



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:42 AM UTC

PDB ID : 4IUA / pdb_00004iua
Title : Crystal Structure of the NK2 Fragment (31-290) of the mouse Hepatocyte Growth Factor/Scatter Factor
Authors : Tolbert, W.D.; Zhou, E.; Kovach, A.; Melcher, K.; Xu, H.E.
Deposited on : 2013-01-20
Resolution : 3.05 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

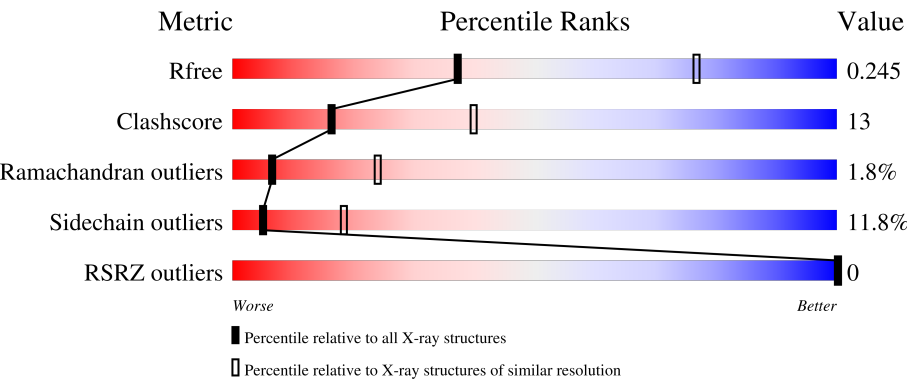
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.05 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	262	63%27%6%.
1	B	262	65%26%6%.
1	C	262	55%34%7%.
1	D	262	65%26%6%.
1	E	262	66%26%5%.

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Mol	Chain	Length	Quality of chain
1	F	262	62%28%6%••
1	G	262	61%26%6%6%
1	H	262	65%25%•6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16628 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 Hepatocyte growth factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			2068	1293	369	386	20			
1	B	254	Total	C	N	O	S	0	0	0
			2068	1293	369	386	20			
1	C	254	Total	C	N	O	S	0	0	0
			2068	1293	369	386	20			
1	D	254	Total	C	N	O	S	0	0	0
			2068	1293	369	386	20			
1	E	254	Total	C	N	O	S	0	0	0
			2068	1293	369	386	20			
1	F	254	Total	C	N	O	S	0	0	0
			2068	1293	369	386	20			
1	G	246	Total	C	N	O	S	0	0	0
			1995	1249	351	375	20			
1	H	246	Total	C	N	O	S	0	0	0
			2000	1251	356	373	20			

There are 24 discrepancies between the modelled and reference sequences:

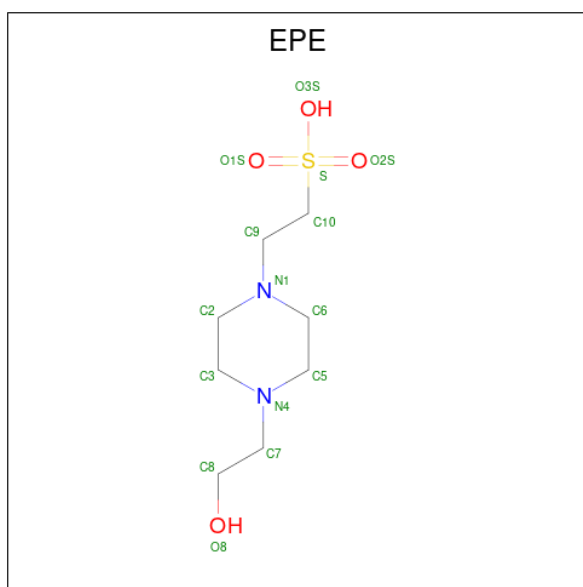
Chain	Residue	Modelled	Actual	Comment	Reference
A	29	GLY	-	expression tag	UNP Q08048
A	30	SER	-	expression tag	UNP Q08048
A	215	ALA	CYS	engineered mutation	UNP Q08048
B	29	GLY	-	expression tag	UNP Q08048
B	30	SER	-	expression tag	UNP Q08048
B	215	ALA	CYS	engineered mutation	UNP Q08048
C	29	GLY	-	expression tag	UNP Q08048
C	30	SER	-	expression tag	UNP Q08048
C	215	ALA	CYS	engineered mutation	UNP Q08048
D	29	GLY	-	expression tag	UNP Q08048
D	30	SER	-	expression tag	UNP Q08048
D	215	ALA	CYS	engineered mutation	UNP Q08048
E	29	GLY	-	expression tag	UNP Q08048

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Chain	Residue	Modelled	Actual	Comment	Reference
E	30	SER	-	expression tag	UNP Q08048
E	215	ALA	CYS	engineered mutation	UNP Q08048
F	29	GLY	-	expression tag	UNP Q08048
F	30	SER	-	expression tag	UNP Q08048
F	215	ALA	CYS	engineered mutation	UNP Q08048
G	29	GLY	-	expression tag	UNP Q08048
G	30	SER	-	expression tag	UNP Q08048
G	215	ALA	CYS	engineered mutation	UNP Q08048
H	29	GLY	-	expression tag	UNP Q08048
H	30	SER	-	expression tag	UNP Q08048
H	215	ALA	CYS	engineered mutation	UNP Q08048

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	G	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	H	1	Total	C	N	O	S	0	0
			15	8	2	4	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	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

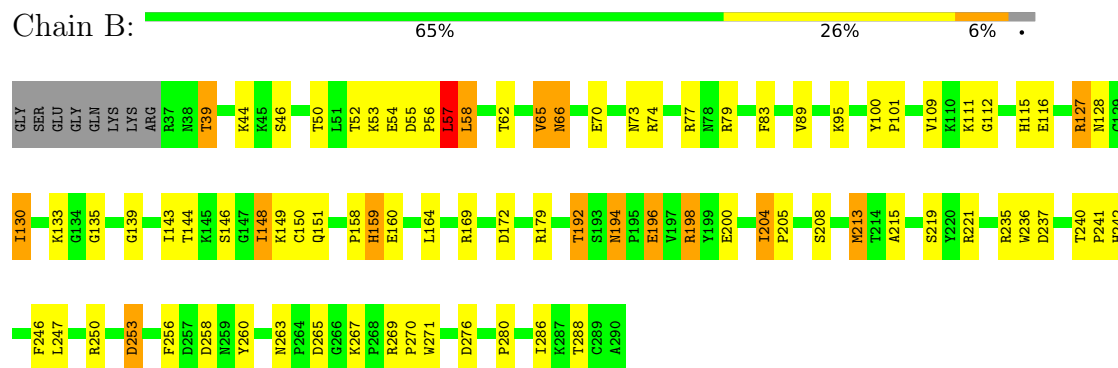
3 Residue-property plots

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.

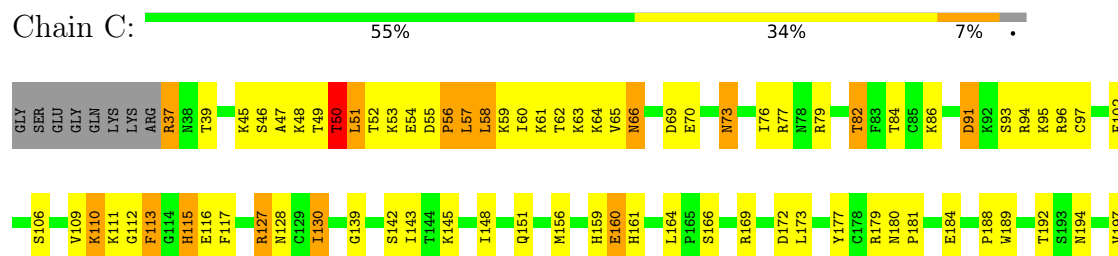
- Molecule 1: Hepatocyte growth factor

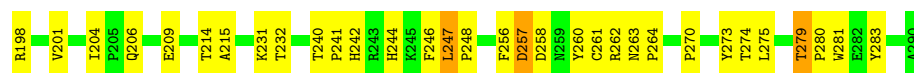


- Molecule 1: Hepatocyte growth factor



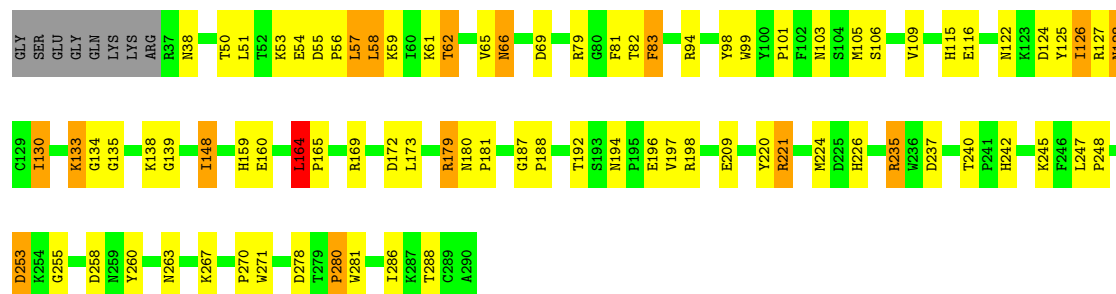
- Molecule 1: Hepatocyte growth factor





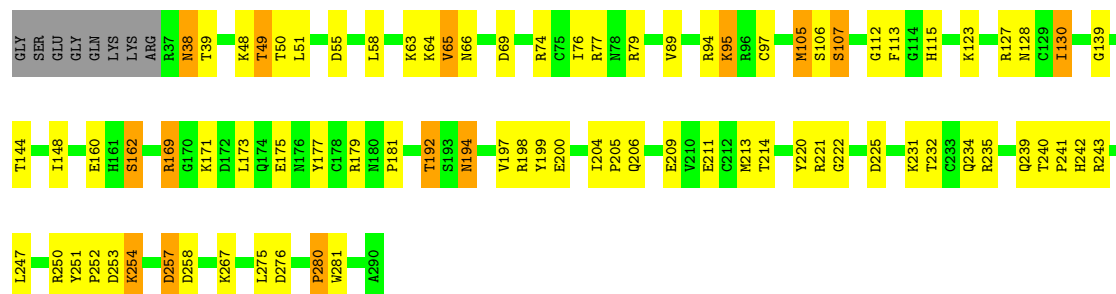
- Molecule 1: Hepatocyte growth factor

Chain D: 65% 26% 6% .



