



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 02:34 PM UTC

PDB ID : 1FUI / pdb_00001fui
Title : L-FUCOSE ISOMERASE FROM ESCHERICHIA COLI
Authors : Seemann, J.E.; Schulz, G.E.
Deposited on : 1997-04-14
Resolution : 2.50 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

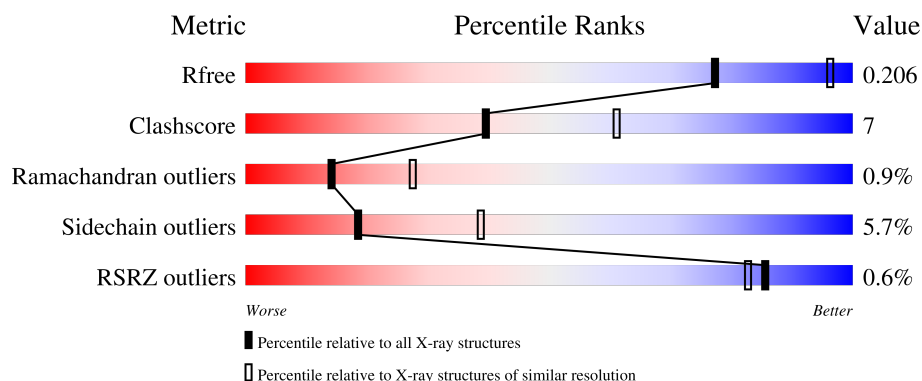
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	591	% 81% 16% .
1	B	591	82% 15% .
1	C	591	% 83% 15% .
1	D	591	% 82% 16% ..
1	E	591	% 82% 16% .

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Mol	Chain	Length	Quality of chain
1	F	591	% 80% 16% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28295 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 L-FUCOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	591	Total	C	N	O	S	50	0	0
			4557	2853	803	866	35			
1	B	591	Total	C	N	O	S	78	0	0
			4557	2853	803	866	35			
1	C	591	Total	C	N	O	S	132	0	0
			4557	2853	803	866	35			
1	D	591	Total	C	N	O	S	198	0	0
			4557	2853	803	866	35			
1	E	591	Total	C	N	O	S	100	0	0
			4557	2853	803	866	35			
1	F	591	Total	C	N	O	S	115	0	0
			4557	2853	803	866	35			

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

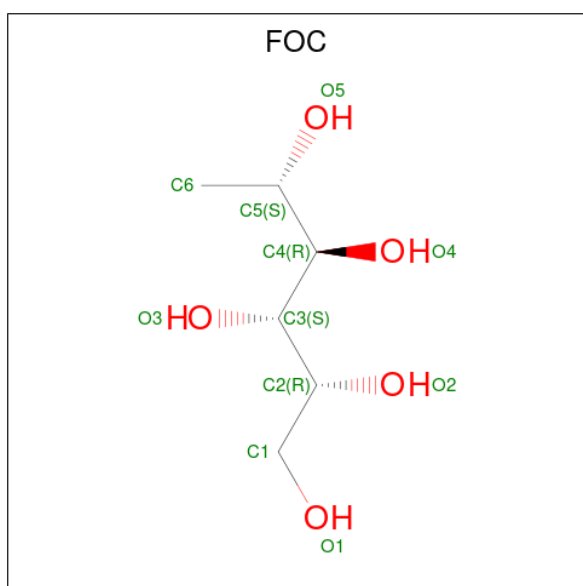
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		
2	E	1	Total	Mn	0	0
			1	1		

- 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	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is FUCITOL (CCD ID: FOC) (formula: C₆H₁₄O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			11	6	5		
4	D	1	Total	C	O	0	0
			11	6	5		
4	E	1	Total	C	O	0	0
			11	6	5		
4	F	1	Total	C	O	0	0
			11	6	5		

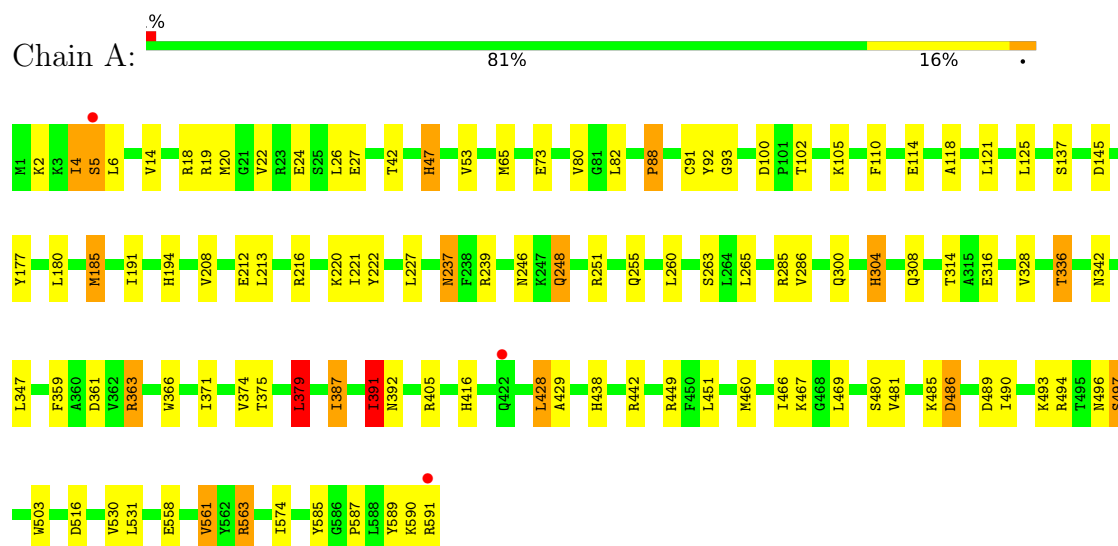
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	163	Total	O	0	0
			163	163		
5	B	126	Total	O	0	0
			126	126		
5	C	158	Total	O	0	0
			158	158		
5	D	142	Total	O	0	0
			142	142		
5	E	152	Total	O	0	0
			152	152		
5	F	131	Total	O	0	0
			131	131		

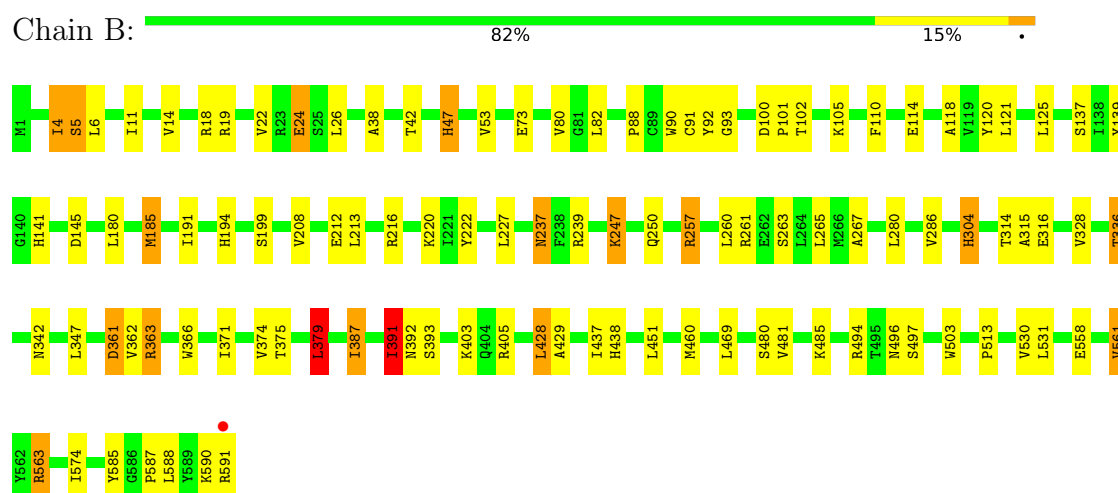
3 Residue-property plots

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.

