



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:48 AM UTC

PDB ID : 2YEP / pdb_00002yep
Title : STRUCTURE OF AN N-TERMINAL NUCLEOPHILE (NTN) HYDROLASE, OAT2, IN COMPLEX WITH GLUTAMATE
Authors : Chowdhury, R.; Iqbal, A.; Clifton, I.J.; Schofield, C.J.
Deposited on : 2011-03-29
Resolution : 2.70 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:

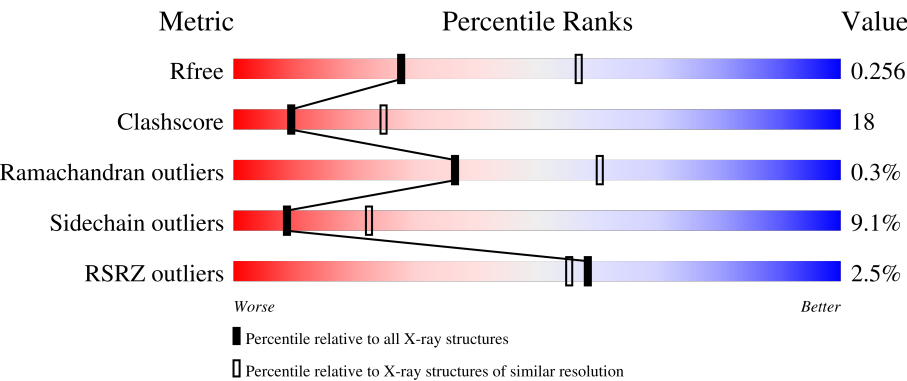
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	180	3% 56% 34% 7% .
1	C	180	% 68% 23% 5% .
1	E	180	2% 56% 36% . .
1	G	180	2% 61% 29% 7% .
2	B	213	2% 64% 31% 5%

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Mol	Chain	Length	Quality of chain
2	D	213	
2	H	213	
3	F	213	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TH5	B	181	-	-	X	-
4	GLU	B	1601	-	-	X	-
4	GLU	C	1602	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11651 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 GLUTAMATE N-ACETYLTRANSFERASE 2 ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	173	Total	C	N	O	S	0	0	0
			1266	783	234	243	6			
1	C	173	Total	C	N	O	S	0	0	0
			1266	783	234	243	6			
1	E	173	Total	C	N	O	S	0	0	0
			1266	783	234	243	6			
1	G	173	Total	C	N	O	S	0	0	0
			1266	783	234	243	6			

- Molecule 2 is a protein called GLUTAMATE N-ACETYLTRANSFERASE 2 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1605	992	279	329	5			
2	D	210	Total	C	N	O	S	0	0	0
			1579	975	276	323	5			
2	H	195	Total	C	N	O	S	0	0	0
			1471	912	253	301	5			

- Molecule 3 is a protein called GLUTAMATE N-ACETYLTRANSFERASE 2 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	197	Total	C	N	O	S	0	0	0
			1487	923	255	304	5			

- Molecule 4 is GLUTAMIC ACID (CCD ID: GLU) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			9	5	1	3		
4	C	1	Total	C	N	O	0	0
			9	5	1	3		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2^-$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			4	2	2		
5	G	1	Total	C	O	0	0
			4	2	2		

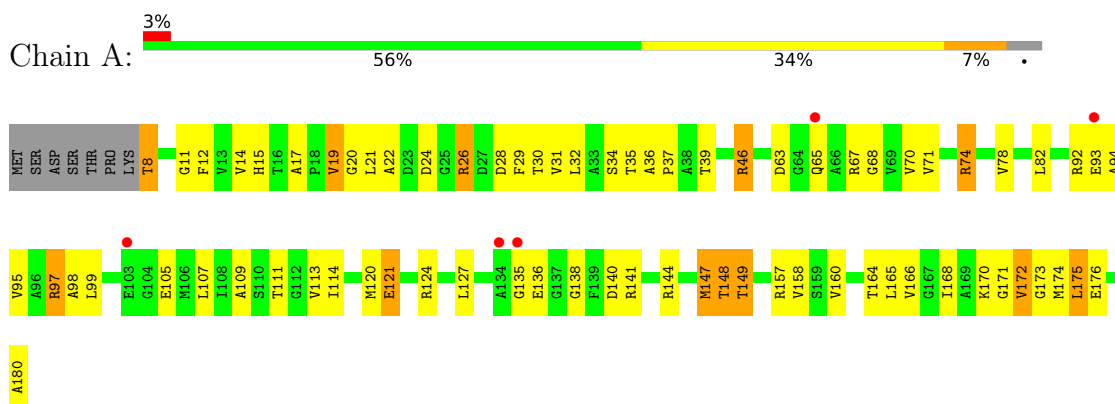
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	71	Total 71	O 71	0	0
6	B	62	Total 62	O 62	0	0
6	C	58	Total 58	O 58	0	0
6	D	55	Total 55	O 55	0	0
6	E	41	Total 41	O 41	0	0
6	F	50	Total 50	O 50	0	0
6	G	43	Total 43	O 43	0	0
6	H	39	Total 39	O 39	0	0