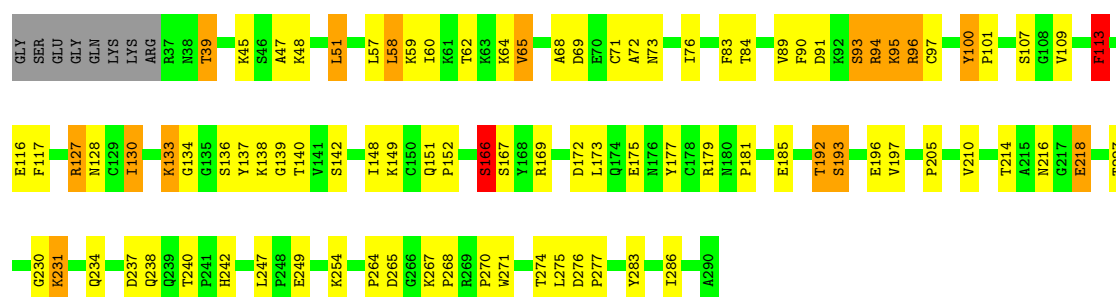
- Molecule 1: Hepatocyte growth factor

Chain E: 66% 26% 5% .



- Molecule 1: Hepatocyte growth factor

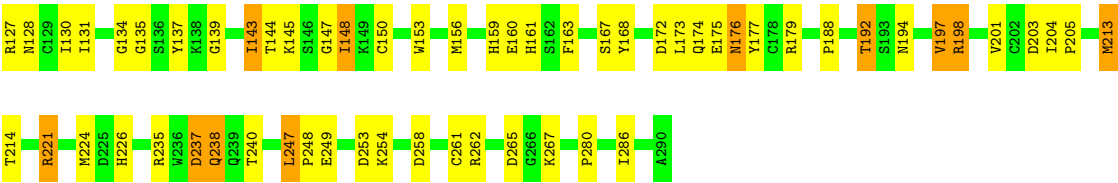
Chain F: 62% 28% 6% .



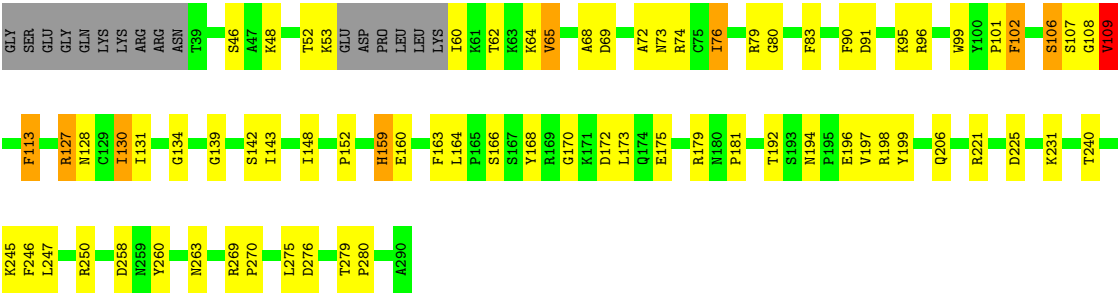
- Molecule 1: Hepatocyte growth factor

Chain G: 61% 26% 6% 6%





• Molecule 1: Hepatocyte growth factor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.62Å 127.33Å 129.60Å 90.00° 90.25° 90.00°	Depositor
Resolution (Å)	29.77 – 3.05 29.77 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.77-3.05) 99.8 (29.77-3.05)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.8_1069, CNS	Depositor
R, R_{free}	0.176 , 0.245 0.180 , 0.245	Depositor DCC
R_{free} test set	5878 reflections (10.18%)	wwPDB-VP
Wilson B-factor (Å ²)	70.7	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 67.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.098 for -h,l,k 0.148 for -h,-l,-k 0.107 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16628	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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: SO4, EPE

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	0.59	0/2129	0.92	3/2871 (0.1%)
1	B	0.63	0/2129	1.00	6/2871 (0.2%)
1	C	0.60	0/2129	1.00	10/2871 (0.3%)
1	D	0.53	0/2129	0.89	2/2871 (0.1%)
1	E	0.54	0/2129	0.96	6/2871 (0.2%)
1	F	0.54	0/2129	0.94	9/2871 (0.3%)
1	G	0.49	0/2053	0.88	3/2768 (0.1%)
1	H	0.48	0/2059	0.85	3/2775 (0.1%)
All	All	0.55	0/16886	0.93	42/22769 (0.2%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	204	ILE	CA-C-N	8.74	128.78	119.78
1	B	204	ILE	C-N-CA	8.74	128.78	119.78
1	B	127	ARG	N-CA-C	8.31	119.97	111.07
1	H	113	PHE	N-CA-C	7.65	118.08	108.45
1	C	127	ARG	N-CA-C	7.17	119.17	111.36
1	C	247	LEU	CA-C-N	6.77	128.31	119.84
1	C	247	LEU	C-N-CA	6.77	128.31	119.84
1	D	164	LEU	CA-C-N	6.58	128.06	119.84
1	D	164	LEU	C-N-CA	6.58	128.06	119.84
1	E	194	ASN	CA-C-N	6.31	126.00	119.82
1	E	194	ASN	C-N-CA	6.31	126.00	119.82
1	G	127	ARG	N-CA-C	6.26	118.90	111.33
1	F	127	ARG	N-CA-C	6.21	118.13	111.36
1	F	113	PHE	N-CA-C	6.14	118.12	108.96
1	E	66	ASN	N-CA-C	6.14	118.89	111.40
1	F	151	GLN	CA-C-N	6.13	126.49	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	151	GLN	C-N-CA	6.13	126.49	119.93
1	C	279	THR	CA-C-N	6.11	125.60	119.24
1	C	279	THR	C-N-CA	6.11	125.60	119.24
1	H	127	ARG	N-CA-C	6.11	117.81	111.03
1	F	247	LEU	CA-C-N	5.93	127.25	119.84
1	F	247	LEU	C-N-CA	5.93	127.25	119.84
1	G	247	LEU	CA-C-N	5.90	127.22	119.84
1	G	247	LEU	C-N-CA	5.90	127.22	119.84
1	E	55	ASP	CA-C-N	5.74	127.02	119.84
1	E	55	ASP	C-N-CA	5.74	127.02	119.84
1	F	100	TYR	CA-C-N	5.59	126.54	120.83
1	F	100	TYR	C-N-CA	5.59	126.54	120.83
1	A	175	GLU	CB-CA-C	-5.53	110.18	116.54
1	C	215	ALA	CB-CA-C	-5.52	110.20	116.54
1	F	218	GLU	N-CA-C	-5.46	105.33	111.28
1	B	194	ASN	CA-C-N	5.40	126.59	119.84
1	B	194	ASN	C-N-CA	5.40	126.59	119.84
1	E	175	GLU	CB-CA-C	-5.36	110.37	116.54
1	H	159	HIS	N-CA-C	5.36	117.97	109.50
1	C	82	THR	N-CA-C	-5.27	106.08	112.88
1	C	50	THR	N-CA-C	5.26	115.23	108.34
1	B	159	HIS	N-CA-C	5.19	117.18	108.73
1	A	171	LYS	N-CA-C	-5.15	105.89	113.61
1	A	215	ALA	CB-CA-C	-5.13	110.64	116.54
1	C	151	GLN	CA-C-N	5.07	125.35	119.93
1	C	151	GLN	C-N-CA	5.07	125.35	119.93

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	2068	0	1951	56	0
1	B	2068	0	1951	46	0
1	C	2068	0	1951	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2068	0	1951	53	0
1	E	2068	0	1951	55	0
1	F	2068	0	1951	56	0
1	G	1995	0	1875	59	0
1	H	2000	0	1879	41	0
2	A	15	0	18	2	0
2	B	30	0	34	1	0
2	C	30	0	34	3	0
2	D	15	0	17	1	0
2	E	15	0	17	1	0
2	F	15	0	17	0	0
2	G	15	0	17	2	0
2	H	15	0	17	0	0
3	A	10	0	0	0	0
3	B	15	0	0	0	0
3	C	5	0	0	0	0
3	D	15	0	0	1	0
3	F	15	0	0	1	0
3	G	10	0	0	1	0
3	H	5	0	0	1	0
All	All	16628	0	15631	418	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 13.

