression tag	UNP P25445
I	336	LEU	-	expression tag	UNP P25445
I	337	GLU	-	expression tag	UNP P25445
K	336	LEU	-	expression tag	UNP P25445
K	337	GLU	-	expression tag	UNP P25445
M	336	LEU	-	expression tag	UNP P25445

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Chain	Residue	Modelled	Actual	Comment	Reference
M	337	GLU	-	expression tag	UNP P25445
O	336	LEU	-	expression tag	UNP P25445
O	337	GLU	-	expression tag	UNP P25445

- Molecule 2 is a protein called Protein FADD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			795	483	154	154	4			
2	D	99	Total	C	N	O	S	0	0	0
			795	483	154	154	4			
2	F	99	Total	C	N	O	S	0	0	0
			795	483	154	154	4			
2	H	99	Total	C	N	O	S	0	0	0
			795	483	154	154	4			
2	J	99	Total	C	N	O	S	0	0	0
			795	483	154	154	4			
2	L	99	Total	C	N	O	S	0	0	0
			795	483	154	154	4			
2	N	99	Total	C	N	O	S	0	0	0
			795	483	154	154	4			
2	P	99	Total	C	N	O	S	0	0	0
			795	483	154	154	4			

There are 48 discrepancies between the modelled and reference sequences:

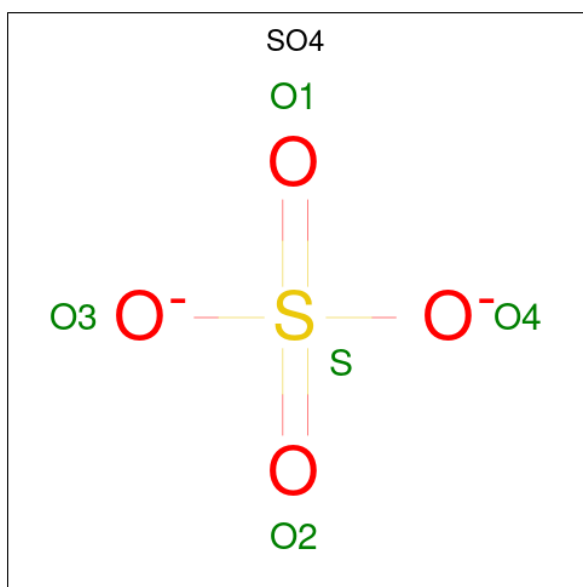
Chain	Residue	Modelled	Actual	Comment	Reference
B	209	HIS	-	expression tag	UNP Q13158
B	210	HIS	-	expression tag	UNP Q13158
B	211	HIS	-	expression tag	UNP Q13158
B	212	HIS	-	expression tag	UNP Q13158
B	213	HIS	-	expression tag	UNP Q13158
B	214	HIS	-	expression tag	UNP Q13158
D	209	HIS	-	expression tag	UNP Q13158
D	210	HIS	-	expression tag	UNP Q13158
D	211	HIS	-	expression tag	UNP Q13158
D	212	HIS	-	expression tag	UNP Q13158
D	213	HIS	-	expression tag	UNP Q13158
D	214	HIS	-	expression tag	UNP Q13158
F	209	HIS	-	expression tag	UNP Q13158
F	210	HIS	-	expression tag	UNP Q13158
F	211	HIS	-	expression tag	UNP Q13158

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Chain	Residue	Modelled	Actual	Comment	Reference
F	212	HIS	-	expression tag	UNP Q13158
F	213	HIS	-	expression tag	UNP Q13158
F	214	HIS	-	expression tag	UNP Q13158
H	209	HIS	-	expression tag	UNP Q13158
H	210	HIS	-	expression tag	UNP Q13158
H	211	HIS	-	expression tag	UNP Q13158
H	212	HIS	-	expression tag	UNP Q13158
H	213	HIS	-	expression tag	UNP Q13158
H	214	HIS	-	expression tag	UNP Q13158
J	209	HIS	-	expression tag	UNP Q13158
J	210	HIS	-	expression tag	UNP Q13158
J	211	HIS	-	expression tag	UNP Q13158
J	212	HIS	-	expression tag	UNP Q13158
J	213	HIS	-	expression tag	UNP Q13158
J	214	HIS	-	expression tag	UNP Q13158
L	209	HIS	-	expression tag	UNP Q13158
L	210	HIS	-	expression tag	UNP Q13158
L	211	HIS	-	expression tag	UNP Q13158
L	212	HIS	-	expression tag	UNP Q13158
L	213	HIS	-	expression tag	UNP Q13158
L	214	HIS	-	expression tag	UNP Q13158
N	209	HIS	-	expression tag	UNP Q13158
N	210	HIS	-	expression tag	UNP Q13158
N	211	HIS	-	expression tag	UNP Q13158
N	212	HIS	-	expression tag	UNP Q13158
N	213	HIS	-	expression tag	UNP Q13158
N	214	HIS	-	expression tag	UNP Q13158
P	209	HIS	-	expression tag	UNP Q13158
P	210	HIS	-	expression tag	UNP Q13158
P	211	HIS	-	expression tag	UNP Q13158
P	212	HIS	-	expression tag	UNP Q13158
P	213	HIS	-	expression tag	UNP Q13158
P	214	HIS	-	expression tag	UNP Q13158

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	M	1	Total	O	S	0	0
			5	4	1		
3	M	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	B	1	Total Na 1 1	0	0
4	E	1	Total Na 1 1	0	0
4	H	1	Total Na 1 1	0	0
4	J	1	Total Na 1 1	0	0
4	K	1	Total Na 1 1	0	0
4	M	1	Total Na 1 1	0	0
4	P	1	Total Na 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	7	Total O 7 7	0	0
5	B	2	Total O 2 2	0	0
5	C	8	Total O 8 8	0	0
5	D	4	Total O 4 4	0	0
5	E	9	Total O 9 9	0	0
5	F	4	Total O 4 4	0	0
5	G	11	Total O 11 11	0	0
5	H	8	Total O 8 8	0	0
5	I	84	Total O 84 84	0	0
5	J	8	Total O 8 8	0	0
5	K	6	Total O 6 6	0	0
5	L	7	Total O 7 7	0	0