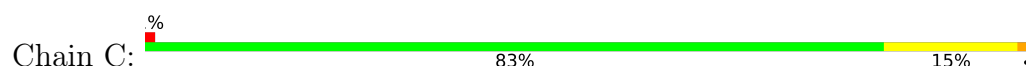
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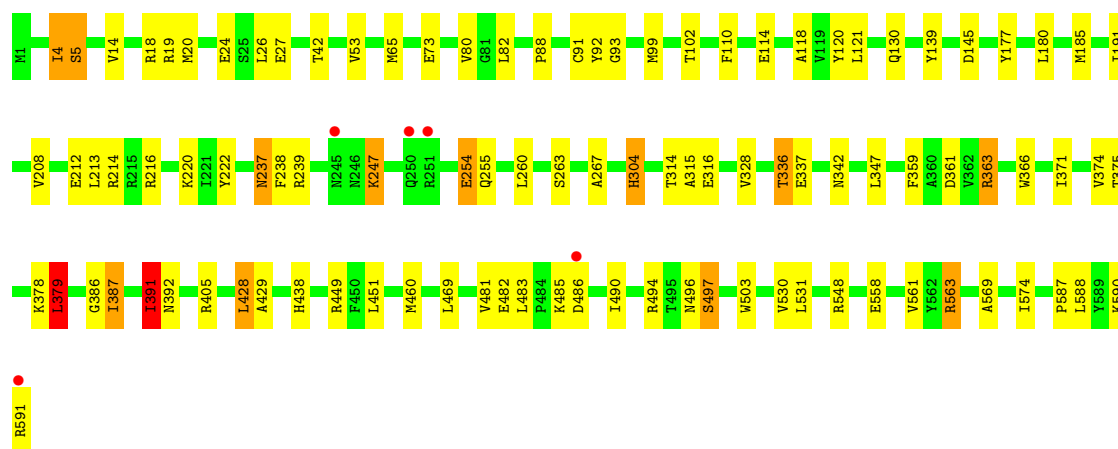


• Molecule 1: L-FUCOSE ISOMERASE

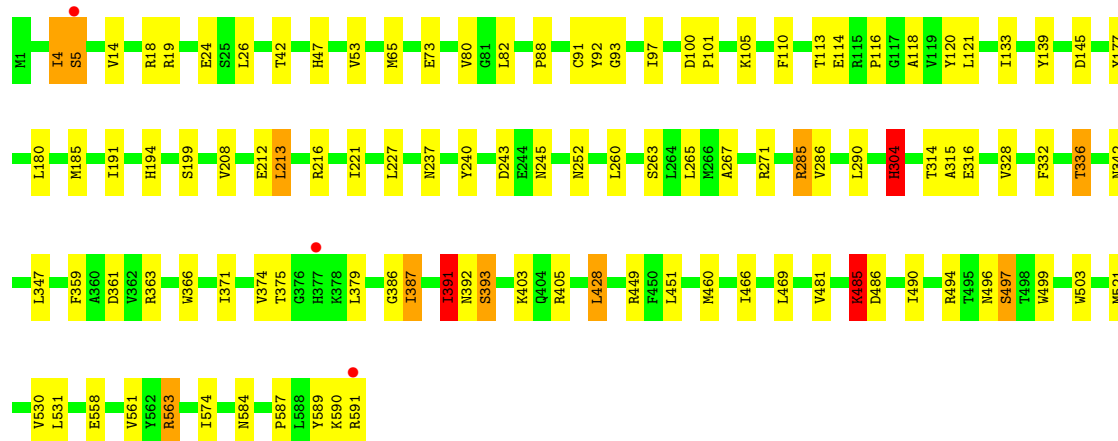
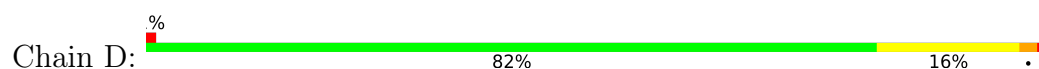


• Molecule 1: L-FUCOSE ISOMERASE

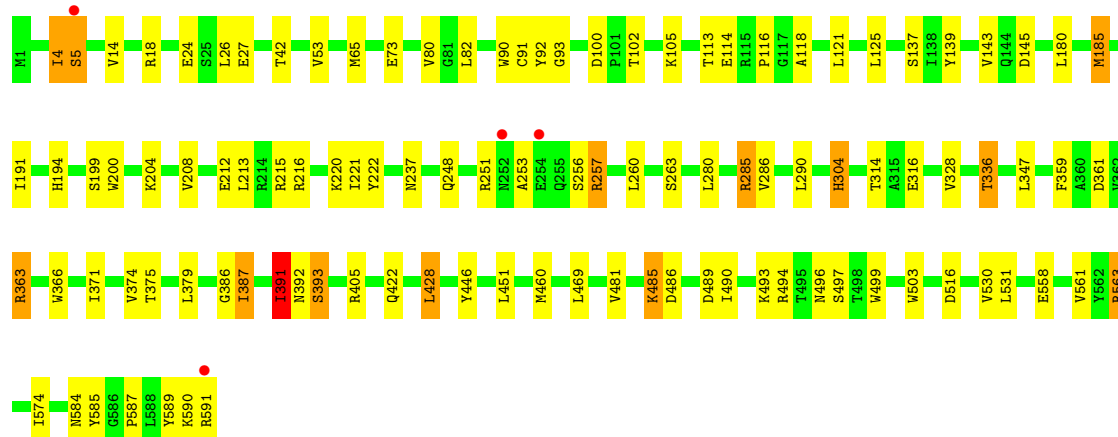
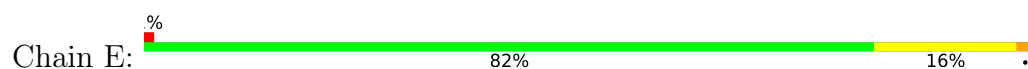




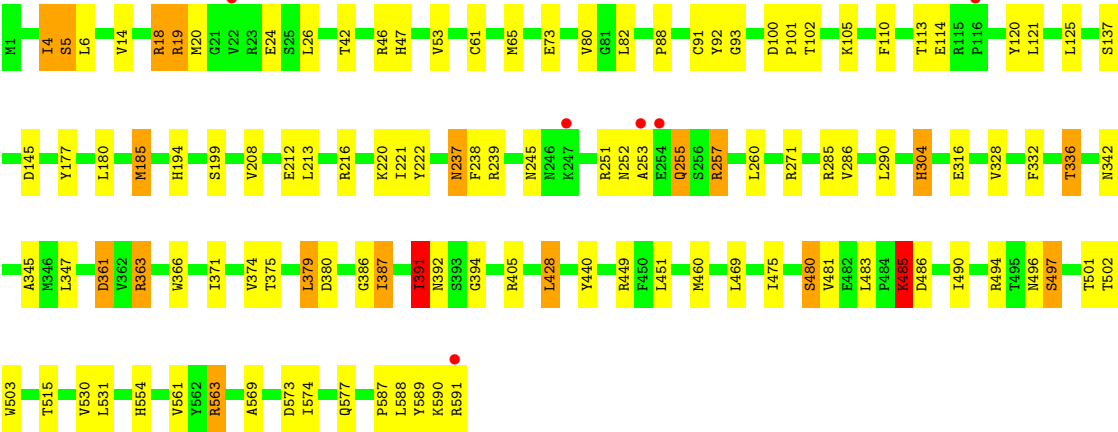
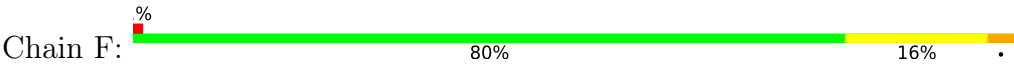
• Molecule 1: L-FUCOSE ISOMERASE



• Molecule 1: L-FUCOSE ISOMERASE



• Molecule 1: L-FUCOSE ISOMERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	127.30Å 128.30Å 239.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	87.0 (20.00-2.50) 86.9 (20.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.162 , 0.209 0.161 , 0.206	Depositor DCC
R_{free} test set	1196 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.2	EDS
L-test for twinning ¹	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	28295	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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: MN, SO4, FOC

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	0.64	1/4657 (0.0%)	1.01	22/6308 (0.3%)
1	B	0.59	1/4657 (0.0%)	0.99	21/6308 (0.3%)
1	C	0.63	0/4657	1.01	24/6308 (0.4%)
1	D	0.61	0/4657	0.99	22/6308 (0.3%)
1	E	0.62	1/4657 (0.0%)	0.99	17/6308 (0.3%)
1	F	0.62	1/4657 (0.0%)	1.01	26/6308 (0.4%)
All	All	0.62	4/27942 (0.0%)	1.00	132/37848 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	MET	SD-CE	-7.33	1.61	1.79
1	B	185	MET	SD-CE	-6.79	1.62	1.79
1	E	185	MET	SD-CE	-6.35	1.63	1.79
1	F	185	MET	SD-CE	-5.24	1.66	1.79