All (418) 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:C:148:ILE:HG21	1:C:192:THR:HG23	1.51	0.93
1:G:143:ILE:HG23	1:G:147:GLY:HA2	1.51	0.91
1:B:139:GLY:O	1:B:179:ARG:NH2	2.04	0.90
1:C:139:GLY:O	1:C:179:ARG:NH2	2.04	0.90
1:A:192:THR:HG22	1:A:194:ASN:H	1.38	0.87
1:H:160:GLU:O	1:H:198:ARG:NH2	2.10	0.83
1:H:192:THR:HG22	1:H:194:ASN:H	1.43	0.82
1:D:139:GLY:O	1:D:179:ARG:NH2	2.11	0.82
1:H:139:GLY:O	1:H:179:ARG:NH2	2.12	0.82
1:D:55:ASP:HB3	1:D:58:LEU:HB2	1.59	0.81
1:C:160:GLU:O	1:C:198:ARG:NH2	2.14	0.81
1:G:235:ARG:NH1	1:G:237:ASP:OD2	2.15	0.79
1:B:192:THR:HG22	1:B:194:ASN:H	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:GLY:O	1:A:179:ARG:NH2	2.17	0.78
1:B:39:THR:OG1	1:B:73:ASN:OD1	2.02	0.77
1:B:160:GLU:O	1:B:198:ARG:NH2	2.17	0.77
1:F:139:GLY:O	1:F:179:ARG:NH2	2.18	0.77
1:E:139:GLY:O	1:E:179:ARG:NH2	2.17	0.77
1:A:160:GLU:O	1:A:198:ARG:NH2	2.18	0.77
1:A:235:ARG:NH2	1:A:258:ASP:OD1	2.19	0.76
1:D:135:GLY:HA2	1:D:180:ASN:HB3	1.67	0.76
1:F:94:ARG:O	1:F:96:ARG:N	2.19	0.75
1:C:130:ILE:HD12	1:C:204:ILE:HB	1.68	0.75
1:B:53:LYS:NZ	1:B:57:LEU:O	2.18	0.74
1:F:231:LYS:NZ	3:F:1004:SO4:O4	2.20	0.74
1:C:231:LYS:HZ3	1:C:275:LEU:HD21	1.53	0.74
1:B:247:LEU:HB2	1:B:250:ARG:HG3	1.69	0.73
1:B:235:ARG:NH2	1:B:258:ASP:OD1	2.21	0.73
1:C:50:THR:OG1	1:C:51:LEU:N	2.19	0.72
1:D:192:THR:HG22	1:D:194:ASN:H	1.54	0.72
1:G:198:ARG:NH1	2:G:1001:EPE:O1S	2.24	0.70
1:C:263:ASN:HB2	1:C:270:PRO:HA	1.73	0.70
1:E:173:LEU:HD21	1:E:181:PRO:HG3	1.75	0.69
1:H:173:LEU:HD21	1:H:181:PRO:HG3	1.75	0.69
1:D:267:LYS:HD2	1:D:271:TRP:CD1	2.28	0.69
1:B:116:GLU:N	1:B:116:GLU:OE2	2.27	0.68
1:E:148:ILE:HG21	1:E:192:THR:HG23	1.74	0.67
1:C:173:LEU:HD21	1:C:181:PRO:HG3	1.76	0.67
1:C:130:ILE:HD11	1:C:188:PRO:HG2	1.76	0.67
1:A:235:ARG:NH1	1:A:237:ASP:OD2	2.28	0.67
1:E:65:VAL:O	1:E:95:LYS:NZ	2.22	0.67
1:H:172:ASP:O	1:H:179:ARG:NH1	2.28	0.66
1:A:59:LYS:NZ	1:A:82:THR:OG1	2.29	0.66
1:F:148:ILE:HG21	1:F:192:THR:HG23	1.77	0.66
1:D:38:ASN:ND2	1:D:69:ASP:OD1	2.25	0.66
1:E:251:TYR:HB3	1:E:254:LYS:HG3	1.78	0.65
1:A:74:ARG:NE	1:A:79:ARG:O	2.29	0.65
1:E:231:LYS:HG2	1:E:276:ASP:HB2	1.76	0.65
1:G:160:GLU:O	1:G:198:ARG:NH2	2.30	0.65
1:D:160:GLU:O	1:D:198:ARG:NH2	2.29	0.65
1:B:77:ARG:HG3	1:B:79:ARG:H	1.62	0.65
1:B:235:ARG:NH1	1:B:237:ASP:OD2	2.30	0.65
1:A:83:PHE:HD1	1:A:101:PRO:HB3	1.61	0.64
2:B:1005:EPE:O1S	1:E:169:ARG:HD2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:LYS:HD3	1:G:113:PHE:HD2	1.62	0.64
1:H:69:ASP:O	1:H:73:ASN:ND2	2.28	0.64
1:E:205:PRO:HD3	1:G:214:THR:HG21	1.79	0.64
1:C:231:LYS:HD3	1:C:275:LEU:HG	1.79	0.64
1:E:257:ASP:OD2	1:E:257:ASP:N	2.30	0.64
1:B:159:HIS:CE1	1:B:198:ARG:HA	2.33	0.64
1:C:56:PRO:O	1:C:58:LEU:N	2.31	0.64
1:C:192:THR:HG22	1:C:194:ASN:H	1.63	0.63
1:H:276:ASP:HB3	1:H:279:THR:HB	1.80	0.63
1:F:149:LYS:O	1:F:193:SER:OG	2.15	0.63
1:C:192:THR:HB	1:C:197:VAL:O	1.99	0.62
1:E:198:ARG:HG2	1:E:199:TYR:HD1	1.63	0.62
1:C:274:THR:OG1	1:C:279:THR:O	2.17	0.62
1:A:55:ASP:HB3	1:A:58:LEU:HD23	1.81	0.62
1:C:198:ARG:NH1	2:C:1001:EPE:O1S	2.32	0.62
1:F:39:THR:OG1	1:F:73:ASN:OD1	2.18	0.62
1:G:134:GLY:HA3	1:G:188:PRO:HD3	1.82	0.62
1:B:144:THR:HB	1:B:200:GLU:HG2	1.82	0.61
1:F:234:GLN:NE2	1:F:238:GLN:O	2.30	0.61
1:A:269:ARG:NH2	1:B:215:ALA:O	2.33	0.61
1:G:221:ARG:HH12	1:G:254:LYS:C	2.09	0.61
1:E:192:THR:HG21	1:E:197:VAL:HB	1.82	0.61
1:G:46:SER:HB3	1:G:119:LEU:HB3	1.82	0.60
1:A:83:PHE:CD1	1:A:101:PRO:HB3	2.36	0.60
1:E:123:LYS:NZ	1:E:225:ASP:OD1	2.34	0.60
1:G:224:MET:HE2	1:G:226:HIS:HB2	1.84	0.60
1:A:173:LEU:HD21	1:A:181:PRO:HG3	1.82	0.60
1:D:94:ARG:NH1	3:D:1002:SO4:O3	2.35	0.60
1:E:241:PRO:HG2	1:E:242:HIS:CD2	2.37	0.59
1:H:263:ASN:HB2	1:H:270:PRO:HA	1.84	0.59
1:D:130:ILE:HD11	1:D:134:GLY:HA3	1.83	0.59
1:B:253:ASP:OD1	1:B:253:ASP:N	2.35	0.59
1:B:57:LEU:HG	1:B:58:LEU:H	1.68	0.59
1:D:159:HIS:CE1	1:D:198:ARG:HA	2.37	0.59
1:G:213:MET:HE2	1:G:286:ILE:HB	1.86	0.58
1:F:130:ILE:HD11	1:F:134:GLY:HA3	1.86	0.58
1:A:249:GLU:CD	1:A:249:GLU:H	2.11	0.58
1:E:280:PRO:HB2	1:E:281:TRP:CE3	2.39	0.58
1:A:148:ILE:HG21	1:A:192:THR:HG23	1.86	0.58
1:A:116:GLU:OE2	1:A:116:GLU:N	2.37	0.57
1:B:196:GLU:HG3	1:E:169:ARG:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:THR:HB	1:E:197:VAL:O	2.04	0.57
1:A:159:HIS:CE1	1:A:198:ARG:HA	2.39	0.57
1:A:192:THR:HB	1:A:197:VAL:O	2.05	0.57
1:B:213:MET:HE2	1:B:286:ILE:HB	1.86	0.57
1:C:257:ASP:N	1:C:257:ASP:OD2	2.34	0.57
1:C:231:LYS:NZ	1:C:275:LEU:HD21	2.18	0.57
1:E:206:GLN:HB2	1:E:209:GLU:HG2	1.87	0.57
1:G:83:PHE:HD1	1:G:101:PRO:HB3	1.70	0.57
1:F:65:VAL:O	1:F:95:LYS:HE2	2.04	0.57
1:A:213:MET:HE2	1:A:286:ILE:HB	1.87	0.56
1:D:133:LYS:O	1:D:187:GLY:HA2	2.06	0.56
1:G:130:ILE:HD12	1:G:204:ILE:HB	1.86	0.56
1:A:56:PRO:O	1:A:58:LEU:N	2.37	0.56
1:A:114:GLY:H	1:F:113:PHE:HZ	1.52	0.56
1:F:173:LEU:HD21	1:F:181:PRO:HG3	1.87	0.56
1:H:198:ARG:HG2	1:H:199:TYR:HD1	1.69	0.56
1:A:114:GLY:N	1:F:113:PHE:HZ	2.03	0.56
1:H:74:ARG:NH1	1:H:79:ARG:O	2.39	0.56
1:C:206:GLN:HB2	1:C:209:GLU:HG2	1.88	0.55
1:D:173:LEU:HD21	1:D:181:PRO:HG3	1.87	0.55
1:F:216:ASN:ND2	1:F:218:GLU:HG3	2.21	0.55
1:D:253:ASP:OD1	1:D:253:ASP:N	2.33	0.55
1:H:64:LYS:HA	1:H:96:ARG:HA	1.86	0.55
1:A:206:GLN:HB2	1:A:209:GLU:HG2	1.86	0.55
1:E:50:THR:HB	1:E:112:GLY:HA3	1.88	0.55
1:E:214:THR:HG21	1:G:205:PRO:HD3	1.89	0.55
1:G:97:CYS:HB3	1:G:99:TRP:CH2	2.42	0.55
1:F:254:LYS:HD2	1:F:264:PRO:HA	1.88	0.54
1:G:159:HIS:CE1	1:G:198:ARG:HA	2.42	0.54
1:C:156:MET:HE1	1:C:161:HIS:O	2.06	0.54
1:A:39:THR:HG21	1:A:76:ILE:HG12	1.89	0.54
1:G:130:ILE:HG23	1:G:134:GLY:HA2	1.89	0.54
1:G:163:PHE:CD1	1:G:168:TYR:HE2	2.26	0.54
1:C:247:LEU:HD12	1:C:248:PRO:HD2	1.88	0.54
1:A:227:THR:HG22	1:A:272:CYS:SG	2.48	0.54
1:F:265:ASP:OD2	1:F:267:LYS:NZ	2.41	0.54
1:F:227:THR:HG21	1:F:274:THR:HG22	1.90	0.54
1:B:213:MET:HE1	1:B:269:ARG:HB2	1.90	0.54
1:H:142:SER:H	1:H:143:ILE:HD12	1.72	0.54
1:A:66:ASN:OD1	1:A:66:ASN:N	2.41	0.54
1:D:103:ASN:O	1:D:109:VAL:HG21	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:MET:HE3	1:D:226:HIS:H	1.72	0.54
1:H:194:ASN:HD22	1:H:197:VAL:HG23	1.73	0.54
1:G:130:ILE:HD11	1:G:188:PRO:HG2	1.89	0.53
1:C:37:ARG:N	1:C:37:ARG:HE	2.06	0.53
1:C:48:LYS:HG2	1:C:115:HIS:HA	1.90	0.53
1:B:50:THR:HG23	1:B:112:GLY:HA3	1.91	0.53