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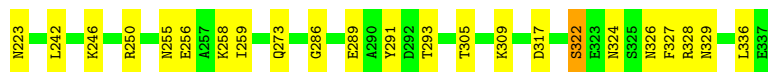
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	9	Total	O	0	0
			9	9		
5	N	3	Total	O	0	0
			3	3		
5	O	5	Total	O	0	0
			5	5		
5	P	2	Total	O	0	0
			2	2		

3 Residue-property plots [i](#)

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

- Molecule 1: Tumor necrosis factor receptor superfamily member 6

Chain A: 



- Molecule 1: Tumor necrosis factor receptor superfamily member 6

Chain C: 



- Molecule 1: Tumor necrosis factor receptor superfamily member 6

Chain E: 



- Molecule 1: Tumor necrosis factor receptor superfamily member 6

Chain G: 



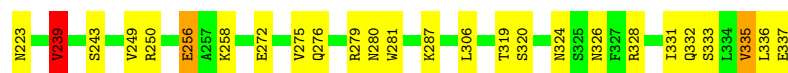
- Molecule 1: Tumor necrosis factor receptor superfamily member 6

Chain I: 



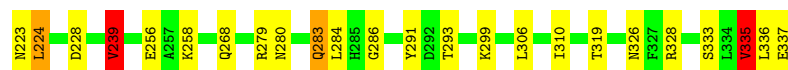
- Molecule 1: Tumor necrosis factor receptor superfamily member 6

Chain K: 



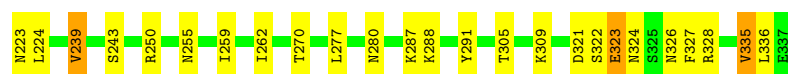
- Molecule 1: Tumor necrosis factor receptor superfamily member 6

Chain M: 79% 17%



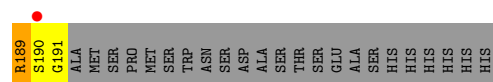
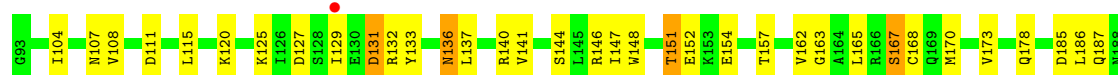
- Molecule 1: Tumor necrosis factor receptor superfamily member 6

Chain O: 78% 19%



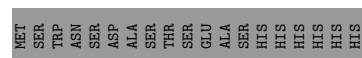
- Molecule 2: Protein FADD

Chain B: 2% 50% 27% 19%



- Molecule 2: Protein FADD

Chain D: 55% 26% 19%



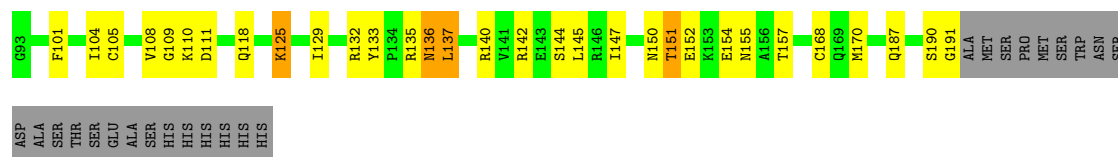
- Molecule 2: Protein FADD

Chain F: 62% 17% 19%

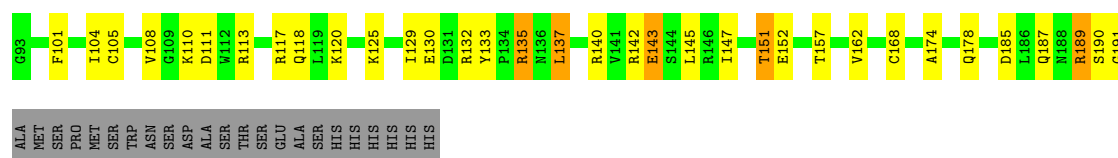


- Molecule 2: Protein FADD

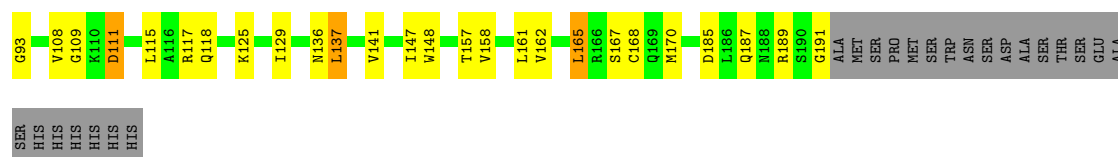
Chain H: 56% 22% 19%



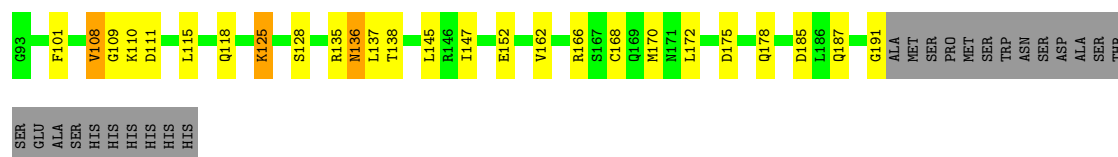
- Molecule 2: Protein FADD



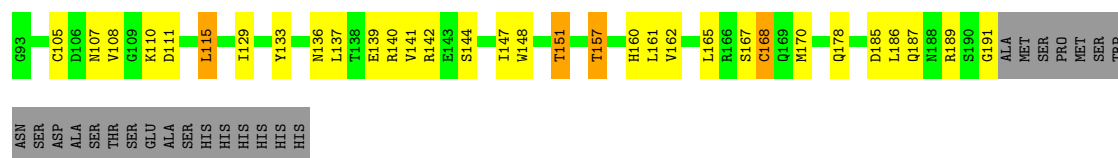
- Molecule 2: Protein FADD



- Molecule 2: Protein FADD



- Molecule 2: Protein FADD



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	126.22Å 126.22Å 299.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.73 30.00 – 2.73	Depositor EDS
% Data completeness (in resolution range)	98.8 (30.00-2.73) 98.8 (30.00-2.73)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.234 , 0.278 0.335 , 0.350	Depositor DCC
R_{free} test set	3556 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	73.2	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.499 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13933	wwPDB-VP
Average B, all atoms (Å ²)	87.0	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 45.65 % 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 1.2821e-04. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NA