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	363	ARG	N-CA-C	10.42	124.11	111.40
1	A	363	ARG	N-CA-C	10.23	123.88	111.40
1	E	363	ARG	N-CA-C	10.02	123.62	111.40
1	C	363	ARG	N-CA-C	9.86	123.43	111.40
1	B	304	HIS	N-CA-C	9.64	122.79	111.71
1	F	363	ARG	N-CA-C	9.51	123.00	111.40
1	F	255	GLN	N-CA-C	-9.42	100.56	112.90
1	D	363	ARG	N-CA-C	9.41	122.88	111.40
1	E	304	HIS	N-CA-C	8.99	122.21	111.33
1	A	304	HIS	N-CA-C	8.70	120.76	111.28
1	F	304	HIS	N-CA-C	8.61	121.74	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	391	ILE	CB-CA-C	-8.45	100.78	110.41
1	C	304	HIS	N-CA-C	8.40	121.38	111.71
1	D	304	HIS	N-CA-C	8.35	121.31	111.71
1	C	254	GLU	N-CA-C	8.11	122.47	112.58
1	B	286	VAL	N-CA-C	8.04	118.14	110.42
1	D	114	GLU	N-CA-C	-8.02	102.51	111.82
1	E	286	VAL	N-CA-C	7.86	118.65	110.72
1	A	438	HIS	N-CA-C	7.85	120.83	111.33
1	C	191	ILE	N-CA-C	-7.76	97.91	106.21
1	C	114	GLU	N-CA-C	-7.70	103.34	112.89
1	F	114	GLU	N-CA-C	-7.68	102.92	111.82
1	B	379	LEU	N-CA-C	7.41	122.11	110.32
1	D	286	VAL	N-CA-C	7.38	117.50	110.42
1	C	255	GLN	N-CA-C	-7.33	103.60	112.54
1	A	379	LEU	N-CA-C	7.31	120.30	110.35
1	A	391	ILE	CB-CA-C	-7.18	100.36	110.12
1	B	114	GLU	N-CA-C	-7.14	103.83	112.54
1	E	114	GLU	N-CA-C	-7.05	103.64	111.82
1	A	114	GLU	N-CA-C	-6.73	104.33	112.54
1	E	391	ILE	CB-CA-C	-6.68	101.04	110.12
1	C	65	MET	N-CA-C	6.46	118.33	111.28
1	E	65	MET	N-CA-C	6.42	118.28	111.28
1	C	391	ILE	CB-CA-C	-6.40	101.41	110.12
1	B	191	ILE	N-CA-C	-6.38	99.38	106.21
1	D	199	SER	N-CA-C	6.35	118.00	111.14
1	F	386	GLY	N-CA-C	-6.35	105.67	112.08
1	C	19	ARG	N-CA-C	6.32	113.96	108.78
1	B	391	ILE	CB-CA-C	-6.28	101.58	110.12
1	E	497	SER	N-CA-C	6.28	120.04	112.38
1	A	65	MET	N-CA-C	6.20	118.11	111.36
1	C	237	ASN	N-CA-C	6.13	121.64	114.04
1	C	177	TYR	N-CA-C	-6.13	99.21	109.07
1	B	497	SER	N-CA-C	6.07	120.23	112.34
1	B	362	VAL	N-CA-C	-6.06	99.73	106.21
1	A	480	SER	N-CA-C	-6.05	100.71	110.32
1	B	438	HIS	N-CA-C	6.01	121.29	111.37
1	C	378	LYS	N-CA-C	-5.97	98.81	108.41
1	A	191	ILE	N-CA-C	-5.95	97.93	106.55
1	F	238	PHE	N-CA-C	5.91	118.28	109.59
1	D	386	GLY	N-CA-C	-5.91	105.59	111.85
1	A	177	TYR	N-CA-C	-5.88	99.59	109.07
1	D	391	ILE	CB-CA-C	-5.88	101.64	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	237	ASN	N-CA-C	5.88	121.34	114.04
1	A	19	ARG	N-CA-C	5.85	113.58	108.78
1	A	27	GLU	N-CA-C	5.84	118.12	111.11
1	C	438	HIS	N-CA-C	5.74	118.00	111.11
1	E	386	GLY	N-CA-C	-5.71	106.31	112.08
1	C	386	GLY	N-CA-C	-5.67	105.83	111.85
1	C	238	PHE	N-CA-C	5.66	117.91	109.59
1	A	102	THR	N-CA-C	5.66	120.31	113.41
1	E	199	SER	N-CA-C	5.61	118.59	111.69
1	F	588	LEU	N-CA-C	5.61	117.39	111.28
1	F	286	VAL	N-CA-C	5.60	116.37	110.72
1	B	585	TYR	N-CA-C	5.56	118.27	111.82
1	E	590	LYS	N-CA-C	5.56	116.96	108.52
1	B	237	ASN	N-CA-C	5.53	120.68	113.88
1	B	588	LEU	N-CA-C	5.52	117.38	111.36
1	E	585	TYR	N-CA-C	5.51	117.36	111.36
1	A	237	ASN	N-CA-C	5.50	121.01	113.97
1	F	199	SER	N-CA-C	5.50	118.45	111.69
1	A	590	LYS	N-CA-C	5.46	116.82	108.52
1	F	290	LEU	N-CA-C	5.45	117.22	111.28
1	F	497	SER	N-CA-C	5.43	119.00	112.38
1	D	191	ILE	N-CA-C	-5.41	97.61	106.32
1	E	290	LEU	N-CA-C	5.41	117.18	111.28
1	E	248	GLN	N-CA-C	5.39	119.12	112.54
1	A	47	HIS	N-CA-C	-5.38	103.42	110.53
1	E	102	THR	N-CA-C	5.38	119.98	113.41
1	B	247	LYS	N-CA-C	5.38	117.84	111.33
1	A	497	SER	N-CA-C	5.38	119.33	112.34
1	D	101	PRO	N-CA-C	5.38	120.58	113.86
1	A	2	LYS	N-CA-C	-5.38	99.34	110.80
1	A	416	HIS	N-CA-C	5.36	118.62	111.75
1	C	27	GLU	N-CA-C	5.36	117.55	111.11
1	A	589	TYR	N-CA-C	5.36	119.92	112.90
1	F	65	MET	N-CA-C	5.35	117.20	111.36
1	B	342	ASN	N-CA-C	-5.35	105.49	112.23
1	A	585	TYR	N-CA-C	5.35	118.03	111.82
1	E	27	GLU	N-CA-C	5.34	117.52	111.11
1	B	590	LYS	N-CA-C	5.33	116.63	108.52
1	D	133	ILE	CA-C-N	5.33	125.34	119.90
1	D	133	ILE	C-N-CA	5.33	125.34	119.90
1	B	141	HIS	N-CA-C	5.32	116.88	111.14
1	C	102	THR	N-CA-C	5.32	119.90	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	379	LEU	N-CA-C	5.31	118.33	110.48
1	D	47	HIS	N-CA-C	-5.30	103.53	110.53
1	D	97	ILE	N-CA-C	5.29	116.19	110.21
1	D	240	TYR	N-CA-C	5.27	118.20	109.46
1	E	589	TYR	N-CA-C	5.27	119.80	112.90
1	F	61	CYS	N-CA-C	-5.25	103.10	110.50
1	F	480	SER	N-CA-C	-5.22	101.19	109.96
1	B	101	PRO	N-CA-C	5.19	120.35	113.86
1	D	590	LYS	N-CA-C	5.19	116.40	108.52
1	C	588	LEU	N-CA-C	5.18	117.00	111.36
1	F	394	GLY	N-CA-C	5.18	120.64	114.48
1	D	177	TYR	N-CA-C	-5.18	100.08	108.52
1	F	590	LYS	N-CA-C	5.16	116.37	108.52
1	C	590	LYS	N-CA-C	5.15	116.35	108.52
1	F	515	THR	N-CA-C	-5.15	105.35	111.69
1	E	191	ILE	N-CA-C	-5.15	100.70	106.21
1	B	199	SER	N-CA-C	5.14	118.01	111.69
1	C	19	ARG	CB-CA-C	-5.14	109.67	117.07
1	F	361	ASP	N-CA-C	-5.14	100.87	109.24
1	C	19	ARG	CA-C-O	5.13	120.92	117.94
1	D	213	LEU	N-CA-C	-5.12	105.78	111.36
1	D	589	TYR	N-CA-C	5.12	119.65	113.41
1	F	101	PRO	N-CA-C	5.11	120.25	113.86
1	F	177	TYR	N-CA-C	-5.11	100.19	108.52
1	F	102	THR	N-CA-C	5.11	119.51	113.12
1	C	497	SER	N-CA-C	5.09	118.95	112.34
1	B	102	THR	N-CA-C	5.08	119.61	113.41
1	F	589	TYR	N-CA-C	5.08	119.61	113.41
1	F	342	ASN	N-CA-C	-5.07	105.93	111.82
1	A	342	ASN	N-CA-C	-5.06	105.47	111.69
1	D	497	SER	N-CA-C	5.06	118.91	112.34
1	B	47	HIS	N-CA-C	-5.05	103.37	110.50
1	C	342	ASN	N-CA-C	-5.05	105.96	111.82
1	D	290	LEU	N-CA-C	5.05	116.87	111.36
1	D	342	ASN	N-CA-C	-5.04	105.88	112.23
1	F	18	ARG	N-CA-C	5.03	118.15	110.20
1	D	65	MET	N-CA-C	5.03	116.84	111.36

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	4557	0	4434	72	0
1	B	4557	0	4434	66	0
1	C	4557	0	4434	63	0
1	D	4557	0	4434	65	0
1	E	4557	0	4434	67	0
1	F	4557	0	4434	77	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
3	A	5	0	0	0	0
3	D	5	0	0	0	0
4	A	11	0	13	0	0
4	B	11	0	12	0	0
4	C	11	0	12	1	0
4	D	11	0	12	0	0
4	E	11	0	13	0	0
4	F	11	0	13	1	0
5	A	163	0	0	6	0
5	B	126	0	0	4	0
5	C	158	0	0	4	0
5	D	142	0	0	5	0
5	E	152	0	0	3	0
5	F	131	0	0	6	0
All	All	28295	0	26679	351	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 7.