1:C:192:THR:HG22	1:C:194:ASN:N	2.24	0.53
1:F:268:PRO:HD2	1:F:283:TYR:OH	2.07	0.53
1:H:130:ILE:HG22	1:H:206:GLN:HA	1.90	0.53
1:D:192:THR:HB	1:D:197:VAL:O	2.09	0.53
1:E:235:ARG:NH2	1:E:258:ASP:OD1	2.41	0.53
1:E:160:GLU:O	1:E:198:ARG:NH2	2.40	0.53
1:G:156:MET:HE1	1:G:161:HIS:H	1.73	0.53
1:F:68:ALA:HB2	1:F:90:PHE:CD2	2.44	0.53
1:F:72:ALA:O	1:F:76:ILE:HG12	2.09	0.53
1:B:258:ASP:HB2	1:B:260:TYR:CE2	2.44	0.52
1:G:261:CYS:O	1:G:262:ARG:NH1	2.39	0.52
1:E:242:HIS:CE1	1:E:280:PRO:HA	2.44	0.52
1:G:105:MET:HE2	1:G:126:ILE:HG22	1.92	0.52
1:A:90:PHE:HD1	1:A:97:CYS:HB3	1.75	0.52
1:F:270:PRO:HG2	1:F:286:ILE:HD13	1.91	0.52
1:C:192:THR:HG21	1:C:197:VAL:HB	1.90	0.52
1:A:205:PRO:HD3	1:F:214:THR:HG21	1.90	0.52
1:A:215:ALA:O	1:B:269:ARG:NH2	2.43	0.52
1:B:213:MET:HG3	1:B:288:THR:HG22	1.91	0.52
1:H:163:PHE:HA	1:H:168:TYR:CE2	2.44	0.52
1:H:192:THR:HB	1:H:197:VAL:O	2.10	0.52
1:F:166:SER:HA	1:F:169:ARG:NE	2.25	0.51
1:G:249:GLU:H	1:G:249:GLU:CD	2.19	0.51
1:E:38:ASN:OD1	1:E:38:ASN:N	2.43	0.51
1:C:231:LYS:HZ3	1:C:275:LEU:HD11	1.75	0.51
1:G:156:MET:CE	1:G:161:HIS:H	2.24	0.51
1:E:39:THR:HG21	1:E:76:ILE:HD11	1.92	0.51
1:A:96:ARG:HG2	1:A:98:TYR:HE1	1.76	0.51
1:F:83:PHE:CD1	1:F:101:PRO:HB3	2.46	0.51
1:E:250:ARG:C	1:E:252:PRO:HD3	2.36	0.51
1:F:231:LYS:HD3	1:F:276:ASP:HB2	1.92	0.51
1:H:163:PHE:HA	1:H:168:TYR:HE2	1.76	0.51
1:H:194:ASN:HD21	1:H:196:GLU:HB2	1.74	0.51
1:D:62:THR:HB	1:D:98:TYR:HD1	1.77	0.51
1:E:280:PRO:HB2	1:E:281:TRP:HE3	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:138:LYS:HD3	1:F:172:ASP:HB2	1.91	0.50
1:C:232:THR:HB	1:C:275:LEU:HD23	1.93	0.50
1:G:265:ASP:OD2	1:G:267:LYS:HE3	2.11	0.50
1:B:70:GLU:OE1	1:B:74:ARG:NH2	2.45	0.50
1:C:261:CYS:O	1:C:262:ARG:NH1	2.41	0.50
1:B:159:HIS:NE2	1:B:198:ARG:HA	2.27	0.50
1:C:86:LYS:HD2	1:C:102:PHE:HA	1.94	0.50
1:A:247:LEU:HB2	1:A:250:ARG:HD2	1.94	0.50
1:C:93:SER:OG	1:C:116:GLU:OE1	2.30	0.50
1:A:211:GLU:HA	1:F:210:VAL:O	2.13	0.49
1:G:50:THR:OG1	1:G:51:LEU:N	2.45	0.49
1:G:64:LYS:HG3	1:G:96:ARG:HD2	1.93	0.49
1:H:159:HIS:CE1	1:H:198:ARG:HA	2.48	0.49
1:C:77:ARG:HH11	1:C:79:ARG:HE	1.60	0.49
1:C:256:PHE:HZ	1:C:264:PRO:HG3	1.77	0.49
1:H:194:ASN:ND2	1:H:197:VAL:HG23	2.28	0.49
1:H:148:ILE:HG21	1:H:192:THR:HG23	1.94	0.49
1:F:69:ASP:O	1:F:73:ASN:ND2	2.46	0.49
1:F:267:LYS:HD2	1:F:271:TRP:CD1	2.48	0.49
1:H:192:THR:HG21	1:H:197:VAL:HB	1.94	0.49
1:A:113:PHE:HB2	1:F:113:PHE:CZ	2.48	0.49
1:C:113:PHE:N	1:C:113:PHE:CD2	2.81	0.49
1:D:192:THR:HG22	1:D:194:ASN:N	2.27	0.48
1:H:258:ASP:HB2	1:H:260:TYR:CE2	2.48	0.48
1:H:172:ASP:OD2	1:H:179:ARG:NH1	2.46	0.48
1:D:133:LYS:HD2	1:D:134:GLY:N	2.28	0.48
1:D:263:ASN:HB2	1:D:270:PRO:HA	1.94	0.48
1:E:211:GLU:HG2	1:E:220:TYR:CE1	2.48	0.48
1:A:281:TRP:CZ2	1:C:145:LYS:HE3	2.49	0.48
1:D:130:ILE:CD1	1:D:134:GLY:HA3	2.43	0.48
1:F:91:ASP:OD2	1:F:94:ARG:HG2	2.13	0.48
1:A:77:ARG:HH11	1:A:79:ARG:HB2	1.78	0.48
1:C:55:ASP:O	1:C:57:LEU:N	2.46	0.48
1:D:165:PRO:HG3	1:D:173:LEU:HB2	1.96	0.48
1:C:242:HIS:ND1	1:C:280:PRO:HA	2.29	0.48
1:E:235:ARG:NH2	1:E:258:ASP:HA	2.29	0.48
1:G:153:TRP:CE3	1:G:173:LEU:HD22	2.48	0.48
1:B:172:ASP:O	1:B:179:ARG:NH1	2.44	0.48
1:A:110:LYS:HD2	1:A:111:LYS:H	1.78	0.47
1:E:214:THR:HB	1:G:205:PRO:HG3	1.95	0.47
1:F:192:THR:HB	1:F:197:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:MET:HE1	1:A:269:ARG:HB2	1.96	0.47
1:C:189:TRP:CE2	2:C:1001:EPE:H51	2.49	0.47
1:G:192:THR:HG21	1:G:197:VAL:HG22	1.96	0.47
1:C:116:GLU:HG3	1:C:117:PHE:CE2	2.50	0.47
1:A:132:GLY:CA	1:A:206:GLN:HE22	2.26	0.47
1:B:83:PHE:CD1	1:B:101:PRO:HB3	2.49	0.47
1:D:55:ASP:CG	1:D:56:PRO:HD2	2.40	0.47
1:F:93:SER:O	1:F:95:LYS:N	2.47	0.47
1:H:72:ALA:O	1:H:76:ILE:HG23	2.15	0.47
1:A:50:THR:OG1	1:A:51:LEU:N	2.46	0.47
1:C:45:LYS:HE2	1:C:47:ALA:HB2	1.97	0.47
1:C:159:HIS:NE2	1:C:197:VAL:O	2.46	0.47
1:D:66:ASN:OD1	1:D:66:ASN:N	2.47	0.47
1:A:247:LEU:HA	1:A:247:LEU:HD13	1.61	0.47
1:D:198:ARG:NH1	2:D:1001:EPE:O1S	2.48	0.47
1:F:64:LYS:HA	1:F:95:LYS:O	2.15	0.47
1:F:64:LYS:HD3	1:F:95:LYS:HB2	1.96	0.47
1:F:130:ILE:CD1	1:F:134:GLY:HA3	2.44	0.47
1:G:65:VAL:HG21	1:G:71:CYS:SG	2.54	0.47
1:E:130:ILE:HD13	1:E:204:ILE:HG21	1.97	0.47
1:G:156:MET:HE3	1:G:160:GLU:HA	1.97	0.47
1:H:53:LYS:HB2	1:H:109:VAL:HB	1.97	0.47
1:C:169:ARG:NH1	2:C:1002:EPE:O3S	2.48	0.47
1:D:83:PHE:N	1:D:83:PHE:CD2	2.82	0.47
1:G:159:HIS:NE2	1:G:198:ARG:HA	2.30	0.47
1:E:177:TYR:O	1:E:179:ARG:HG2	2.15	0.46
1:C:110:LYS:HE2	1:C:111:LYS:H	1.80	0.46
1:D:130:ILE:CG1	1:D:134:GLY:HA3	2.45	0.46
1:E:231:LYS:HE3	1:E:275:LEU:HB2	1.98	0.46
1:G:51:LEU:HB2	1:G:100:TYR:CE2	2.50	0.46
1:E:221:ARG:NH2	1:E:253:ASP:O	2.49	0.46
1:E:241:PRO:HG2	1:E:242:HIS:HD2	1.78	0.46
1:G:144:THR:OG1	1:G:148:ILE:HG12	2.16	0.46
1:G:150:CYS:O	1:G:176:ASN:HB3	2.16	0.46
1:A:208:SER:HB3	1:A:224:MET:HE3	1.97	0.46
1:E:49:THR:HG22	1:E:50:THR:H	1.81	0.46
1:H:127:ARG:NH2	1:H:225:ASP:OD1	2.48	0.46
1:B:205:PRO:HD3	1:C:214:THR:HG21	1.97	0.46
1:B:247:LEU:HD12	1:B:250:ARG:HE	1.81	0.46
1:A:263:ASN:HB2	1:A:270:PRO:HA	1.97	0.45
1:D:105:MET:HE2	1:D:126:ILE:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:LYS:HD2	1:D:61:LYS:HA	1.75	0.45
1:G:101:PRO:HG2	1:G:102:PHE:HD2	1.80	0.45
1:D:172:ASP:O	1:D:179:ARG:HD2	2.16	0.45
1:F:65:VAL:HG21	1:F:71:CYS:SG	2.55	0.45
1:G:192:THR:OG1	1:G:197:VAL:O	2.32	0.45
1:G:237:ASP:HB3	1:G:248:PRO:HG2	1.99	0.45
1:G:247:LEU:HB3	1:G:249:GLU:OE1	2.17	0.45
1:A:156:MET:HE1	1:A:161:HIS:O	2.17	0.45
1:C:172:ASP:OD2	1:C:179:ARG:NH1	2.49	0.45
1:D:267:LYS:HE3	1:D:281:TRP:CH2	2.52	0.45
1:A:172:ASP:O	1:A:179:ARG:HD2	2.16	0.45
1:D:125:TYR:CZ	1:D:138:LYS:HD2	2.51	0.45
1:E:77:ARG:NH2	1:E:79:ARG:HG3	2.32	0.45
1:F:140:THR:HA	1:F:177:TYR:CD1	2.52	0.45
1:A:210:VAL:HG13	1:A:211:GLU:H	1.81	0.45
1:B:65:VAL:O	1:B:95:LYS:HB3	2.16	0.45
1:H:231:LYS:HZ1	1:H:275:LEU:HB2	1.82	0.45
1:H:68:ALA:HB2	1:H:90:PHE:CD2	2.52	0.45
1:H:247:LEU:HD22	1:H:250:ARG:NE	2.32	0.45
1:D:122:ASN:OD1	1:D:124:ASP:HB2	2.17	0.45
1:F:242:HIS:NE2	1:F:277:PRO:HA	2.32	0.45
1:G:137:TYR:CZ	1:G:139:GLY:HA3	2.52	0.45
1:F:90:PHE:CG	1:F:91:ASP:N	2.84	0.45
1:F:227:THR:O	1:F:230:GLY:N	2.50	0.45
1:H:65:VAL:O	1:H:95:LYS:HB3	2.17	0.45
1:B:151:GLN:OE1	1:B:158:PRO:HD2	2.18	0.44
1:C:66:ASN:O	1:C:95:LYS:HG3	2.17	0.44