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	0.76	0/923	0.90	0/1241
1	C	0.90	1/923 (0.1%)	0.93	1/1241 (0.1%)
1	E	0.85	0/923	0.91	0/1241
1	G	0.87	0/923	1.00	2/1241 (0.2%)
1	I	0.88	0/923	0.95	0/1241
1	K	0.85	0/923	0.93	1/1241 (0.1%)
1	M	0.91	3/923 (0.3%)	0.96	2/1241 (0.2%)
1	O	0.76	0/923	0.90	0/1241
2	B	0.67	1/802 (0.1%)	0.80	1/1080 (0.1%)
2	D	0.66	2/802 (0.2%)	0.80	0/1080
2	F	0.62	0/802	0.80	0/1080
2	H	0.68	0/802	0.87	0/1080
2	J	0.66	1/802 (0.1%)	0.83	0/1080
2	L	0.63	0/802	0.80	0/1080
2	N	0.61	0/802	0.82	0/1080
2	P	0.62	0/802	0.80	0/1080
All	All	0.76	8/13800 (0.1%)	0.88	7/18568 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	228	ASP	CG-OD1	6.77	1.38	1.25
1	C	279	ARG	NE-CZ	6.73	1.40	1.33
2	D	131	ASP	CG-OD2	6.40	1.37	1.25
2	J	135	ARG	NE-CZ	5.54	1.39	1.33
2	B	127	ASP	CG-OD1	5.39	1.35	1.25
1	M	310	ILE	CA-CB	-5.18	1.47	1.54
2	D	131	ASP	CG-OD1	5.08	1.34	1.25
1	M	224	LEU	CG-CD1	5.04	1.69	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	268	GLN	OE1-CD-NE2	-9.84	112.76	122.60
1	G	268	GLN	CG-CD-NE2	6.66	126.38	116.40
1	M	335	VAL	N-CA-CB	-6.07	104.05	111.94
1	C	335	VAL	N-CA-CB	-5.88	104.30	111.94
1	K	239	VAL	N-CA-CB	-5.86	104.48	112.28
1	M	239	VAL	N-CA-CB	-5.27	105.27	112.28
2	B	136	ASN	N-CA-C	5.26	117.30	108.73

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	916	0	939	18	0
1	C	916	0	939	17	0
1	E	916	0	939	15	0
1	G	916	0	939	13	0
1	I	916	0	939	16	0
1	K	916	0	939	21	0
1	M	916	0	939	15	0
1	O	916	0	939	26	0
2	B	795	0	793	24	0
2	D	795	0	793	15	0
2	F	795	0	793	20	0
2	H	795	0	793	20	0
2	J	795	0	793	23	0
2	L	795	0	793	23	0
2	N	795	0	793	19	0
2	P	795	0	793	28	0
3	A	5	0	0	0	0
3	C	5	0	0	0	0
3	E	10	0	0	0	0
3	G	5	0	0	0	0
3	I	5	0	0	0	0
3	J	5	0	0	0	0
3	K	10	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	M	10	0	0	1	0
3	O	5	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	H	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	M	1	0	0	0	0
4	P	1	0	0	0	0
5	A	7	0	0	1	0
5	B	2	0	0	0	0
5	C	8	0	0	1	0
5	D	4	0	0	0	0
5	E	9	0	0	0	0
5	F	4	0	0	0	0
5	G	11	0	0	0	0
5	H	8	0	0	1	0
5	I	84	0	0	4	0
5	J	8	0	0	0	0
5	K	6	0	0	0	0
5	L	7	0	0	1	0
5	M	9	0	0	1	0
5	N	3	0	0	0	0
5	O	5	0	0	0	0
5	P	2	0	0	3	0
All	All	13933	0	13856	259	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 9.