All (351) 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:F:14:VAL:HG12	1:F:91:CYS:SG	2.07	0.94
1:D:14:VAL:HG12	1:D:91:CYS:SG	2.06	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14:VAL:HG12	1:E:91:CYS:SG	2.07	0.94
1:E:221:ILE:HG23	1:E:285:ARG:HG2	1.48	0.92
1:A:14:VAL:HG12	1:A:91:CYS:SG	2.11	0.90
1:B:14:VAL:HG12	1:B:91:CYS:SG	2.12	0.90
1:F:336:THR:HG21	1:F:392:ASN:HD21	1.36	0.89
1:D:336:THR:HG21	1:D:392:ASN:HD21	1.41	0.86
1:B:336:THR:HG21	1:B:392:ASN:HD21	1.40	0.86
1:C:14:VAL:HG12	1:C:91:CYS:SG	2.16	0.85
1:C:336:THR:HG21	1:C:392:ASN:HD21	1.42	0.84
1:A:336:THR:HG21	1:A:392:ASN:HD21	1.42	0.84
1:E:336:THR:HG22	5:E:628:HOH:O	1.81	0.81
1:E:336:THR:HG21	1:E:392:ASN:HD21	1.46	0.80
1:F:257:ARG:HG2	1:F:257:ARG:HH11	1.49	0.77
1:C:336:THR:HG22	5:C:627:HOH:O	1.84	0.77
1:C:374:VAL:HG23	1:C:375:THR:HG23	1.68	0.76
1:F:336:THR:HG22	5:F:633:HOH:O	1.85	0.75
1:D:221:ILE:HG23	1:D:285:ARG:HG2	1.70	0.74
1:A:336:THR:HG22	5:A:620:HOH:O	1.88	0.73
1:B:374:VAL:HG23	1:B:375:THR:HG23	1.71	0.72
1:B:336:THR:HG22	5:B:620:HOH:O	1.90	0.72
1:C:387:ILE:HD11	1:C:481:VAL:CG2	2.20	0.71
1:F:387:ILE:HD11	1:F:503:TRP:HB3	1.72	0.71
1:E:387:ILE:HD11	1:E:481:VAL:CG2	2.21	0.71
1:D:145:ASP:HA	1:E:494:ARG:HH22	1.56	0.70
1:D:336:THR:HG22	5:D:630:HOH:O	1.91	0.70
1:D:374:VAL:HG23	1:D:375:THR:HG23	1.74	0.69
1:F:19:ARG:HG3	1:F:19:ARG:HH11	1.57	0.69
1:B:247:LYS:HA	1:B:250:GLN:HG3	1.74	0.69
1:A:194:HIS:HD2	5:D:670:HOH:O	1.76	0.68
5:A:675:HOH:O	1:D:194:HIS:HD2	1.76	0.68
1:A:374:VAL:HG23	1:A:375:THR:HG23	1.75	0.67
1:B:366:TRP:HB2	1:B:387:ILE:HG22	1.77	0.66
1:A:304:HIS:CD2	1:A:304:HIS:H	2.12	0.65
1:F:374:VAL:HG23	1:F:375:THR:HG23	1.77	0.65
1:D:19:ARG:HD2	5:D:667:HOH:O	1.97	0.64
1:B:387:ILE:HD11	1:B:481:VAL:CG2	2.28	0.64
1:C:5:SER:HB2	1:E:73:GLU:OE2	1.98	0.63
1:C:366:TRP:HB2	1:C:387:ILE:HG22	1.80	0.63
1:D:366:TRP:HB2	1:D:387:ILE:HG22	1.79	0.63
1:E:374:VAL:HG23	1:E:375:THR:HG23	1.81	0.63
1:A:42:THR:HG22	1:A:53:VAL:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:LEU:HD11	1:B:137:SER:HB2	1.79	0.63
1:D:116:PRO:HD2	5:D:724:HOH:O	1.98	0.63
1:F:366:TRP:HB2	1:F:387:ILE:HG22	1.81	0.63
1:A:387:ILE:HD11	1:A:481:VAL:CG2	2.30	0.62
5:B:666:HOH:O	1:F:194:HIS:HD2	1.79	0.62
1:B:304:HIS:HE1	1:D:208:VAL:HA	1.64	0.62
1:F:251:ARG:C	1:F:253:ALA:H	2.07	0.62
1:A:5:SER:HB2	1:D:73:GLU:OE2	1.99	0.61
1:C:361:ASP:HB2	1:C:391:ILE:O	2.00	0.61
1:D:387:ILE:HD11	1:D:481:VAL:CG2	2.30	0.61
1:E:361:ASP:HB2	1:E:391:ILE:O	2.01	0.61
1:B:73:GLU:OE2	1:F:5:SER:HB2	2.00	0.60
1:A:237:ASN:HB3	1:A:428:LEU:HD13	1.84	0.59
1:E:256:SER:HB3	1:E:446:TYR:OH	2.02	0.59
1:F:563:ARG:NH2	1:F:574:ILE:O	2.36	0.59
1:F:387:ILE:HD11	1:F:481:VAL:CG2	2.33	0.59
1:F:486:ASP:O	1:F:490:ILE:HG12	2.03	0.59
1:C:563:ARG:NH2	1:C:574:ILE:O	2.35	0.59
5:C:665:HOH:O	1:E:194:HIS:HD2	1.84	0.59
1:D:42:THR:HG22	1:D:53:VAL:O	2.03	0.59
1:A:239:ARG:HH21	1:A:429:ALA:HA	1.66	0.58
5:C:669:HOH:O	1:F:591:ARG:HB3	2.03	0.58
1:F:42:THR:HG22	1:F:53:VAL:O	2.04	0.58
1:F:253:ALA:HB3	1:F:255:GLN:OE1	2.03	0.58
1:B:194:HIS:HD2	5:F:685:HOH:O	1.86	0.58
1:D:237:ASN:HB3	1:D:428:LEU:HD13	1.85	0.58
1:E:145:ASP:HA	1:F:494:ARG:HH22	1.69	0.58
1:E:366:TRP:HB2	1:E:387:ILE:HG22	1.85	0.57
1:B:366:TRP:HB3	1:B:371:ILE:HD11	1.86	0.57
1:E:516:ASP:HB2	5:E:674:HOH:O	2.05	0.57
1:E:387:ILE:HD11	1:E:481:VAL:HG21	1.85	0.57
1:A:366:TRP:HB2	1:A:387:ILE:HG22	1.87	0.57
1:C:587:PRO:HG2	1:C:591:ARG:OXT	2.04	0.57
1:E:257:ARG:HH11	1:E:257:ARG:HG2	1.70	0.57
1:F:221:ILE:HG23	1:F:285:ARG:HG3	1.86	0.57
1:A:73:GLU:OE2	1:D:5:SER:HB2	2.05	0.56
1:F:387:ILE:CD1	1:F:503:TRP:HB3	2.34	0.56
1:B:18:ARG:HH22	1:C:185:MET:HE1	1.70	0.56
1:B:361:ASP:HB2	1:B:391:ILE:O	2.05	0.56
1:B:42:THR:HG22	1:B:53:VAL:O	2.05	0.56
1:D:316:GLU:OE1	1:D:336:THR:HB	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:ARG:NH2	1:B:574:ILE:O	2.39	0.56
1:A:486:ASP:O	1:A:490:ILE:HG12	2.06	0.55
1:A:125:LEU:HD11	1:A:137:SER:HB2	1.87	0.55
1:F:251:ARG:O	1:F:253:ALA:N	2.39	0.55
1:B:5:SER:HB2	1:F:73:GLU:OE2	2.06	0.55
1:F:485:LYS:HD2	1:F:486:ASP:H	1.71	0.55
1:B:591:ARG:HB3	5:D:720:HOH:O	2.04	0.55
1:C:387:ILE:HD11	1:C:481:VAL:HG21	1.87	0.55
1:D:212:GLU:O	1:D:216:ARG:HG2	2.06	0.55
1:C:73:GLU:OE2	1:E:5:SER:HB2	2.06	0.55
1:C:208:VAL:HA	1:F:304:HIS:CE1	2.42	0.55
1:A:18:ARG:HH22	1:B:185:MET:CE	2.20	0.55
1:A:304:HIS:CE1	1:E:208:VAL:HG13	2.41	0.55
1:F:125:LEU:HD11	1:F:137:SER:HB2	1.88	0.55
1:F:316:GLU:OE1	1:F:336:THR:HB	2.07	0.55
1:B:208:VAL:HA	1:D:304:HIS:CE1	2.42	0.55
1:E:42:THR:HG22	1:E:53:VAL:O	2.06	0.54
1:B:208:VAL:HA	1:D:304:HIS:HE1	1.71	0.54
1:A:361:ASP:HB2	1:A:391:ILE:O	2.07	0.54
1:C:379:LEU:HD21	1:C:483:LEU:HD22	1.89	0.54
1:D:18:ARG:HH22	1:E:185:MET:HE1	1.72	0.54
1:D:486:ASP:O	1:D:490:ILE:HG12	2.07	0.54
1:E:489:ASP:O	1:E:493:LYS:HG2	2.08	0.54
1:F:379:LEU:HD21	1:F:483:LEU:HD22	1.90	0.54
1:F:220:LYS:HA	1:F:222:TYR:CE2	2.43	0.54
1:B:239:ARG:HH21	1:B:429:ALA:HA	1.73	0.54
1:B:304:HIS:N	1:B:304:HIS:CD2	2.75	0.54
1:E:558:GLU:HG3	1:E:574:ILE:HG13	1.91	0.53
1:F:257:ARG:HH11	1:F:257:ARG:CG	2.18	0.53
1:E:237:ASN:HB3	1:E:428:LEU:HD13	1.90	0.53
1:E:422:GLN:HG3	5:E:732:HOH:O	2.08	0.53
1:E:316:GLU:OE1	1:E:336:THR:HB	2.08	0.53
1:E:563:ARG:NH2	1:E:574:ILE:O	2.42	0.53
1:B:145:ASP:HA	1:C:494:ARG:HH22	1.74	0.53
1:B:304:HIS:CE1	1:D:208:VAL:HA	2.44	0.52
1:D:563:ARG:NH2	1:D:574:ILE:O	2.43	0.52
1:C:237:ASN:HB3	1:C:428:LEU:HD13	1.91	0.52
1:F:212:GLU:O	1:F:216:ARG:HG2	2.09	0.52
1:B:212:GLU:OE2	1:B:216:ARG:HD3	2.10	0.52
1:F:587:PRO:HG2	1:F:591:ARG:O	2.09	0.52
1:D:304:HIS:N	1:D:304:HIS:CD2	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:ARG:NH2	1:A:574:ILE:O	2.43	0.52
1:B:387:ILE:HD11	1:B:503:TRP:HB3	1.91	0.52
1:A:185:MET:HE1	1:C:18:ARG:HH22	1.74	0.52
1:A:387:ILE:HD11	1:A:503:TRP:HB3	1.92	0.52
1:C:239:ARG:HH21	1:C:429:ALA:HA	1.74	0.52
1:B:212:GLU:O	1:B:216:ARG:HG2	2.09	0.52
1:C:208:VAL:HA	1:F:304:HIS:HE1	1.75	0.52
1:F:46:ARG:HD3	5:F:717:HOH:O	2.09	0.51
1:D:366:TRP:HB3	1:D:371:ILE:HD11	1.91	0.51
1:D:387:ILE:HD11	1:D:503:TRP:HB3	1.92	0.51
1:B:558:GLU:HG3	1:B:574:ILE:HG13	1.92	0.51
1:C:212:GLU:O	1:C:216:ARG:HG2	2.10	0.51
1:F:251:ARG:C	1:F:253:ALA:N	2.67	0.51
1:F:253:ALA:O	1:F:255:GLN:HG3	2.11	0.51
1:C:486:ASP:O	1:C:490:ILE:HG12	2.11	0.51
1:A:316:GLU:OE1	1:A:336:THR:HB	2.11	0.51
1:E:363:ARG:HD2	1:E:391:ILE:HD11	1.91	0.51
1:A:18:ARG:HH22	1:B:185:MET:HE1	1.75	0.51
1:B:237:ASN:HB3	1:B:428:LEU:HD13	1.93	0.51
1:C:316:GLU:OE1	1:C:336:THR:HB	2.10	0.51
1:E:92:TYR:CE1	1:F:185:MET:HE2	2.46	0.51
1:A:359:PHE:O	1:A:392:ASN:HB2	2.11	0.51
1:A:558:GLU:HG3	1:A:574:ILE:HG13	1.93	0.51
1:D:92:TYR:CE1	1:E:185:MET:HE2	2.46	0.51
1:D:361:ASP:HB2	1:D:391:ILE:O	2.11	0.51
1:A:363:ARG:HD2	1:A:391:ILE:HD11	1.92	0.50
1:C:482:GLU:HA	5:C:743:HOH:O	2.11	0.50
1:F:363:ARG:HD2	1:F:391:ILE:HD11	1.93	0.50
1:A:442:ARG:HD3	1:C:20:MET:HE1	1.92	0.50
1:E:212:GLU:OE2	1:E:216:ARG:HD3	2.09	0.50
1:A:220:LYS:HA	1:A:222:TYR:CE2	2.47	0.50
1:B:257:ARG:HG2	1:B:257:ARG:HH11	1.76	0.50
1:C:387:ILE:HD11	1:C:503:TRP:HB3	1.93	0.49
1:E:113:THR:OG1	1:F:494:ARG:NH1	2.45	0.49
1:A:185:MET:CE	1:C:18:ARG:HH22	2.25	0.49
1:A:227:LEU:HD22	1:A:265:LEU:HD21	1.94	0.49
1:D:14:VAL:CG1	1:D:91:CYS:SG	2.89	0.49
1:D:460:MET:HA	1:D:530:VAL:O	2.12	0.49
1:E:387:ILE:HD11	1:E:503:TRP:HB3	1.93	0.49
1:B:363:ARG:HD2	1:B:391:ILE:HD11	1.94	0.49
1:E:587:PRO:HG2	1:E:591:ARG:O	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:PRO:HG2	1:A:591:ARG:OXT	2.13	0.49
1:D:185:MET:HE2	1:F:92:TYR:CE1	2.47	0.49
1:B:18:ARG:HH22	1:C:185:MET:CE	2.25	0.49
1:F:237:ASN:HB3	1:F:428:LEU:HD13	1.95	0.49
1:B:387:ILE:HD11	1:B:481:VAL:HG21	1.95	0.49
1:B:513:PRO:HG3	5:B:684:HOH:O	2.12	0.49
1:E:212:GLU:O	1:E:216:ARG:HG2	2.12	0.48
1:B:558:GLU:O	1:B:561:VAL:HG13	2.13	0.48
1:D:494:ARG:HH22	1:F:145:ASP:HA	1.78	0.48
1:A:212:GLU:O	1:A:216:ARG:HG2	2.14	0.48
1:C:359:PHE:O	1:C:392:ASN:HB2	2.14	0.48
1:E:359:PHE:O	1:E:392:ASN:HB2	2.13	0.48
1:E:387:ILE:HD11	1:E:481:VAL:HG22	1.95	0.48