1:B:235:ARG:HB2	1:B:237:ASP:OD1	2.17	0.44
1:G:145:LYS:HE3	1:G:203:ASP:OD1	2.17	0.44
1:B:236:TRP:CD1	1:B:236:TRP:H	2.35	0.44
1:C:192:THR:CG2	1:C:194:ASN:H	2.28	0.44
1:D:148:ILE:HG21	1:D:192:THR:HG23	1.99	0.44
1:E:177:TYR:HB3	1:E:179:ARG:NH2	2.32	0.44
1:F:133:LYS:HG2	1:F:185:GLU:HA	1.99	0.44
1:A:51:LEU:HD23	1:A:51:LEU:HA	1.81	0.44
1:A:256:PHE:CZ	1:A:264:PRO:HG3	2.53	0.44
1:G:137:TYR:CE1	1:G:139:GLY:HA3	2.53	0.44
1:F:89:VAL:HG23	1:F:100:TYR:HE2	1.82	0.44
1:G:174:GLN:NE2	3:G:1002:SO4:O1	2.51	0.44
1:F:51:LEU:HD12	1:F:51:LEU:HA	1.83	0.44
1:H:245:LYS:HE3	1:H:246:PHE:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:LYS:HG2	1:C:54:GLU:H	1.82	0.44
1:E:239:GLN:HE21	1:E:247:LEU:HD11	1.81	0.44
1:H:170:GLY:N	3:H:1002:SO4:O3	2.44	0.44
1:D:247:LEU:HD13	1:D:247:LEU:HA	1.65	0.44
1:B:246:PHE:HB3	1:B:256:PHE:CE1	2.53	0.43
1:C:61:LYS:HZ1	1:C:63:LYS:HE3	1.82	0.43
1:F:249:GLU:H	1:F:249:GLU:CD	2.25	0.43
1:A:256:PHE:HZ	1:A:264:PRO:HG3	1.83	0.43
1:B:204:ILE:HA	1:B:205:PRO:HD3	1.74	0.43
1:D:164:LEU:HD13	1:D:164:LEU:HA	1.82	0.43
1:D:242:HIS:CE1	1:D:280:PRO:HA	2.53	0.43
1:F:237:ASP:OD1	1:F:237:ASP:N	2.51	0.43
1:G:194:ASN:HB3	1:G:197:VAL:HG13	2.00	0.43
1:C:281:TRP:HZ3	1:C:283:TYR:CE2	2.36	0.43
1:E:173:LEU:HD23	1:E:179:ARG:HG3	2.00	0.43
1:G:145:LYS:HG2	1:G:203:ASP:HB2	2.00	0.43
1:B:89:VAL:HG23	1:B:100:TYR:HE2	1.83	0.43
1:G:51:LEU:HA	1:G:51:LEU:HD23	1.71	0.43
1:G:63:LYS:HE2	1:G:63:LYS:HB3	1.84	0.43
1:D:53:LYS:HG3	1:D:109:VAL:HG12	2.01	0.43
1:D:235:ARG:NH1	1:D:237:ASP:OD2	2.52	0.43
1:A:73:ASN:O	1:A:77:ARG:HG2	2.18	0.43
1:C:258:ASP:HB2	1:C:260:TYR:CE2	2.54	0.43
1:D:133:LYS:HD2	1:D:135:GLY:H	1.83	0.43
1:B:133:LYS:NZ	1:B:135:GLY:HA3	2.34	0.43
1:B:149:LYS:HG3	1:B:150:CYS:N	2.34	0.43
1:C:91:ASP:OD1	1:C:116:GLU:HB2	2.17	0.43
1:D:81:PHE:CG	1:D:83:PHE:HE2	2.37	0.43
1:F:90:PHE:HZ	1:F:95:LYS:HZ2	1.62	0.43
1:F:177:TYR:HB2	1:F:179:ARG:NH1	2.33	0.43
1:H:198:ARG:HG2	1:H:199:TYR:CD1	2.50	0.43
1:H:231:LYS:NZ	1:H:275:LEU:HB2	2.34	0.43
1:C:58:LEU:CG	1:C:59:LYS:H	2.32	0.43
1:C:110:LYS:CE	1:C:111:LYS:H	2.32	0.43
1:C:244:HIS:HE1	1:C:246:PHE:O	2.02	0.43
1:D:62:THR:HB	1:D:98:TYR:CD1	2.54	0.43
1:G:62:THR:OG1	1:G:96:ARG:HG2	2.19	0.43
1:A:51:LEU:HB2	1:A:100:TYR:CE2	2.53	0.42
1:D:81:PHE:HZ	1:D:99:TRP:CD2	2.36	0.42
1:E:192:THR:HG22	1:E:194:ASN:N	2.33	0.42
1:F:267:LYS:HD2	1:F:271:TRP:NE1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:235:ARG:NH2	1:G:258:ASP:HA	2.34	0.42
1:B:241:PRO:HG2	1:B:242:HIS:ND1	2.35	0.42
1:G:63:LYS:C	1:G:96:ARG:HG3	2.43	0.42
1:G:224:MET:HE3	1:G:224:MET:HA	2.01	0.42
1:E:198:ARG:NH1	2:E:1001:EPE:O1S	2.48	0.42
1:G:172:ASP:HB3	1:G:179:ARG:HE	1.84	0.42
1:G:237:ASP:O	1:G:238:GLN:HG2	2.20	0.42
1:D:55:ASP:OD1	1:D:56:PRO:HD2	2.20	0.42
1:A:267:LYS:HE2	1:A:271:TRP:CE2	2.55	0.42
1:B:267:LYS:HE2	1:B:271:TRP:CE2	2.54	0.42
1:B:146:SER:HB3	1:B:200:GLU:OE1	2.19	0.42
1:B:263:ASN:HB2	1:B:270:PRO:HA	2.02	0.42
1:C:58:LEU:HG	1:C:59:LYS:H	1.84	0.42
1:C:70:GLU:HA	1:C:73:ASN:HB2	2.02	0.42
1:E:63:LYS:HG2	1:E:64:LYS:O	2.19	0.42
1:E:63:LYS:NZ	1:E:74:ARG:HH12	2.18	0.42
1:E:144:THR:HB	1:E:200:GLU:OE1	2.19	0.42
1:F:137:TYR:CZ	1:F:139:GLY:HA3	2.54	0.42
1:D:247:LEU:HA	1:D:248:PRO:HD3	1.90	0.42
1:E:64:LYS:HE3	1:E:94:ARG:O	2.19	0.42
1:B:242:HIS:HE1	1:B:276:ASP:O	2.02	0.42
1:F:152:PRO:HA	1:F:175:GLU:O	2.20	0.42
1:G:46:SER:N	1:G:119:LEU:O	2.42	0.42
1:A:133:LYS:O	1:A:187:GLY:HA2	2.20	0.41
1:A:206:GLN:O	1:A:209:GLU:HG3	2.20	0.41
1:B:130:ILE:HD13	1:B:130:ILE:HG21	1.88	0.41
1:B:148:ILE:HG21	1:B:192:THR:HG23	2.02	0.41
1:C:48:LYS:HE3	1:C:115:HIS:HD1	1.85	0.41
1:E:105:MET:HE2	1:E:105:MET:HB2	1.77	0.41
1:H:74:ARG:HG2	1:H:99:TRP:CZ2	2.55	0.41
1:C:73:ASN:O	1:C:77:ARG:HG2	2.20	0.41
1:D:83:PHE:CD1	1:D:101:PRO:HB3	2.54	0.41
1:F:268:PRO:HD2	1:F:283:TYR:HH	1.84	0.41
2:A:1001:EPE:S	1:E:162:SER:OG	2.73	0.41
1:C:91:ASP:OD2	1:C:94:ARG:NH1	2.54	0.41
1:C:244:HIS:HB2	1:C:273:TYR:CZ	2.55	0.41
1:D:164:LEU:HA	1:D:165:PRO:HD3	1.84	0.41
1:E:171:LYS:HE2	1:E:181:PRO:HA	2.02	0.41
2:G:1001:EPE:H82	2:G:1001:EPE:H52	1.89	0.41
1:H:48:LYS:O	1:H:113:PHE:HA	2.20	0.41
1:B:265:ASP:OD2	1:B:267:LYS:NZ	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:THR:HA	1:C:112:GLY:O	2.20	0.41
1:D:220:TYR:CE1	1:D:286:ILE:HD13	2.56	0.41
1:G:177:TYR:HB3	1:G:179:ARG:NH1	2.35	0.41
1:H:152:PRO:HA	1:H:175:GLU:O	2.19	0.41
1:A:234:GLN:HB2	1:A:275:LEU:HD23	2.01	0.41
1:C:179:ARG:C	1:C:181:PRO:HD3	2.46	0.41
1:D:258:ASP:HB2	1:D:260:TYR:CE2	2.55	0.41
1:E:220:TYR:CZ	1:E:222:GLY:HA3	2.55	0.41
1:C:177:TYR:HB3	1:C:179:ARG:NH2	2.35	0.41
1:C:231:LYS:HZ3	1:C:275:LEU:CD2	2.29	0.41
1:F:91:ASP:HB2	1:F:117:PHE:CE1	2.55	0.41
1:E:64:LYS:HA	1:E:95:LYS:O	2.20	0.41
1:H:102:PHE:HB2	1:H:106:SER:CB	2.51	0.41
1:A:148:ILE:HG21	1:A:192:THR:CG2	2.49	0.41
2:A:1001:EPE:O1S	1:E:162:SER:OG	2.39	0.41
1:C:102:PHE:HB2	1:C:106:SER:CB	2.50	0.41
1:D:130:ILE:HD11	1:D:188:PRO:HD3	2.03	0.41
1:E:231:LYS:HD2	1:E:231:LYS:HA	1.90	0.41
1:F:45:LYS:HE2	1:F:47:ALA:HB2	2.03	0.41
1:F:175:GLU:HB2	1:F:177:TYR:CE2	2.56	0.41
1:G:51:LEU:HB2	1:G:100:TYR:HE2	1.84	0.41
1:C:63:LYS:C	1:C:64:LYS:HD3	2.46	0.41
1:E:130:ILE:HD13	1:E:204:ILE:CG2	2.51	0.41
1:F:216:ASN:HD21	1:F:218:GLU:HG3	1.83	0.41
1:G:55:ASP:OD1	1:G:57:LEU:HG	2.20	0.40
1:G:175:GLU:HB3	1:G:176:ASN:H	1.61	0.40
1:H:83:PHE:CD1	1:H:101:PRO:HB3	2.55	0.40
1:D:221:ARG:HD3	1:D:255:GLY:HA3	2.03	0.40
1:B:66:ASN:OD1	1:B:66:ASN:N	2.53	0.40
1:D:50:THR:O	1:D:51:LEU:HD23	2.21	0.40
1:D:130:ILE:HG12	1:D:134:GLY:HA3	2.03	0.40
1:E:251:TYR:N	1:E:252:PRO:HD3	2.36	0.40
1:A:214:THR:HG21	1:F:205:PRO:HD3	2.04	0.40
1:A:258:ASP:HB2	1:A:260:TYR:CE2	2.56	0.40
1:H:130:ILE:HD11	1:H:134:GLY:HA3	2.02	0.40
1:C:180:ASN:HD21	1:C:184:GLU:N	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	252/262 (96%)	224 (89%)	22 (9%)	6 (2%)	4	18
1	B	252/262 (96%)	227 (90%)	21 (8%)	4 (2%)	7	26
1	C	252/262 (96%)	223 (88%)	25 (10%)	4 (2%)	7	26
1	D	252/262 (96%)	223 (88%)	24 (10%)	5 (2%)	6	21
1	E	252/262 (96%)	223 (88%)	27 (11%)	2 (1%)	16	42
1	F	252/262 (96%)	222 (88%)	24 (10%)	6 (2%)	4	18
1	G	240/262 (92%)	210 (88%)	26 (11%)	4 (2%)	7	25
1	H	242/262 (92%)	225 (93%)	12 (5%)	5 (2%)	5	21
All	All	1994/2096 (95%)	1777 (89%)	181 (9%)	36 (2%)	6	24