All (259) 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)
2:B:108:VAL:HG13	2:B:170:MET:HE1	1.35	1.04
2:L:109:GLY:HA2	2:L:137:LEU:HD21	1.37	1.04
2:H:108:VAL:HG13	2:H:170:MET:HE1	1.38	1.03
2:B:115:LEU:HD11	2:B:165:LEU:HD23	1.42	1.01
1:K:328:ARG:HE	1:K:332:GLN:HE22	1.13	0.95
2:F:109:GLY:HA2	2:F:137:LEU:HD21	1.47	0.91
1:A:289:GLU:O	1:A:293:THR:HG22	1.73	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:258:LYS:HG2	1:K:280:ASN:ND2	1.86	0.89
1:A:328:ARG:HG3	1:C:335:VAL:HG13	1.60	0.83
2:D:108:VAL:HG13	2:D:170:MET:HE1	1.59	0.83
1:K:258:LYS:HG2	1:K:280:ASN:HD21	1.44	0.80
1:K:328:ARG:NE	1:K:332:GLN:HE22	1.78	0.79
2:P:162:VAL:HG11	2:P:178:GLN:HE21	1.47	0.79
1:K:328:ARG:HE	1:K:332:GLN:NE2	1.79	0.79
2:N:108:VAL:HG13	2:N:170:MET:HE1	1.66	0.76
2:D:162:VAL:HG11	2:D:178:GLN:HE21	1.51	0.75
1:I:223:ASN:HB2	2:J:135:ARG:CZ	2.17	0.74
2:L:129:ILE:HD11	2:L:147:ILE:HD12	1.69	0.74
1:K:250:ARG:CZ	1:K:256:GLU:OE2	2.36	0.73
1:M:328:ARG:HG3	1:O:335:VAL:HG13	1.70	0.73
1:I:309:LYS:HZ2	2:J:189:ARG:HB3	1.52	0.73
1:G:223:ASN:HB2	2:H:135:ARG:CZ	2.18	0.73
2:F:115:LEU:HD11	2:F:165:LEU:HD12	1.70	0.73
2:J:137:LEU:HG	2:J:140:ARG:NH2	2.04	0.72
2:H:151:THR:HG22	2:H:152:GLU:OE1	1.90	0.72
2:L:108:VAL:HG23	2:L:109:GLY:H	1.55	0.71
2:H:136:ASN:HB2	5:H:19:HOH:O	1.90	0.71
2:B:115:LEU:CD1	2:B:165:LEU:HD23	2.20	0.71
2:F:108:VAL:HG13	2:F:170:MET:HE1	1.72	0.70
1:M:291:TYR:HB3	2:N:172:LEU:HD12	1.74	0.70
2:F:93:GLY:N	5:I:175:HOH:O	2.24	0.70
1:O:309:LYS:NZ	2:P:189:ARG:HB3	2.07	0.69
1:G:248:PHE:CZ	1:G:293:THR:HG22	2.27	0.68
5:I:106:HOH:O	2:N:136:ASN:ND2	2.27	0.68
2:F:129:ILE:HD11	2:F:147:ILE:HD12	1.77	0.67
2:N:175:ASP:CG	1:O:323:GLU:HG2	2.20	0.66
1:G:248:PHE:CE1	1:G:293:THR:HG22	2.30	0.66
2:P:115:LEU:HD11	2:P:165:LEU:HD23	1.78	0.65
1:A:322:SER:O	1:C:299:LYS:NZ	2.29	0.65
2:B:129:ILE:HD11	2:B:147:ILE:HD12	1.78	0.65
2:N:101:PHE:CD1	2:N:145:LEU:HD13	2.32	0.65
2:F:108:VAL:HG22	2:F:170:MET:HE1	1.77	0.65
1:O:323:GLU:OE2	1:O:323:GLU:HA	1.96	0.64
2:J:151:THR:HG23	2:J:152:GLU:OE2	1.97	0.64
2:D:157:THR:HG23	2:D:160:HIS:H	1.62	0.63
1:C:291:TYR:HB3	2:D:172:LEU:HD12	1.79	0.63
2:B:162:VAL:HG11	2:B:178:GLN:HE21	1.61	0.63
2:B:115:LEU:HD11	2:B:165:LEU:CD2	2.26	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:108:VAL:CG1	2:H:170:MET:HE1	2.21	0.62
2:P:148:TRP:O	2:P:151:THR:HG22	1.99	0.62
1:G:223:ASN:HB2	2:H:135:ARG:NE	2.14	0.62
2:B:178:GLN:NE2	5:I:97:HOH:O	2.31	0.62
1:G:239:VAL:O	1:G:239:VAL:HG13	2.00	0.62
2:N:162:VAL:HG11	2:N:178:GLN:HE21	1.64	0.62
2:H:132:ARG:HD3	2:H:133:TYR:CE1	2.35	0.61
2:P:129:ILE:HD11	2:P:147:ILE:HD12	1.80	0.61
1:A:291:TYR:OH	2:B:107:ASN:HB3	2.01	0.61
1:E:239:VAL:HA	2:F:187:GLN:HE22	1.64	0.61
1:A:255:ASN:OD1	1:A:258:LYS:HG3	2.00	0.61
2:L:115:LEU:HD11	2:L:165:LEU:HD12	1.83	0.60
2:J:151:THR:CG2	2:J:152:GLU:OE2	2.49	0.60
2:F:109:GLY:C	2:F:137:LEU:HD11	2.26	0.60
2:L:109:GLY:C	2:L:137:LEU:HD11	2.27	0.60
2:B:148:TRP:O	2:B:151:THR:HG22	2.02	0.60
2:D:118:GLN:HG3	2:D:168:CYS:SG	2.42	0.60
2:L:109:GLY:HA2	2:L:137:LEU:CD2	2.24	0.60
2:J:118:GLN:HG3	2:J:168:CYS:SG	2.42	0.59
2:L:108:VAL:HG21	2:L:141:VAL:HG11	1.84	0.59
1:M:279:ARG:O	1:M:283:GLN:HG3	2.02	0.59
1:C:270:THR:HG23	5:C:199:HOH:O	2.02	0.59
1:O:239:VAL:HG13	1:O:239:VAL:O	2.01	0.59
1:I:336:LEU:O	2:J:185:ASP:OD2	2.21	0.59
2:P:115:LEU:HD12	2:P:168:CYS:SG	2.44	0.58
2:H:118:GLN:HG3	2:H:168:CYS:SG	2.43	0.58
2:L:108:VAL:HG23	2:L:141:VAL:HG21	1.85	0.58
1:O:309:LYS:NZ	2:P:189:ARG:CD	2.67	0.57
2:F:118:GLN:HG3	2:F:168:CYS:SG	2.44	0.57
2:N:118:GLN:HG3	2:N:168:CYS:SG	2.44	0.57
2:P:189:ARG:HB2	5:P:217:HOH:O	2.04	0.57
2:L:129:ILE:HD11	2:L:147:ILE:CD1	2.35	0.57
2:L:115:LEU:CD1	2:L:165:LEU:HD12	2.35	0.57
1:O:323:GLU:OE2	1:O:323:GLU:CA	2.53	0.57
1:I:250:ARG:NE	1:I:256:GLU:OE1	2.38	0.56
1:M:306:LEU:HD13	1:O:327:PHE:CE2	2.41	0.56
1:O:309:LYS:NZ	2:P:189:ARG:HD2	2.22	0.55
1:A:327:PHE:CE2	1:C:306:LEU:HD13	2.42	0.55
1:O:309:LYS:HZ2	2:P:189:ARG:HD2	1.70	0.55
2:J:187:GLN:O	2:J:191:GLY:N	2.38	0.55
2:N:125:LYS:HG2	2:N:147:ILE:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:137:LEU:HD12	2:N:137:LEU:H	1.71	0.55
2:P:189:ARG:CB	5:P:217:HOH:O	2.54	0.55
1:I:239:VAL:O	1:I:239:VAL:HG13	2.06	0.55
1:O:305:THR:HB	2:P:186:LEU:HD13	1.88	0.54
2:D:187:GLN:O	2:D:191:GLY:N	2.39	0.54
1:O:291:TYR:OH	2:P:107:ASN:HB3	2.07	0.54
1:A:309:LYS:HZ2	2:B:189:ARG:HD2	1.72	0.54
2:F:129:ILE:HD11	2:F:147:ILE:CD1	2.37	0.54
1:O:335:VAL:HG13	1:O:335:VAL:O	2.06	0.54
1:A:317:ASP:OD1	1:A:324:ASN:ND2	2.40	0.53
2:H:187:GLN:O	2:H:191:GLY:N	2.39	0.53
2:F:109:GLY:HA2	2:F:137:LEU:CD2	2.32	0.53
1:A:250:ARG:HG3	1:A:259:ILE:HD11	1.91	0.53
1:A:223:ASN:HB3	2:B:136:ASN:HD21	1.74	0.53
1:M:326:ASN:HB2	3:M:12:SO4:S	2.49	0.53
1:E:239:VAL:HA	2:F:187:GLN:NE2	2.24	0.52
1:O:250:ARG:HG3	1:O:259:ILE:HD11	1.92	0.52
2:L:187:GLN:O	2:L:191:GLY:N	2.42	0.52
1:K:239:VAL:HG13	1:K:239:VAL:O	2.09	0.52
2:L:108:VAL:CG2	2:L:141:VAL:HG11	2.39	0.52
2:B:125:LYS:HG2	2:B:147:ILE:HD13	1.92	0.52
2:B:187:GLN:O	2:B:191:GLY:N	2.40	0.52
2:D:97:LEU:HD11	2:D:156:ALA:O	2.10	0.52
1:K:336:LEU:O	2:L:185:ASP:OD2	2.28	0.52
1:M:336:LEU:O	2:N:185:ASP:OD2	2.28	0.52
2:F:115:LEU:CD1	2:F:165:LEU:HD12	2.39	0.51
1:I:327:PHE:CE2	1:K:306:LEU:HD13	2.45	0.51
1:O:309:LYS:HZ1	2:P:189:ARG:HB3	1.74	0.51
1:O:336:LEU:O	2:P:185:ASP:OD2	2.29	0.51
2:P:129:ILE:HD11	2:P:147:ILE:CD1	2.40	0.51
1:C:250:ARG:HE	1:C:256:GLU:HG3	1.75	0.51
1:K:249:VAL:HG12	1:K:281:TRP:HB2	1.93	0.51
1:K:326:ASN:HB2	3:K:13:SO4:S	2.51	0.51
1:G:239:VAL:O	1:G:239:VAL:CG1	2.59	0.51
2:H:101:PHE:CD1	2:H:145:LEU:HD13	2.46	0.51
2:P:187:GLN:O	2:P:191:GLY:N	2.41	0.51
1:O:262:ILE:HD12	1:O:277:LEU:HD23	1.92	0.51
2:P:115:LEU:HD11	2:P:165:LEU:CD2	2.41	0.51
2:F:187:GLN:O	2:F:191:GLY:N	2.42	0.51
2:N:175:ASP:OD2	1:O:323:GLU:HG2	2.10	0.50
1:O:309:LYS:HZ2	2:P:189:ARG:HB3	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:223:ASN:HB2	2:J:135:ARG:NE	2.26	0.50
2:H:137:LEU:HD12	2:H:140:ARG:HH22	1.75	0.50
2:N:125:LYS:CG	2:N:147:ILE:HD13	2.42	0.50
2:P:133:TYR:O	2:P:140:ARG:HD3	2.11	0.50
2:J:113:ARG:NH1	2:J:130:GLU:OE1	2.45	0.50
1:A:305:THR:HB	2:B:186:LEU:HD13	1.92	0.50
2:B:129:ILE:HD11	2:B:147:ILE:CD1	2.41	0.50
2:H:108:VAL:HG13	2:H:170:MET:CE	2.25	0.50