1:A:460:MET:HA	1:A:530:VAL:O	2.14	0.48
1:B:460:MET:HA	1:B:530:VAL:O	2.14	0.48
1:A:286:VAL:HG22	5:A:738:HOH:O	2.13	0.48
1:A:118:ALA:HB1	5:A:725:HOH:O	2.13	0.47
1:A:246:ASN:HB3	1:A:248:GLN:OE1	2.15	0.47
1:A:371:ILE:HG21	1:A:379:LEU:HD22	1.96	0.47
1:A:558:GLU:O	1:A:561:VAL:HG13	2.15	0.47
1:D:145:ASP:HA	1:E:494:ARG:NH2	2.27	0.47
1:E:220:LYS:N	1:E:220:LYS:HD2	2.29	0.47
1:F:336:THR:HG21	1:F:392:ASN:ND2	2.17	0.47
1:E:460:MET:HA	1:E:530:VAL:O	2.14	0.47
1:E:366:TRP:HB3	1:E:371:ILE:HD11	1.97	0.47
1:A:466:ILE:HG13	1:C:569:ALA:HB1	1.97	0.47
1:C:304:HIS:CE1	1:F:208:VAL:HA	2.49	0.47
1:D:18:ARG:HH22	1:E:185:MET:CE	2.28	0.47
1:F:449:ARG:HD3	1:F:497:SER:O	2.15	0.47
1:A:92:TYR:CE1	1:B:185:MET:HE2	2.50	0.47
1:C:387:ILE:HD11	1:C:481:VAL:HG22	1.95	0.47
1:B:92:TYR:CE1	1:C:185:MET:HE2	2.50	0.46
1:F:361:ASP:HB2	1:F:391:ILE:O	2.15	0.46
1:A:387:ILE:HD11	1:A:481:VAL:HG22	1.96	0.46
1:F:251:ARG:HB2	1:F:255:GLN:OE1	2.15	0.46
1:F:387:ILE:HD11	1:F:481:VAL:HG22	1.97	0.46
1:A:221:ILE:HG23	1:A:285:ARG:HG3	1.97	0.46
1:B:437:ILE:HD11	5:B:680:HOH:O	2.15	0.46
1:C:220:LYS:HA	1:C:222:TYR:CE2	2.50	0.46
1:B:90:TRP:HE1	1:C:185:MET:HE2	1.81	0.46
1:B:263:SER:HB3	1:B:314:THR:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:HIS:HE1	1:F:208:VAL:HA	1.81	0.46
1:F:91:CYS:HB2	1:F:120:TYR:CD1	2.51	0.46
1:E:92:TYR:CD1	1:E:92:TYR:N	2.83	0.46
1:B:19:ARG:HA	1:B:24:GLU:OE2	2.15	0.46
1:C:92:TYR:N	1:C:92:TYR:CD1	2.82	0.46
1:D:185:MET:HE1	1:F:18:ARG:HH22	1.80	0.46
1:F:460:MET:HA	1:F:530:VAL:O	2.15	0.46
1:A:449:ARG:HD3	1:A:497:SER:O	2.16	0.46
1:D:263:SER:HB3	1:D:314:THR:HB	1.97	0.46
1:F:100:ASP:O	1:F:105:LYS:CE	2.64	0.46
1:A:366:TRP:HB3	1:A:371:ILE:HD11	1.96	0.46
1:C:363:ARG:HD2	1:C:391:ILE:HD11	1.96	0.46
1:C:558:GLU:HG3	1:C:574:ILE:HG13	1.97	0.46
1:E:143:VAL:HG23	5:F:622:HOH:O	2.16	0.46
1:D:91:CYS:HB2	1:D:120:TYR:CD1	2.51	0.46
1:B:91:CYS:HB2	1:B:120:TYR:CD1	2.52	0.45
1:F:6:LEU:HD13	1:F:47:HIS:CD2	2.52	0.45
1:A:92:TYR:N	1:A:92:TYR:CD1	2.82	0.45
1:E:486:ASP:O	1:E:490:ILE:HG12	2.17	0.45
1:C:99:MET:HG3	1:E:204:LYS:HE2	1.98	0.45
1:D:88:PRO:HA	1:D:110:PHE:HB3	1.98	0.45
1:D:387:ILE:HD11	1:D:481:VAL:HG21	1.98	0.45
1:A:125:LEU:CD1	1:A:137:SER:HB2	2.46	0.45
1:E:257:ARG:HH11	1:E:257:ARG:CG	2.29	0.45
1:F:363:ARG:HD2	1:F:391:ILE:CD1	2.47	0.45
1:C:591:ARG:NH1	1:E:584:ASN:OD1	2.50	0.45
1:D:359:PHE:O	1:D:392:ASN:HB2	2.17	0.45
1:E:363:ARG:HD2	1:E:391:ILE:CD1	2.47	0.45
1:A:387:ILE:HD11	1:A:481:VAL:HG21	1.99	0.45
1:D:212:GLU:OE2	1:D:216:ARG:HD3	2.17	0.45
1:D:91:CYS:HB2	1:D:120:TYR:CE1	2.52	0.44
1:D:387:ILE:HD11	1:D:481:VAL:HG22	1.99	0.44
1:D:587:PRO:HG2	1:D:591:ARG:O	2.16	0.44
1:A:216:ARG:NH1	5:A:748:HOH:O	2.51	0.44
1:B:227:LEU:HD22	1:B:265:LEU:HD21	1.99	0.44
1:C:214:ARG:HG2	5:F:723:HOH:O	2.17	0.44
1:F:88:PRO:HA	1:F:110:PHE:HB3	2.00	0.44
1:F:475:ILE:O	1:F:554:HIS:HA	2.18	0.44
1:A:265:LEU:HD23	1:A:265:LEU:HA	1.87	0.44
1:D:271:ARG:HG3	1:D:332:PHE:CZ	2.52	0.44
1:C:263:SER:HB3	1:C:314:THR:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:TYR:N	1:B:92:TYR:CD1	2.84	0.44
1:D:466:ILE:HG13	1:F:569:ALA:HB1	2.00	0.44
1:C:254:GLU:OE2	1:C:254:GLU:HA	2.13	0.44
1:C:267:ALA:HB2	1:C:315:ALA:HA	1.98	0.44
1:A:20:MET:HB2	1:A:20:MET:HE3	1.67	0.44
1:A:208:VAL:HA	1:E:304:HIS:CE1	2.53	0.44
1:A:18:ARG:NH2	1:B:185:MET:CE	2.81	0.44
1:A:467:LYS:HB2	1:C:130:GLN:O	2.18	0.44
1:C:91:CYS:HB2	1:C:120:TYR:CE1	2.53	0.44
1:A:591:ARG:NH1	1:D:584:ASN:OD1	2.50	0.43
1:A:489:ASP:O	1:A:493:LYS:HG2	2.17	0.43
1:A:494:ARG:HH22	1:C:145:ASP:HA	1.83	0.43
1:F:92:TYR:N	1:F:92:TYR:CD1	2.84	0.43
1:F:345:ALA:HB3	1:F:530:VAL:HG21	1.99	0.43
1:B:387:ILE:HD11	1:B:481:VAL:HG22	2.01	0.43
1:A:285:ARG:HG2	1:A:285:ARG:HH11	1.83	0.43
1:C:42:THR:HG22	1:C:53:VAL:O	2.17	0.43
1:D:118:ALA:HB2	1:D:139:TYR:CE1	2.53	0.43
1:A:145:ASP:HA	1:B:494:ARG:HH22	1.83	0.43
1:C:337:GLU:OE2	4:C:593:FOC:H2	2.19	0.43
1:C:449:ARG:HD3	1:C:497:SER:O	2.18	0.43
1:B:403:LYS:HA	1:B:403:LYS:HD3	1.86	0.43
1:D:494:ARG:NH1	1:F:113:THR:OG1	2.52	0.43
1:C:304:HIS:CD2	1:C:304:HIS:N	2.85	0.43
1:D:100:ASP:O	1:D:105:LYS:CE	2.67	0.43
1:C:212:GLU:OE2	1:C:216:ARG:HD3	2.19	0.43
1:D:449:ARG:HD3	1:D:497:SER:O	2.18	0.43
1:E:90:TRP:HE1	1:F:185:MET:HE2	1.84	0.43
1:F:573:ASP:O	1:F:577:GLN:HG2	2.19	0.43
1:A:100:ASP:O	1:A:105:LYS:HE3	2.18	0.42
1:A:304:HIS:CD2	1:A:304:HIS:N	2.85	0.42
1:B:587:PRO:CG	1:B:591:ARG:OXT	2.67	0.42
1:D:267:ALA:HB2	1:D:315:ALA:HA	1.99	0.42
1:B:11:ILE:HD12	1:B:38:ALA:HB2	2.01	0.42
1:B:480:SER:HA	1:B:503:TRP:O	2.20	0.42
1:C:587:PRO:CG	1:C:591:ARG:OXT	2.67	0.42
1:D:92:TYR:CD1	1:D:92:TYR:N	2.82	0.42
1:D:145:ASP:OD1	1:E:494:ARG:NH2	2.52	0.42
1:A:6:LEU:HD13	1:A:47:HIS:CD2	2.54	0.42
1:B:91:CYS:HB2	1:B:120:TYR:CE1	2.54	0.42
1:D:393:SER:HA	1:D:499:TRP:CE3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:TYR:HE1	1:E:185:MET:HE2	1.85	0.42
1:E:145:ASP:OD1	1:F:494:ARG:NH2	2.52	0.42
1:A:145:ASP:OD1	1:B:494:ARG:NH2	2.53	0.42
1:D:113:THR:O	1:E:363:ARG:NH1	2.53	0.42
1:D:485:LYS:HD2	1:D:486:ASP:H	1.85	0.42
1:B:100:ASP:O	1:B:105:LYS:CE	2.68	0.42
1:B:220:LYS:HA	1:B:222:TYR:CE2	2.54	0.42
1:E:118:ALA:HB2	1:E:139:TYR:CE1	2.55	0.42
1:E:125:LEU:HD11	1:E:137:SER:HB2	2.01	0.42
1:E:387:ILE:CD1	1:E:503:TRP:HB3	2.50	0.42
1:F:19:ARG:HH11	1:F:19:ARG:CG	2.30	0.42
1:A:308:GLN:NE2	1:E:215:ARG:HB2	2.35	0.42
1:C:91:CYS:HB2	1:C:120:TYR:CD1	2.55	0.42
1:F:14:VAL:CG1	1:F:91:CYS:SG	2.95	0.42
1:C:366:TRP:HB3	1:C:371:ILE:HD11	2.02	0.42
1:F:91:CYS:HB2	1:F:120:TYR:CE1	2.55	0.42
1:D:403:LYS:HD3	1:D:403:LYS:HA	1.88	0.41
1:A:100:ASP:O	1:A:105:LYS:CE	2.68	0.41
1:B:118:ALA:HB2	1:B:139:TYR:CE1	2.55	0.41
1:A:251:ARG:HB3	1:A:255:GLN:HB2	2.03	0.41
1:B:222:TYR:HA	1:B:280:LEU:HD21	2.02	0.41
1:D:494:ARG:NH2	1:F:145:ASP:OD1	2.53	0.41
1:F:125:LEU:CD1	1:F:137:SER:HB2	2.51	0.41
1:B:88:PRO:HA	1:B:110:PHE:HB3	2.02	0.41
1:F:257:ARG:CG	1:F:257:ARG:NH1	2.81	0.41
1:A:88:PRO:HA	1:A:110:PHE:HB3	2.03	0.41
1:B:267:ALA:HB2	1:B:315:ALA:HA	2.02	0.41
1:F:304:HIS:CD2	1:F:304:HIS:N	2.88	0.41
1:A:185:MET:HE2	1:C:92:TYR:CE1	2.55	0.41
1:A:516:ASP:HB2	5:A:750:HOH:O	2.20	0.41
1:B:371:ILE:HG21	1:B:379:LEU:HD22	2.02	0.41
1:C:88:PRO:HA	1:C:110:PHE:HB3	2.03	0.41
1:B:261:ARG:NH1	1:B:261:ARG:HG2	2.36	0.41
1:F:271:ARG:HG3	1:F:332:PHE:CZ	2.55	0.41
1:E:222:TYR:HA	1:E:280:LEU:HD21	2.02	0.41
1:A:300:GLN:HE22	1:A:304:HIS:CD2	2.38	0.41
1:B:6:LEU:HD13	1:B:47:HIS:CD2	2.56	0.41
1:C:387:ILE:CD1	1:C:503:TRP:HB3	2.50	0.41
1:D:227:LEU:HD22	1:D:265:LEU:HD21	2.01	0.41
1:E:100:ASP:O	1:E:105:LYS:CE	2.69	0.41
1:E:200:TRP:CE2	1:E:587:PRO:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:393:SER:HA	1:E:499:TRP:CE3	2.56	0.41
1:F:366:TRP:HB3	1:F:371:ILE:HD11	2.02	0.41
1:B:316:GLU:OE1	1:B:336:THR:HB	2.21	0.41
1:E:116:PRO:HG3	5:F:661:HOH:O	2.21	0.41
1:F:440:TYR:CD1	4:F:592:FOC:H61	2.55	0.41
1:C:363:ARG:HD2	1:C:391:ILE:CD1	2.51	0.40
1:D:387:ILE:CD1	1:D:503:TRP:HB3	2.50	0.40
1:A:263:SER:HB3	1:A:314:THR:HB	2.04	0.40
1:C:118:ALA:HB2	1:C:139:TYR:CE1	2.56	0.40
1:C:460:MET:HA	1:C:530:VAL:O	2.21	0.40
1:D:304:HIS:CD2	1:D:304:HIS:H	2.39	0.40
1:D:558:GLU:HG3	1:D:574:ILE:HG13	2.04	0.40
1:E:363:ARG:O	1:E:363:ARG:HG2	2.22	0.40
1:F:501:THR:CG2	1:F:502:THR:N	2.83	0.40
1:A:363:ARG:HD2	1:A:391:ILE:CD1	2.50	0.40
1:A:387:ILE:CD1	1:A:503:TRP:HB3	2.50	0.40
1:E:18:ARG:HH22	1:F:185:MET:CE	2.34	0.40
1:E:90:TRP:HE1	1:F:185:MET:CE	2.35	0.40
1:E:263:SER:HB3	1:E:314:THR:HB	2.03	0.40
1:C:548:ARG:HD2	1:C:548:ARG:N	2.37	0.40
1:F:480:SER:HA	1:F:503:TRP:O	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	589/591 (100%)	567 (96%)	17 (3%)	5 (1%)	16	31
1	B	589/591 (100%)	562 (95%)	22 (4%)	5 (1%)	16	31
1	C	589/591 (100%)	561 (95%)	24 (4%)	4 (1%)	18	34
1	D	589/591 (100%)	557 (95%)	24 (4%)	8 (1%)	9	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	589/591 (100%)	561 (95%)	22 (4%)	6 (1%)	12	24
1	F	589/591 (100%)	556 (94%)	28 (5%)	5 (1%)	16	31
All	All	3534/3546 (100%)	3364 (95%)	137 (4%)	33 (1%)	14	27