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	B	58	LEU
1	C	57	LEU
1	C	66	ASN
1	C	241	PRO
1	F	93	SER
1	F	95	LYS
1	A	56	PRO
1	E	107	SER
1	E	280	PRO
1	F	94	ARG
1	F	166	SER
1	G	58	LEU
1	H	280	PRO
1	A	53	LYS
1	A	54	GLU
1	A	58	LEU

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Mol	Chain	Res	Type
1	A	108	GLY
1	B	56	PRO
1	B	57	LEU
1	D	58	LEU
1	D	128	ASN
1	F	167	SER
1	C	56	PRO
1	D	57	LEU
1	D	127	ARG
1	F	58	LEU
1	G	135	GLY
1	B	280	PRO
1	G	280	PRO
1	H	80	GLY
1	H	107	SER
1	D	280	PRO
1	G	109	VAL
1	H	108	GLY
1	H	109	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	229/235 (97%)	204 (89%)	25 (11%)	6	21
1	B	229/235 (97%)	200 (87%)	29 (13%)	4	16
1	C	229/235 (97%)	196 (86%)	33 (14%)	3	12
1	D	229/235 (97%)	200 (87%)	29 (13%)	4	16
1	E	229/235 (97%)	201 (88%)	28 (12%)	5	17
1	F	229/235 (97%)	200 (87%)	29 (13%)	4	16
1	G	222/235 (94%)	198 (89%)	24 (11%)	6	22
1	H	221/235 (94%)	203 (92%)	18 (8%)	11	33
All	All	1817/1880 (97%)	1602 (88%)	215 (12%)	5	18