2:L:118:GLN:HG3	2:L:168:CYS:SG	2.52	0.50
1:O:239:VAL:O	1:O:239:VAL:CG1	2.59	0.50
1:M:239:VAL:HG13	1:M:239:VAL:O	2.12	0.49
1:A:326:ASN:HA	1:A:329:ASN:HD22	1.76	0.49
1:C:242:LEU:HD12	1:C:274:LYS:HG3	1.94	0.49
1:C:337:GLU:OE1	2:D:178:GLN:HG2	2.11	0.49
1:K:337:GLU:HG3	2:L:158:VAL:HG23	1.94	0.49
2:N:108:VAL:HG12	2:N:109:GLY:N	2.28	0.49
2:N:187:GLN:O	2:N:191:GLY:N	2.41	0.49
1:A:336:LEU:O	2:B:185:ASP:OD2	2.30	0.49
2:B:132:ARG:HG2	2:B:133:TYR:CE2	2.47	0.49
2:F:108:VAL:HG22	2:F:170:MET:CE	2.42	0.49
2:D:101:PHE:CD1	2:D:145:LEU:HD13	2.46	0.49
2:H:132:ARG:HD3	2:H:133:TYR:CZ	2.48	0.49
1:I:256:GLU:OE2	1:I:256:GLU:HA	2.12	0.49
1:I:335:VAL:HG13	1:K:328:ARG:HG3	1.93	0.49
2:J:125:LYS:HG2	2:J:147:ILE:HD13	1.95	0.49
1:I:328:ARG:HG3	1:K:335:VAL:HG13	1.95	0.49
2:J:137:LEU:CG	2:J:140:ARG:NH2	2.76	0.48
1:A:246:LYS:NZ	5:A:64:HOH:O	2.45	0.48
1:E:305:THR:HB	2:F:186:LEU:HD13	1.96	0.48
1:E:328:ARG:HG3	1:G:335:VAL:HG13	1.95	0.48
1:M:335:VAL:HG13	1:O:328:ARG:HG3	1.96	0.48
1:E:336:LEU:O	2:F:185:ASP:OD2	2.31	0.47
1:C:272:GLU:HA	1:C:275:VAL:HG22	1.94	0.47
2:J:101:PHE:CD1	2:J:145:LEU:HD13	2.50	0.47
2:J:105:CYS:SG	2:J:142:ARG:HB2	2.54	0.47
2:L:158:VAL:O	2:L:162:VAL:HG23	2.14	0.47
1:C:280:ASN:O	1:C:284:LEU:HG	2.14	0.47
2:D:129:ILE:HD11	2:D:147:ILE:HD12	1.97	0.47
1:K:239:VAL:O	1:K:239:VAL:CG1	2.62	0.47
2:L:108:VAL:CG2	2:L:141:VAL:HG21	2.44	0.47
2:H:105:CYS:SG	2:H:142:ARG:HB2	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:272:GLU:HA	1:K:272:GLU:OE1	2.14	0.47
1:C:336:LEU:O	2:D:185:ASP:OD2	2.33	0.47
2:J:104:ILE:HG23	2:J:108:VAL:CG2	2.44	0.47
1:M:223:ASN:HB2	2:N:135:ARG:HE	1.80	0.47
1:A:242:LEU:HD11	1:A:273:GLN:HE21	1.79	0.46
1:I:239:VAL:O	1:I:239:VAL:CG1	2.62	0.46
1:C:242:LEU:HD21	1:C:273:GLN:OE1	2.16	0.46
2:H:109:GLY:HA2	2:H:137:LEU:HD23	1.97	0.46
2:P:157:THR:CG2	2:P:160:HIS:ND1	2.79	0.46
1:E:306:LEU:HD13	1:G:327:PHE:CE2	2.51	0.46
1:M:337:GLU:OE1	2:N:178:GLN:HG2	2.15	0.46
1:E:315:LEU:O	1:E:319:THR:HG22	2.16	0.46
2:B:165:LEU:HD13	2:B:173:VAL:HG12	1.98	0.46
2:D:137:LEU:HD12	2:D:137:LEU:H	1.81	0.46
1:G:250:ARG:HG3	1:G:259:ILE:HD11	1.98	0.45
2:J:104:ILE:HG23	2:J:108:VAL:HG21	1.98	0.45
2:B:189:ARG:HD3	2:B:189:ARG:C	2.41	0.45
2:H:125:LYS:HG2	2:H:147:ILE:HD13	1.98	0.45
2:L:115:LEU:HD11	2:L:165:LEU:CD1	2.46	0.45
2:H:152:GLU:HB3	2:H:155:ASN:HB2	1.99	0.45
1:C:255:ASN:OD1	1:C:258:LYS:HG3	2.16	0.45
1:M:299:LYS:NZ	1:O:322:SER:O	2.47	0.45
1:E:316:LYS:O	1:E:319:THR:HG22	2.17	0.44
1:E:328:ARG:HH21	1:E:332:GLN:HE22	1.65	0.44
2:J:189:ARG:HD3	2:J:189:ARG:C	2.42	0.44
5:I:106:HOH:O	2:N:138:THR:HG23	2.18	0.44
2:P:133:TYR:CG	2:P:139:GLU:HG3	2.53	0.44
1:E:335:VAL:HG13	1:G:328:ARG:HG3	1.98	0.44
1:E:337:GLU:OE1	2:F:178:GLN:HG2	2.18	0.44
2:B:131:ASP:OD2	2:B:132:ARG:N	2.51	0.44
2:J:162:VAL:HG11	2:J:178:GLN:HE21	1.83	0.44
1:O:223:ASN:HB3	5:P:61:HOH:O	2.18	0.44
2:B:137:LEU:O	2:B:141:VAL:HG23	2.17	0.44
2:F:128:SER:O	2:F:131:ASP:OD2	2.36	0.43
2:H:104:ILE:HG23	2:H:108:VAL:CG2	2.48	0.43
1:A:328:ARG:HG3	1:C:335:VAL:CG1	2.42	0.43
1:I:335:VAL:HG13	1:I:335:VAL:O	2.18	0.43
2:L:111:ASP:OD2	2:L:170:MET:HE3	2.18	0.43
1:G:242:LEU:HD21	1:G:273:GLN:NE2	2.34	0.43
1:G:324:ASN:C	1:G:326:ASN:H	2.26	0.43
1:O:309:LYS:HZ2	2:P:189:ARG:CD	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:129:ILE:HD11	2:J:147:ILE:HD12	2.00	0.43
1:M:258:LYS:CD	1:M:280:ASN:HD21	2.32	0.43
1:C:242:LEU:CD1	1:C:274:LYS:HG3	2.49	0.43
1:O:224:LEU:HB2	2:P:136:ASN:HD22	1.84	0.43
2:H:108:VAL:HG22	2:H:170:MET:HE1	2.01	0.42
1:I:258:LYS:HA	1:I:258:LYS:HD3	1.89	0.42
1:A:286:GLY:H	1:I:260:ASP:CG	2.27	0.42
2:J:137:LEU:HG	2:J:140:ARG:HH22	1.81	0.42
1:E:249:VAL:HG12	1:E:281:TRP:HB2	2.02	0.42
2:L:108:VAL:HG21	2:L:141:VAL:CG1	2.48	0.42
1:E:328:ARG:HE	1:E:332:GLN:NE2	2.17	0.42
1:K:328:ARG:NE	1:K:332:GLN:NE2	2.52	0.42
2:D:108:VAL:HG12	2:D:109:GLY:N	2.35	0.42
2:H:129:ILE:HD11	2:H:147:ILE:HD12	2.01	0.42
2:P:133:TYR:HB3	2:P:139:GLU:CG	2.50	0.42
2:J:132:ARG:HG2	2:J:133:TYR:CE2	2.55	0.42
2:J:133:TYR:HE1	2:J:143:GLU:HG3	1.85	0.42
2:F:108:VAL:HG12	2:F:109:GLY:N	2.35	0.41
1:I:324:ASN:C	1:I:326:ASN:H	2.28	0.41
1:K:275:VAL:O	1:K:279:ARG:HG3	2.20	0.41
1:A:289:GLU:O	1:A:293:THR:CG2	2.56	0.41
1:K:249:VAL:HG12	1:K:281:TRP:CB	2.50	0.41
1:K:324:ASN:ND2	3:K:13:SO4:O3	2.45	0.41
2:P:129:ILE:HG22	2:P:140:ARG:HG2	2.01	0.41
2:P:157:THR:HG23	2:P:160:HIS:ND1	2.34	0.41
1:C:239:VAL:HB	2:D:183:ALA:HB1	2.01	0.41
1:E:324:ASN:C	1:E:326:ASN:H	2.27	0.41
1:M:280:ASN:O	1:M:284:LEU:HG	2.21	0.41
2:D:173:VAL:O	2:D:177:VAL:HG23	2.21	0.41
1:G:248:PHE:CE1	1:G:293:THR:CG2	3.00	0.41
1:M:239:VAL:O	1:M:239:VAL:CG1	2.67	0.41
2:N:162:VAL:HG11	2:N:178:GLN:NE2	2.33	0.41
1:O:324:ASN:C	1:O:326:ASN:H	2.29	0.41
2:L:93:GLY:N	5:L:90:HOH:O	2.54	0.40
2:J:162:VAL:HG13	2:J:174:ALA:HB1	2.03	0.40
2:B:137:LEU:HG	2:B:140:ARG:NH2	2.37	0.40
2:B:163:GLY:O	2:B:167:SER:OG	2.38	0.40
1:C:335:VAL:HG13	1:C:335:VAL:O	2.21	0.40
1:E:250:ARG:HD2	1:E:256:GLU:OE2	2.21	0.40
1:K:331:ILE:HD13	1:K:331:ILE:HA	1.93	0.40
2:L:148:TRP:CH2	2:L:161:LEU:HG	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:286:GLY:N	5:M:222:HOH:O	2.29	0.40
2:N:162:VAL:O	2:N:166:ARG:HG3	2.21	0.40
2:B:104:ILE:HG23	2:B:108:VAL:CG2	2.51	0.40
2:L:108:VAL:HG23	2:L:109:GLY:N	2.28	0.40
1:I:316:LYS:O	1:I:319:THR:HG22	2.20	0.40
2:P:137:LEU:O	2:P:141:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	113/115 (98%)	106 (94%)	6 (5%)	1 (1%)	14	26
1	C	113/115 (98%)	106 (94%)	6 (5%)	1 (1%)	14	26
1	E	113/115 (98%)	106 (94%)	7 (6%)	0	100	100
1	G	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
1	I	113/115 (98%)	108 (96%)	4 (4%)	1 (1%)	14	26
1	K	113/115 (98%)	106 (94%)	6 (5%)	1 (1%)	14	26
1	M	113/115 (98%)	106 (94%)	6 (5%)	1 (1%)	14	26
1	O	113/115 (98%)	106 (94%)	7 (6%)	0	100	100
2	B	97/122 (80%)	92 (95%)	5 (5%)	0	100	100
2	D	97/122 (80%)	92 (95%)	5 (5%)	0	100	100
2	F	97/122 (80%)	93 (96%)	3 (3%)	1 (1%)	12	22
2	H	97/122 (80%)	92 (95%)	5 (5%)	0	100	100
2	J	97/122 (80%)	93 (96%)	4 (4%)	0	100	100
2	L	97/122 (80%)	92 (95%)	5 (5%)	0	100	100
2	N	97/122 (80%)	93 (96%)	3 (3%)	1 (1%)	12	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	97/122 (80%)	93 (96%)	3 (3%)	1 (1%)	12	22
All	All	1680/1896 (89%)	1592 (95%)	80 (5%)	8 (0%)	24	40