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	GLY
1	B	93	GLY
1	C	5	SER
1	D	93	GLY
1	E	93	GLY
1	E	253	ALA
1	F	93	GLY
1	A	4	ILE
1	A	5	SER
1	B	4	ILE
1	B	5	SER
1	C	93	GLY
1	D	4	ILE
1	D	5	SER
1	D	245	ASN
1	E	4	ILE
1	E	5	SER
1	F	4	ILE
1	F	5	SER
1	B	22	VAL
1	D	252	ASN
1	E	393	SER
1	F	252	ASN
1	B	393	SER
1	C	247	LYS
1	C	4	ILE
1	D	243	ASP
1	D	393	SER
1	D	485	LYS
1	E	485	LYS
1	F	485	LYS
1	A	22	VAL
1	A	88	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	474/474 (100%)	448 (94%)	26 (6%)	19	40
1	B	474/474 (100%)	448 (94%)	26 (6%)	19	40
1	C	474/474 (100%)	449 (95%)	25 (5%)	20	42
1	D	474/474 (100%)	447 (94%)	27 (6%)	18	39
1	E	474/474 (100%)	447 (94%)	27 (6%)	18	39
1	F	474/474 (100%)	444 (94%)	30 (6%)	16	34
All	All	2844/2844 (100%)	2683 (94%)	161 (6%)	18	39