All (215) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	THR
1	A	46	SER
1	A	50	THR
1	A	52	THR
1	A	54	GLU
1	A	55	ASP
1	A	57	LEU
1	A	58	LEU
1	A	62	THR
1	A	65	VAL
1	A	66	ASN
1	A	109	VAL
1	A	133	LYS
1	A	166	SER
1	A	167	SER
1	A	179	ARG
1	A	209	GLU
1	A	210	VAL
1	A	213	MET
1	A	214	THR
1	A	221	ARG
1	A	234	GLN
1	A	245	LYS
1	A	247	LEU
1	A	253	ASP
1	B	39	THR
1	B	44	LYS
1	B	46	SER
1	B	52	THR
1	B	54	GLU
1	B	55	ASP
1	B	57	LEU
1	B	62	THR
1	B	65	VAL
1	B	66	ASN
1	B	109	VAL
1	B	111	LYS
1	B	115	HIS
1	B	127	ARG
1	B	128	ASN
1	B	130	ILE
1	B	143	ILE

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Mol	Chain	Res	Type
1	B	148	ILE
1	B	164	LEU
1	B	169	ARG
1	B	192	THR
1	B	196	GLU
1	B	198	ARG
1	B	208	SER
1	B	213	MET
1	B	219	SER
1	B	221	ARG
1	B	240	THR
1	B	253	ASP
1	C	37	ARG
1	C	39	THR
1	C	46	SER
1	C	50	THR
1	C	51	LEU
1	C	52	THR
1	C	58	LEU
1	C	60	ILE
1	C	62	THR
1	C	65	VAL
1	C	69	ASP
1	C	73	ASN
1	C	76	ILE
1	C	82	THR
1	C	84	THR
1	C	91	ASP
1	C	96	ARG
1	C	97	CYS
1	C	109	VAL
1	C	110	LYS
1	C	113	PHE
1	C	115	HIS
1	C	127	ARG
1	C	128	ASN
1	C	130	ILE
1	C	142	SER
1	C	143	ILE
1	C	160	GLU
1	C	164	LEU
1	C	166	SER

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Mol	Chain	Res	Type
1	C	201	VAL
1	C	240	THR
1	C	257	ASP
1	D	54	GLU
1	D	57	LEU
1	D	59	LYS
1	D	62	THR
1	D	65	VAL
1	D	66	ASN
1	D	79	ARG
1	D	82	THR
1	D	83	PHE
1	D	106	SER
1	D	115	HIS
1	D	116	GLU
1	D	126	ILE
1	D	128	ASN
1	D	130	ILE
1	D	133	LYS
1	D	148	ILE
1	D	164	LEU
1	D	169	ARG
1	D	179	ARG
1	D	196	GLU
1	D	209	GLU
1	D	221	ARG
1	D	235	ARG
1	D	240	THR
1	D	245	LYS
1	D	253	ASP
1	D	278	ASP
1	D	288	THR
1	E	38	ASN
1	E	49	THR
1	E	51	LEU
1	E	58	LEU
1	E	65	VAL
1	E	69	ASP
1	E	89	VAL
1	E	95	LYS
1	E	97	CYS
1	E	105	MET

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Mol	Chain	Res	Type
1	E	106	SER
1	E	107	SER
1	E	113	PHE
1	E	115	HIS
1	E	127	ARG
1	E	128	ASN
1	E	130	ILE
1	E	162	SER
1	E	169	ARG
1	E	192	THR
1	E	213	MET
1	E	232	THR
1	E	234	GLN
1	E	240	THR
1	E	243	ARG
1	E	254	LYS
1	E	257	ASP
1	E	267	LYS
1	F	39	THR
1	F	48	LYS
1	F	51	LEU
1	F	57	LEU
1	F	58	LEU
1	F	59	LYS
1	F	60	ILE
1	F	62	THR
1	F	65	VAL
1	F	84	THR
1	F	96	ARG
1	F	97	CYS
1	F	107	SER
1	F	109	VAL
1	F	113	PHE
1	F	116	GLU
1	F	127	ARG
1	F	128	ASN
1	F	130	ILE
1	F	133	LYS
1	F	136	SER
1	F	142	SER
1	F	166	SER
1	F	192	THR

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Mol	Chain	Res	Type
1	F	193	SER
1	F	196	GLU
1	F	231	LYS
1	F	240	THR
1	F	275	LEU
1	G	39	THR
1	G	50	THR
1	G	57	LEU
1	G	59	LYS
1	G	60	ILE
1	G	62	THR
1	G	83	PHE
1	G	109	VAL
1	G	128	ASN
1	G	131	ILE
1	G	143	ILE
1	G	148	ILE
1	G	167	SER
1	G	176	ASN
1	G	192	THR
1	G	197	VAL
1	G	198	ARG
1	G	201	VAL
1	G	213	MET
1	G	221	ARG
1	G	237	ASP
1	G	238	GLN
1	G	240	THR
1	G	253	ASP
1	H	46	SER
1	H	52	THR
1	H	60	ILE
1	H	62	THR
1	H	65	VAL
1	H	76	ILE
1	H	91	ASP
1	H	102	PHE
1	H	106	SER
1	H	109	VAL
1	H	128	ASN
1	H	130	ILE
1	H	131	ILE

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Mol	Chain	Res	Type
1	H	164	LEU
1	H	166	SER
1	H	221	ARG
1	H	240	THR
1	H	269	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	GLN
1	A	238	GLN
1	B	128	ASN
1	C	41	HIS
1	C	128	ASN
1	E	242	HIS
1	F	226	HIS
1	G	154	ASN
1	H	41	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](#)

25 ligands 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
3	SO4	C	1003	-	4,4,4	0.29	0	6,6,6	0.18	0
3	SO4	F	1004	-	4,4,4	0.23	0	6,6,6	0.12	0
3	SO4	D	1003	-	4,4,4	0.27	0	6,6,6	0.15	0
2	EPE	E	1001	-	15,15,15	0.90	1 (6%)	19,20,20	1.82	6 (31%)
3	SO4	F	1002	-	4,4,4	0.30	0	6,6,6	0.15	0
2	EPE	C	1001	-	15,15,15	0.78	0	19,20,20	1.99	6 (31%)
3	SO4	G	1002	-	4,4,4	0.26	0	6,6,6	0.13	0
2	EPE	F	1001	-	15,15,15	0.76	1 (6%)	19,20,20	2.00	5 (26%)
3	SO4	H	1002	-	4,4,4	0.32	0	6,6,6	0.29	0
2	EPE	B	1005	-	15,15,15	0.89	1 (6%)	19,20,20	1.85	5 (26%)
3	SO4	F	1003	-	4,4,4	0.26	0	6,6,6	0.08	0
3	SO4	A	1003	-	4,4,4	0.27	0	6,6,6	0.17	0
3	SO4	G	1003	-	4,4,4	0.26	0	6,6,6	0.06	0
2	EPE	H	1001	-	15,15,15	0.85	1 (6%)	19,20,20	2.18	6 (31%)
2	EPE	A	1001	-	15,15,15	0.96	1 (6%)	19,20,20	2.46	10 (52%)
3	SO4	B	1004	-	4,4,4	0.25	0	6,6,6	0.20	0
2	EPE	C	1002	-	15,15,15	0.78	1 (6%)	19,20,20	2.18	6 (31%)
3	SO4	B	1002	-	4,4,4	0.29	0	6,6,6	0.08	0
2	EPE	B	1001	-	15,15,15	0.94	2 (13%)	19,20,20	2.08	9 (47%)
3	SO4	D	1004	-	4,4,4	0.24	0	6,6,6	0.10	0
2	EPE	G	1001	-	15,15,15	0.82	1 (6%)	19,20,20	1.82	6 (31%)
3	SO4	B	1003	-	4,4,4	0.29	0	6,6,6	0.32	0
2	EPE	D	1001	-	15,15,15	0.73	1 (6%)	19,20,20	1.81	5 (26%)
3	SO4	D	1002	-	4,4,4	0.25	0	6,6,6	0.10	0
3	SO4	A	1002	-	4,4,4	0.30	0	6,6,6	0.28	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EPE	E	1001	-	-	4/9/19/19	0/1/1/1
2	EPE	G	1001	-	-	5/9/19/19	0/1/1/1
2	EPE	H	1001	-	-	2/9/19/19	0/1/1/1
2	EPE	A	1001	-	-	5/9/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EPE	C	1001	-	-	3/9/19/19	0/1/1/1
2	EPE	C	1002	-	-	2/9/19/19	0/1/1/1
2	EPE	D	1001	-	-	4/9/19/19	0/1/1/1
2	EPE	F	1001	-	-	5/9/19/19	0/1/1/1
2	EPE	B	1001	-	-	3/9/19/19	0/1/1/1
2	EPE	B	1005	-	-	0/9/19/19	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1005	EPE	C10-S	2.99	1.81	1.77
2	A	1001	EPE	C10-S	2.98	1.81	1.77
2	E	1001	EPE	C10-S	2.71	1.81	1.77
2	H	1001	EPE	C10-S	2.56	1.81	1.77
2	G	1001	EPE	C10-S	2.56	1.81	1.77
2	C	1002	EPE	C10-S	2.45	1.81	1.77
2	F	1001	EPE	C10-S	2.39	1.80	1.77
2	D	1001	EPE	C10-S	2.38	1.80	1.77
2	B	1001	EPE	C10-S	2.21	1.80	1.77
2	B	1001	EPE	C7-N4	-2.01	1.42	1.47