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	GLU
1	C	256	GLU
1	K	256	GLU
1	M	256	GLU
1	I	256	GLU
2	F	108	VAL
2	N	108	VAL
2	P	108	VAL

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	105/105 (100%)	104 (99%)	1 (1%)	68	80
1	C	105/105 (100%)	99 (94%)	6 (6%)	18	34
1	E	105/105 (100%)	97 (92%)	8 (8%)	12	22
1	G	105/105 (100%)	99 (94%)	6 (6%)	18	34
1	I	105/105 (100%)	96 (91%)	9 (9%)	10	18
1	K	105/105 (100%)	96 (91%)	9 (9%)	10	18
1	M	105/105 (100%)	97 (92%)	8 (8%)	12	22
1	O	105/105 (100%)	95 (90%)	10 (10%)	8	15
2	B	87/107 (81%)	74 (85%)	13 (15%)	3	4
2	D	87/107 (81%)	79 (91%)	8 (9%)	8	16
2	F	87/107 (81%)	81 (93%)	6 (7%)	14	26
2	H	87/107 (81%)	76 (87%)	11 (13%)	4	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	87/107 (81%)	77 (88%)	10 (12%)	5	10
2	L	87/107 (81%)	78 (90%)	9 (10%)	7	13
2	N	87/107 (81%)	80 (92%)	7 (8%)	11	20
2	P	87/107 (81%)	75 (86%)	12 (14%)	3	5
All	All	1536/1696 (91%)	1403 (91%)	133 (9%)	9	17