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	24	GLU
1	A	26	LEU
1	A	80	VAL
1	A	82	LEU
1	A	121	LEU
1	A	180	LEU
1	A	213	LEU
1	A	248	GLN
1	A	260	LEU
1	A	328	VAL
1	A	336	THR
1	A	347	LEU
1	A	379	LEU
1	A	387	ILE
1	A	391	ILE
1	A	405	ARG
1	A	428	LEU
1	A	451	LEU
1	A	469	LEU
1	A	485	LYS
1	A	486	ASP

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Mol	Chain	Res	Type
1	A	496	ASN
1	A	531	LEU
1	A	561	VAL
1	A	563	ARG
1	B	4	ILE
1	B	24	GLU
1	B	26	LEU
1	B	80	VAL
1	B	82	LEU
1	B	121	LEU
1	B	180	LEU
1	B	213	LEU
1	B	257	ARG
1	B	260	LEU
1	B	328	VAL
1	B	336	THR
1	B	347	LEU
1	B	361	ASP
1	B	379	LEU
1	B	387	ILE
1	B	391	ILE
1	B	405	ARG
1	B	428	LEU
1	B	451	LEU
1	B	469	LEU
1	B	485	LYS
1	B	496	ASN
1	B	531	LEU
1	B	561	VAL
1	B	563	ARG
1	C	4	ILE
1	C	24	GLU
1	C	26	LEU
1	C	80	VAL
1	C	82	LEU
1	C	121	LEU
1	C	180	LEU
1	C	213	LEU
1	C	247	LYS
1	C	260	LEU
1	C	328	VAL
1	C	336	THR

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Mol	Chain	Res	Type
1	C	347	LEU
1	C	379	LEU
1	C	387	ILE
1	C	391	ILE
1	C	405	ARG
1	C	428	LEU
1	C	451	LEU
1	C	469	LEU
1	C	485	LYS
1	C	496	ASN
1	C	531	LEU
1	C	561	VAL
1	C	563	ARG
1	D	4	ILE
1	D	24	GLU
1	D	26	LEU
1	D	80	VAL
1	D	82	LEU
1	D	121	LEU
1	D	180	LEU
1	D	213	LEU
1	D	260	LEU
1	D	285	ARG
1	D	304	HIS
1	D	328	VAL
1	D	336	THR
1	D	347	LEU
1	D	379	LEU
1	D	387	ILE
1	D	391	ILE
1	D	405	ARG
1	D	428	LEU
1	D	451	LEU
1	D	469	LEU
1	D	485	LYS
1	D	496	ASN
1	D	521	MET
1	D	531	LEU
1	D	561	VAL
1	D	563	ARG
1	E	4	ILE
1	E	24	GLU

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Mol	Chain	Res	Type
1	E	26	LEU
1	E	80	VAL
1	E	82	LEU
1	E	121	LEU
1	E	180	LEU
1	E	213	LEU
1	E	251	ARG
1	E	257	ARG
1	E	260	LEU
1	E	285	ARG
1	E	328	VAL
1	E	336	THR
1	E	347	LEU
1	E	379	LEU
1	E	387	ILE
1	E	391	ILE
1	E	405	ARG
1	E	428	LEU
1	E	451	LEU
1	E	469	LEU
1	E	485	LYS
1	E	496	ASN
1	E	531	LEU
1	E	561	VAL
1	E	563	ARG
1	F	4	ILE
1	F	19	ARG
1	F	20	MET
1	F	24	GLU
1	F	26	LEU
1	F	80	VAL
1	F	82	LEU
1	F	121	LEU
1	F	180	LEU
1	F	213	LEU
1	F	239	ARG
1	F	245	ASN
1	F	257	ARG
1	F	260	LEU
1	F	328	VAL
1	F	336	THR
1	F	347	LEU