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1002	EPE	C5-N4-C3	6.65	123.17	108.84
2	H	1001	EPE	C5-N4-C3	4.97	119.56	108.84
2	H	1001	EPE	O2S-S-C10	4.91	114.15	106.73
2	F	1001	EPE	C5-N4-C3	4.89	119.37	108.84
2	A	1001	EPE	C5-C6-N1	-4.61	101.34	110.65
2	B	1005	EPE	C5-N4-C3	4.56	118.65	108.84
2	G	1001	EPE	C5-N4-C3	4.47	118.47	108.84
2	A	1001	EPE	C5-N4-C3	4.33	118.17	108.84
2	C	1001	EPE	C5-C6-N1	-4.11	102.36	110.65
2	D	1001	EPE	O3S-S-C10	4.07	113.96	106.00
2	A	1001	EPE	C9-N1-C2	3.80	121.36	111.24
2	E	1001	EPE	C5-N4-C3	3.73	116.87	108.84
2	C	1002	EPE	C5-C6-N1	-3.59	103.40	110.65
2	D	1001	EPE	C5-N4-C3	3.58	116.55	108.84
2	A	1001	EPE	C9-N1-C6	3.56	120.72	111.24
2	H	1001	EPE	C7-N4-C5	3.52	120.62	111.24
2	B	1001	EPE	C7-N4-C3	3.49	120.53	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1001	EPE	C5-N4-C3	3.47	116.31	108.84
2	F	1001	EPE	O2S-S-C10	3.38	111.84	106.73
2	E	1001	EPE	O2S-S-C10	3.35	111.78	106.73
2	B	1005	EPE	O2S-S-C10	3.30	111.72	106.73
2	E	1001	EPE	C7-N4-C3	3.28	119.99	111.24
2	B	1001	EPE	O3S-S-C10	3.27	112.41	106.00
2	B	1001	EPE	C5-N4-C3	3.27	115.88	108.84
2	H	1001	EPE	C7-N4-C3	3.16	119.65	111.24
2	C	1001	EPE	C7-N4-C3	3.08	119.43	111.24
2	A	1001	EPE	C7-N4-C3	2.88	118.92	111.24
2	B	1005	EPE	C7-N4-C5	2.87	118.89	111.24
2	G	1001	EPE	C7-N4-C5	2.82	118.76	111.24
2	C	1001	EPE	O1S-S-C10	2.78	110.94	106.73
2	A	1001	EPE	O3S-S-C10	2.78	111.45	106.00
2	A	1001	EPE	O2S-S-C10	2.78	110.92	106.73
2	C	1002	EPE	C7-N4-C3	2.76	118.60	111.24
2	D	1001	EPE	C7-N4-C3	2.74	118.54	111.24
2	H	1001	EPE	C6-N1-C2	2.72	114.70	108.84
2	A	1001	EPE	C7-N4-C5	2.71	118.47	111.24
2	G	1001	EPE	C3-C2-N1	-2.70	105.21	110.65
2	C	1002	EPE	C2-C3-N4	2.66	116.01	110.65
2	F	1001	EPE	C7-N4-C5	2.65	118.30	111.24
2	C	1001	EPE	C3-C2-N1	-2.61	105.39	110.65
2	G	1001	EPE	O1S-S-C10	2.60	110.65	106.73
2	B	1005	EPE	O1S-S-C10	2.58	110.62	106.73
2	B	1001	EPE	C2-C3-N4	-2.53	105.54	110.65
2	C	1002	EPE	O3S-S-C10	2.53	110.95	106.00
2	E	1001	EPE	C6-N1-C2	2.52	114.26	108.84
2	F	1001	EPE	C6-N1-C2	2.48	114.18	108.84
2	E	1001	EPE	O1S-S-C10	2.48	110.47	106.73
2	B	1001	EPE	C8-C7-N4	-2.45	104.86	113.44
2	H	1001	EPE	C3-C2-N1	-2.39	105.84	110.65
2	B	1001	EPE	C3-C2-N1	-2.37	105.86	110.65
2	B	1001	EPE	O1S-S-C10	2.33	110.24	106.73
2	E	1001	EPE	O2S-S-O1S	-2.31	106.29	113.82
2	G	1001	EPE	C7-N4-C3	2.31	117.40	111.24
2	D	1001	EPE	C3-C2-N1	-2.30	106.02	110.65
2	B	1001	EPE	C6-C5-N4	-2.29	106.04	110.65
2	A	1001	EPE	O2S-S-O1S	-2.26	106.46	113.82
2	C	1002	EPE	C7-N4-C5	2.23	117.18	111.24
2	B	1005	EPE	C7-N4-C3	2.20	117.11	111.24
2	B	1001	EPE	C7-N4-C5	2.18	117.06	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1001	EPE	C7-N4-C5	2.13	116.92	111.24
2	A	1001	EPE	O1S-S-C10	2.13	109.94	106.73
2	C	1001	EPE	C7-N4-C5	2.13	116.91	111.24
2	F	1001	EPE	C7-N4-C3	2.10	116.82	111.24
2	G	1001	EPE	O2S-S-C10	2.08	109.87	106.73

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	EPE	C9-C10-S-O2S
2	A	1001	EPE	C9-C10-S-O3S
2	B	1001	EPE	C9-C10-S-O2S
2	B	1001	EPE	C9-C10-S-O3S
2	C	1002	EPE	C10-C9-N1-C2
2	D	1001	EPE	C9-C10-S-O2S
2	D	1001	EPE	C9-C10-S-O3S
2	E	1001	EPE	C9-C10-S-O2S
2	F	1001	EPE	C8-C7-N4-C5
2	G	1001	EPE	C8-C7-N4-C5
2	G	1001	EPE	C9-C10-S-O2S
2	G	1001	EPE	C9-C10-S-O3S
2	D	1001	EPE	N4-C7-C8-O8
2	E	1001	EPE	N4-C7-C8-O8
2	F	1001	EPE	C9-C10-S-O3S
2	E	1001	EPE	C9-C10-S-O3S
2	A	1001	EPE	C9-C10-S-O1S
2	B	1001	EPE	C9-C10-S-O1S
2	C	1001	EPE	C9-C10-S-O1S
2	D	1001	EPE	C9-C10-S-O1S
2	E	1001	EPE	C9-C10-S-O1S
2	F	1001	EPE	C9-C10-S-O1S
2	F	1001	EPE	C9-C10-S-O2S
2	G	1001	EPE	C9-C10-S-O1S
2	A	1001	EPE	N4-C7-C8-O8
2	G	1001	EPE	N4-C7-C8-O8
2	A	1001	EPE	C8-C7-N4-C3
2	C	1001	EPE	C9-C10-S-O3S
2	C	1001	EPE	C9-C10-S-O2S
2	C	1002	EPE	C8-C7-N4-C5
2	H	1001	EPE	C8-C7-N4-C5
2	F	1001	EPE	C8-C7-N4-C3

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Mol	Chain	Res	Type	Atoms
2	H	1001	EPE	C8-C7-N4-C3

There are no ring outliers.

11 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1004	SO4	1	0
2	E	1001	EPE	1	0
2	C	1001	EPE	2	0
3	G	1002	SO4	1	0
3	H	1002	SO4	1	0
2	B	1005	EPE	1	0
2	A	1001	EPE	2	0
2	C	1002	EPE	1	0
2	G	1001	EPE	2	0
2	D	1001	EPE	1	0
3	D	1002	SO4	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 [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	254/262 (96%)	-0.73	0 100 100	15, 37, 91, 136	0
1	B	254/262 (96%)	-0.71	0 100 100	16, 36, 92, 149	0
1	C	254/262 (96%)	-0.64	0 100 100	14, 44, 98, 135	0
1	D	254/262 (96%)	-0.67	0 100 100	24, 52, 107, 152	0
1	E	254/262 (96%)	-0.54	0 100 100	23, 62, 112, 133	0
1	F	254/262 (96%)	-0.55	0 100 100	16, 54, 105, 133	0
1	G	246/262 (93%)	-0.40	0 100 100	37, 71, 120, 137	0
1	H	246/262 (93%)	-0.55	0 100 100	32, 64, 106, 129	0
All	All	2016/2096 (96%)	-0.60	0 100 100	14, 54, 108, 152	0

There are no RSRZ outliers to report.

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
3	SO4	D	1002	5/5	0.51	0.09	204,204,205,207	0
3	SO4	F	1002	5/5	0.66	0.13	157,157,158,160	0
3	SO4	F	1004	5/5	0.67	0.14	156,159,159,160	0
3	SO4	B	1002	5/5	0.82	0.08	115,116,118,118	0
3	SO4	G	1003	5/5	0.86	0.12	92,93,94,97	0
3	SO4	F	1003	5/5	0.87	0.15	140,142,143,143	0
3	SO4	G	1002	5/5	0.88	0.09	107,109,110,111	0
3	SO4	A	1002	5/5	0.88	0.13	68,70,78,85	0
3	SO4	D	1004	5/5	0.91	0.10	90,92,93,97	0
3	SO4	C	1003	5/5	0.92	0.09	81,83,86,89	0
3	SO4	H	1002	5/5	0.92	0.14	63,72,74,76	0
3	SO4	D	1003	5/5	0.93	0.07	70,76,78,80	0
3	SO4	A	1003	5/5	0.93	0.12	58,63,66,68	0
3	SO4	B	1003	5/5	0.94	0.07	57,64,74,81	0
3	SO4	B	1004	5/5	0.94	0.13	79,84,84,88	0
2	EPE	H	1001	15/15	0.95	0.08	44,56,64,65	0
2	EPE	B	1005	15/15	0.95	0.08	31,50,68,77	0
2	EPE	C	1002	15/15	0.95	0.09	29,49,64,68	0
2	EPE	D	1001	15/15	0.95	0.09	36,53,58,61	0
2	EPE	F	1001	15/15	0.96	0.07	0,18,43,48	0
2	EPE	G	1001	15/15	0.97	0.07	25,53,60,61	0
2	EPE	C	1001	15/15	0.98	0.07	4,13,29,30	0
2	EPE	B	1001	15/15	0.98	0.05	0,14,22,25	0
2	EPE	A	1001	15/15	0.98	0.06	0,9,23,28	0
2	EPE	E	1001	15/15	0.99	0.06	12,24,31,31	0

6.5 Other polymers

There are no such residues in this entry.