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	322	SER
2	B	111	ASP
2	B	120	LYS
2	B	131	ASP
2	B	144	SER
2	B	146	ARG
2	B	151	THR
2	B	152	GLU
2	B	154	GLU
2	B	157	THR
2	B	167	SER
2	B	168	CYS
2	B	189	ARG
2	B	190	SER
1	C	270	THR
1	C	319	THR
1	C	322	SER
1	C	333	SER
1	C	335	VAL
1	C	336	LEU
2	D	110	LYS
2	D	111	ASP
2	D	125	LYS
2	D	128	SER
2	D	136	ASN
2	D	149	LYS
2	D	167	SER
2	D	189	ARG
1	E	261	GLU
1	E	268	GLN
1	E	283	GLN
1	E	284	LEU

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Mol	Chain	Res	Type
1	E	322	SER
1	E	326	ASN
1	E	335	VAL
1	E	336	LEU
2	F	136	ASN
2	F	137	LEU
2	F	151	THR
2	F	153	LYS
2	F	157	THR
2	F	167	SER
1	G	225	SER
1	G	239	VAL
1	G	243	SER
1	G	270	THR
1	G	287	LYS
1	G	335	VAL
2	H	110	LYS
2	H	111	ASP
2	H	125	LYS
2	H	136	ASN
2	H	137	LEU
2	H	144	SER
2	H	150	ASN
2	H	151	THR
2	H	154	GLU
2	H	157	THR
2	H	190	SER
1	I	239	VAL
1	I	243	SER
1	I	258	LYS
1	I	267	VAL
1	I	270	THR
1	I	283	GLN
1	I	287	LYS
1	I	319	THR
1	I	335	VAL
2	J	110	LYS
2	J	111	ASP
2	J	117	ARG
2	J	120	LYS
2	J	137	LEU
2	J	143	GLU

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Mol	Chain	Res	Type
2	J	151	THR
2	J	157	THR
2	J	189	ARG
2	J	190	SER
1	K	223	ASN
1	K	239	VAL
1	K	243	SER
1	K	276	GLN
1	K	287	LYS
1	K	319	THR
1	K	320	SER
1	K	333	SER
1	K	335	VAL
2	L	111	ASP
2	L	117	ARG
2	L	125	LYS
2	L	136	ASN
2	L	137	LEU
2	L	157	THR
2	L	165	LEU
2	L	167	SER
2	L	189	ARG
1	M	224	LEU
1	M	239	VAL
1	M	268	GLN
1	M	283	GLN
1	M	293	THR
1	M	319	THR
1	M	333	SER
1	M	335	VAL
2	N	110	LYS
2	N	111	ASP
2	N	115	LEU
2	N	125	LYS
2	N	128	SER
2	N	136	ASN
2	N	152	GLU
1	O	239	VAL
1	O	243	SER
1	O	255	ASN
1	O	270	THR
1	O	280	ASN