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Mol	Chain	Res	Type
1	F	379	LEU
1	F	380	ASP
1	F	387	ILE
1	F	391	ILE
1	F	405	ARG
1	F	428	LEU
1	F	451	LEU
1	F	469	LEU
1	F	485	LYS
1	F	496	ASN
1	F	531	LEU
1	F	561	VAL
1	F	563	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	194	HIS
1	A	195	ASN
1	A	304	HIS
1	A	392	ASN
1	A	416	HIS
1	A	438	HIS
1	B	47	HIS
1	B	79	ASN
1	B	130	GLN
1	B	195	ASN
1	B	308	GLN
1	B	392	ASN
1	B	416	HIS
1	B	438	HIS
1	C	79	ASN
1	C	195	ASN
1	C	206	GLN
1	C	304	HIS
1	C	308	GLN
1	C	392	ASN
1	C	416	HIS
1	D	79	ASN
1	D	130	GLN
1	D	194	HIS

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Mol	Chain	Res	Type
1	D	195	ASN
1	D	377	HIS
1	D	392	ASN
1	D	416	HIS
1	E	79	ASN
1	E	130	GLN
1	E	194	HIS
1	E	195	ASN
1	E	308	GLN
1	E	351	GLN
1	E	416	HIS
1	F	79	ASN
1	F	130	GLN
1	F	194	HIS
1	F	195	ASN
1	F	416	HIS

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 13 ligands modelled in this entry, 5 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
4	FOC	F	592	-	10,10,10	0.98	1 (10%)	13,13,13	1.48	3 (23%)
4	FOC	D	594	2	10,10,10	0.94	1 (10%)	13,13,13	1.68	3 (23%)
3	SO4	A	593	-	4,4,4	0.65	0	6,6,6	0.80	0
3	SO4	D	593	-	4,4,4	0.61	0	6,6,6	0.87	0
4	FOC	A	594	2	10,10,10	0.87	1 (10%)	13,13,13	1.58	2 (15%)
4	FOC	B	593	2	10,10,10	0.88	1 (10%)	13,13,13	1.55	2 (15%)
4	FOC	E	593	2	10,10,10	0.87	0	13,13,13	1.62	2 (15%)
4	FOC	C	593	2	10,10,10	0.85	1 (10%)	13,13,13	1.58	3 (23%)

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
4	FOC	F	592	-	-	8/14/14/14	-
4	FOC	D	594	2	-	8/14/14/14	-
4	FOC	A	594	2	-	9/14/14/14	-
4	FOC	B	593	2	-	7/14/14/14	-
4	FOC	E	593	2	-	8/14/14/14	-
4	FOC	C	593	2	-	8/14/14/14	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	592	FOC	O1-C1	-2.17	1.33	1.42
4	C	593	FOC	O1-C1	-2.14	1.33	1.42
4	D	594	FOC	O1-C1	-2.08	1.33	1.42
4	B	593	FOC	O1-C1	-2.06	1.33	1.42
4	A	594	FOC	O1-C1	-2.00	1.34	1.42

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	593	FOC	C6-C5-C4	-4.82	106.21	112.11
4	D	594	FOC	C6-C5-C4	-4.72	106.34	112.11
4	C	593	FOC	C6-C5-C4	-4.42	106.70	112.11
4	A	594	FOC	C6-C5-C4	-4.29	106.87	112.11
4	B	593	FOC	C6-C5-C4	-4.18	107.00	112.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	592	FOC	C6-C5-C4	-3.82	107.44	112.11
4	A	594	FOC	O5-C5-C4	-2.81	105.12	109.77
4	B	593	FOC	O5-C5-C4	-2.75	105.22	109.77
4	D	594	FOC	O5-C5-C4	-2.63	105.42	109.77
4	F	592	FOC	O5-C5-C4	-2.43	105.75	109.77
4	E	593	FOC	O5-C5-C4	-2.10	106.30	109.77
4	F	592	FOC	O1-C1-C2	-2.07	106.81	111.16
4	D	594	FOC	O1-C1-C2	-2.06	106.83	111.16
4	C	593	FOC	O5-C5-C4	-2.01	106.44	109.77
4	C	593	FOC	O1-C1-C2	-2.00	106.95	111.16

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	594	FOC	O1-C1-C2-O2
4	A	594	FOC	O1-C1-C2-C3
4	B	593	FOC	O1-C1-C2-O2
4	B	593	FOC	O1-C1-C2-C3
4	C	593	FOC	O1-C1-C2-O2
4	C	593	FOC	O1-C1-C2-C3
4	D	594	FOC	O1-C1-C2-O2
4	D	594	FOC	O1-C1-C2-C3
4	E	593	FOC	O1-C1-C2-O2
4	E	593	FOC	O1-C1-C2-C3
4	F	592	FOC	O1-C1-C2-O2
4	F	592	FOC	O1-C1-C2-C3
4	A	594	FOC	O2-C2-C3-O3
4	A	594	FOC	O3-C3-C4-O4
4	B	593	FOC	O3-C3-C4-O4
4	C	593	FOC	O3-C3-C4-O4
4	D	594	FOC	O3-C3-C4-O4
4	E	593	FOC	O3-C3-C4-O4
4	F	592	FOC	O3-C3-C4-O4
4	A	594	FOC	O2-C2-C3-C4
4	C	593	FOC	O2-C2-C3-O3
4	D	594	FOC	O2-C2-C3-O3
4	F	592	FOC	O2-C2-C3-O3
4	F	592	FOC	O2-C2-C3-C4
4	A	594	FOC	C1-C2-C3-O3
4	C	593	FOC	O2-C2-C3-C4
4	B	593	FOC	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	E	593	FOC	O2-C2-C3-O3
4	D	594	FOC	C1-C2-C3-O3
4	D	594	FOC	O2-C2-C3-C4
4	A	594	FOC	C3-C4-C5-O5
4	B	593	FOC	O2-C2-C3-C4
4	A	594	FOC	C1-C2-C3-C4
4	E	593	FOC	C2-C3-C4-O4
4	E	593	FOC	O2-C2-C3-C4
4	C	593	FOC	C1-C2-C3-O3
4	F	592	FOC	C1-C2-C3-O3
4	F	592	FOC	C1-C2-C3-C4
4	E	593	FOC	C1-C2-C3-O3
4	C	593	FOC	C1-C2-C3-C4
4	D	594	FOC	C1-C2-C3-C4
4	B	593	FOC	C2-C3-C4-O4
4	D	594	FOC	C2-C3-C4-O4
4	F	592	FOC	C2-C3-C4-O4
4	B	593	FOC	C1-C2-C3-O3
4	A	594	FOC	C2-C3-C4-O4
4	C	593	FOC	C2-C3-C4-O4
4	E	593	FOC	C1-C2-C3-C4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	592	FOC	1	0
4	C	593	FOC	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	587/591 (99%)	-0.81	3 (0%) 87 85	12, 25, 52, 80	3 (0%)
1	B	587/591 (99%)	-0.64	1 (0%) 91 89	13, 31, 57, 79	9 (1%)
1	C	581/591 (98%)	-0.73	5 (0%) 81 78	11, 26, 55, 77	9 (1%)
1	D	569/591 (96%)	-0.67	3 (0%) 87 85	12, 29, 59, 97	3 (0%)
1	E	586/591 (99%)	-0.74	4 (0%) 84 81	11, 26, 55, 78	11 (1%)
1	F	583/591 (98%)	-0.58	6 (1%) 79 76	14, 31, 59, 87	10 (1%)
All	All	3493/3546 (98%)	-0.70	22 (0%) 85 83	11, 28, 57, 97	45 (1%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	252	ASN	6.8
1	F	247	LYS	4.8
1	D	591	ARG	3.8
1	E	591	ARG	3.7
1	A	5	SER	3.5
1	A	591	ARG	3.5
1	B	591	ARG	3.4
1	F	591	ARG	3.2
1	F	116	PRO	2.9
1	C	591	ARG	2.8
1	F	253	ALA	2.7
1	E	254	GLU	2.6
1	C	250	GLN	2.6
1	A	422	GLN	2.3
1	F	254	GLU	2.3
1	D	5	SER	2.2
1	E	5	SER	2.2
1	C	486	ASP	2.2
1	F	22	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	251	ARG	2.1
1	C	245	ASN	2.1
1	D	377	HIS	2.1

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(Å ²)	Q<0.9
4	FOC	F	592	11/11	0.59	0.18	55,72,77,87	0
4	FOC	A	594	11/11	0.84	0.16	56,69,77,82	0
4	FOC	D	594	11/11	0.85	0.12	68,71,83,88	0
4	FOC	B	593	11/11	0.87	0.13	59,77,84,86	0
4	FOC	C	593	11/11	0.89	0.17	67,74,77,83	0
2	MN	C	592	1/1	0.93	0.08	43,43,43,43	0
4	FOC	E	593	11/11	0.94	0.13	43,63,69,77	0
2	MN	D	592	1/1	0.95	0.06	49,49,49,49	0
2	MN	A	592	1/1	0.97	0.04	39,39,39,39	0
2	MN	E	592	1/1	0.97	0.06	31,31,31,31	0
2	MN	B	592	1/1	0.98	0.07	41,41,41,41	0
3	SO4	D	593	5/5	0.99	0.04	17,20,22,25	0
3	SO4	A	593	5/5	1.00	0.02	12,12,21,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.