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Mol	Chain	Res	Type
1	O	287	LYS
1	O	288	LYS
1	O	321	ASP
1	O	323	GLU
1	O	335	VAL
2	P	105	CYS
2	P	110	LYS
2	P	111	ASP
2	P	115	LEU
2	P	142	ARG
2	P	144	SER
2	P	151	THR
2	P	157	THR
2	P	161	LEU
2	P	167	SER
2	P	168	CYS
2	P	170	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	GLN
1	A	282	HIS
1	A	311	GLN
1	A	324	ASN
1	A	329	ASN
2	B	136	ASN
2	B	178	GLN
1	C	252	ASN
1	C	280	ASN
1	C	311	GLN
1	C	324	ASN
1	C	332	GLN
2	D	160	HIS
2	D	178	GLN
1	E	268	GLN
1	E	311	GLN
1	E	332	GLN
2	F	136	ASN
2	F	187	GLN
1	G	273	GLN
1	G	282	HIS

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Mol	Chain	Res	Type
1	G	311	GLN
1	G	324	ASN
2	H	171	ASN
1	I	311	GLN
1	I	329	ASN
2	J	178	GLN
1	K	252	ASN
1	K	276	GLN
1	K	282	HIS
1	K	332	GLN
2	L	102	ASN
1	M	252	ASN
1	M	266	ASN
1	M	280	ASN
1	M	324	ASN
2	N	178	GLN
1	O	280	ASN
1	O	283	GLN
1	O	311	GLN
1	O	326	ASN
2	P	178	GLN

5.3.3 RNA [i](#)

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 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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	SO4	E	1	-	4,4,4	0.30	0	6,6,6	0.55	0
3	SO4	O	4	-	4,4,4	0.22	0	6,6,6	0.28	0
3	SO4	G	2	-	4,4,4	0.19	0	6,6,6	0.40	0
3	SO4	I	6	-	4,4,4	0.19	0	6,6,6	0.44	0
3	SO4	E	11	-	4,4,4	0.25	0	6,6,6	0.07	0
3	SO4	M	9	-	4,4,4	0.24	0	6,6,6	0.36	0
3	SO4	C	7	-	4,4,4	0.25	0	6,6,6	0.51	0
3	SO4	J	8	-	4,4,4	0.25	0	6,6,6	0.24	0
3	SO4	K	13	-	4,4,4	0.25	0	6,6,6	0.36	0
3	SO4	A	10	-	4,4,4	0.29	0	6,6,6	0.23	0
3	SO4	M	12	-	4,4,4	0.28	0	6,6,6	0.12	0
3	SO4	K	3	-	4,4,4	0.28	0	6,6,6	0.64	0

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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	13	SO4	2	0
3	M	12	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	115/115 (100%)	-0.99	0 100 100	72, 85, 99, 103	0
1	C	115/115 (100%)	-0.85	0 100 100	72, 85, 99, 103	0
1	E	115/115 (100%)	-0.96	0 100 100	72, 85, 99, 103	0
1	G	115/115 (100%)	-0.92	0 100 100	72, 85, 99, 104	0
1	I	115/115 (100%)	-0.92	0 100 100	72, 85, 99, 104	0
1	K	115/115 (100%)	-0.98	0 100 100	72, 85, 99, 103	0
1	M	115/115 (100%)	-0.87	0 100 100	72, 85, 99, 103	0
1	O	115/115 (100%)	-0.93	0 100 100	72, 85, 99, 103	0
2	B	99/122 (81%)	-0.76	2 (2%) 65 62	77, 89, 95, 108	0
2	D	99/122 (81%)	-0.99	0 100 100	76, 88, 95, 108	0
2	F	99/122 (81%)	-0.94	0 100 100	76, 89, 95, 108	0
2	H	99/122 (81%)	-0.97	0 100 100	77, 89, 96, 108	0
2	J	99/122 (81%)	-0.97	0 100 100	77, 89, 96, 108	0
2	L	99/122 (81%)	-0.93	0 100 100	76, 89, 95, 108	0
2	N	99/122 (81%)	-0.91	0 100 100	77, 89, 95, 108	0
2	P	99/122 (81%)	-0.86	0 100 100	77, 89, 95, 108	0
All	All	1712/1896 (90%)	-0.92	2 (0%) 92 93	72, 88, 99, 108	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	190	SER	2.3
2	B	129	ILE	2.2

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
4	NA	H	20	1/1	0.97	0.15	77,77,77,77	0
3	SO4	C	7	5/5	0.98	0.04	120,120,121,124	0
3	SO4	E	11	5/5	0.98	0.04	135,135,135,136	0
3	SO4	J	8	5/5	0.98	0.04	127,127,128,128	0
3	SO4	K	13	5/5	0.98	0.05	109,109,110,110	0
3	SO4	M	9	5/5	0.98	0.05	111,111,114,116	0
3	SO4	A	10	5/5	0.98	0.05	114,114,117,117	0
4	NA	J	19	1/1	0.98	0.12	76,76,76,76	0
4	NA	P	18	1/1	0.98	0.17	88,88,88,88	0
3	SO4	I	6	5/5	0.99	0.05	91,94,96,97	0
3	SO4	M	12	5/5	0.99	0.03	117,117,117,118	0
3	SO4	O	4	5/5	0.99	0.05	116,117,119,120	0
4	NA	A	15	1/1	0.99	0.12	62,62,62,62	0
4	NA	B	21	1/1	0.99	0.17	84,84,84,84	0
4	NA	E	14	1/1	0.99	0.14	63,63,63,63	0
3	SO4	E	1	5/5	0.99	0.05	95,96,99,101	0
3	SO4	K	3	5/5	0.99	0.04	92,95,97,99	0
4	NA	K	16	1/1	0.99	0.14	62,62,62,62	0
4	NA	M	17	1/1	0.99	0.11	64,64,64,64	0
3	SO4	G	2	5/5	0.99	0.05	95,95,97,98	0

6.5 Other polymers [i](#)

There are no such residues in this entry.