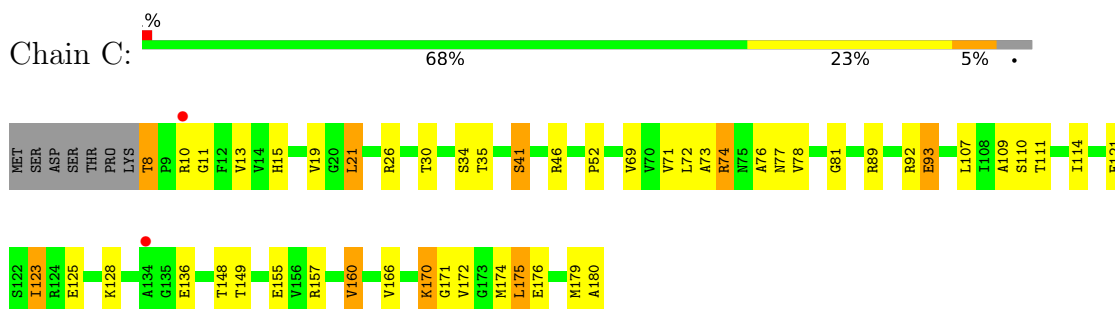
3 Residue-property plots [i](#)

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

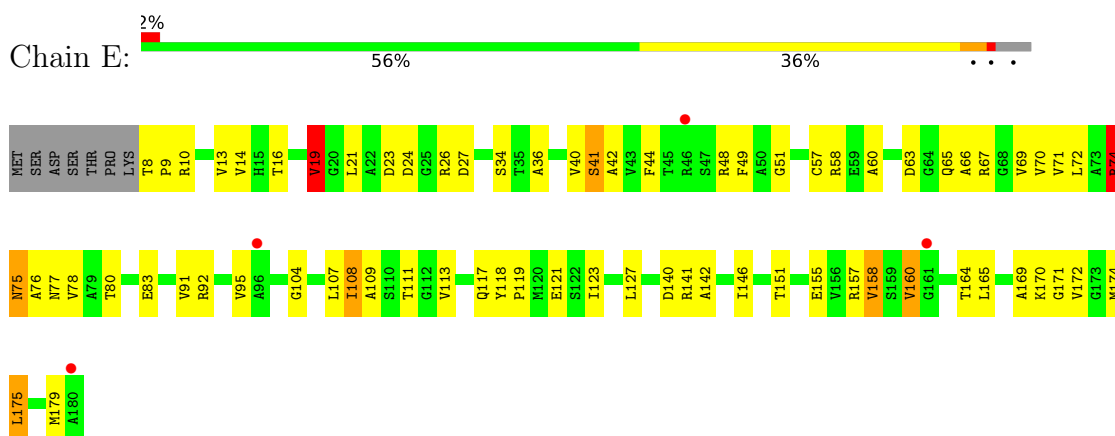
• Molecule 1: GLUTAMATE N-ACETYLTRANSFERASE 2 ALPHA CHAIN



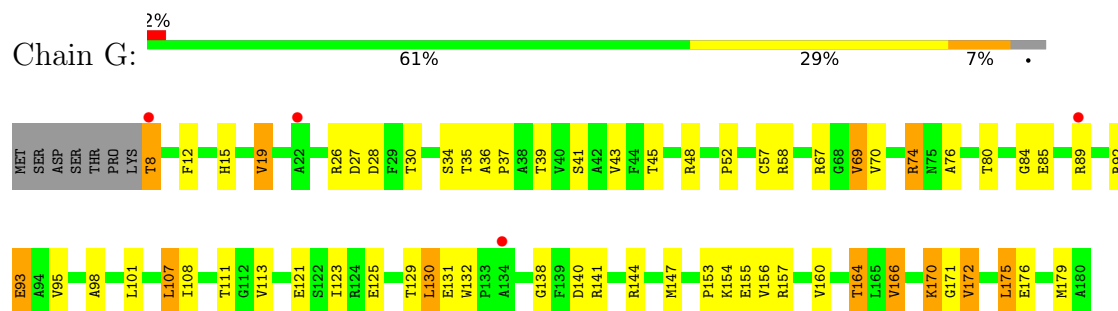
• Molecule 1: GLUTAMATE N-ACETYLTRANSFERASE 2 ALPHA CHAIN



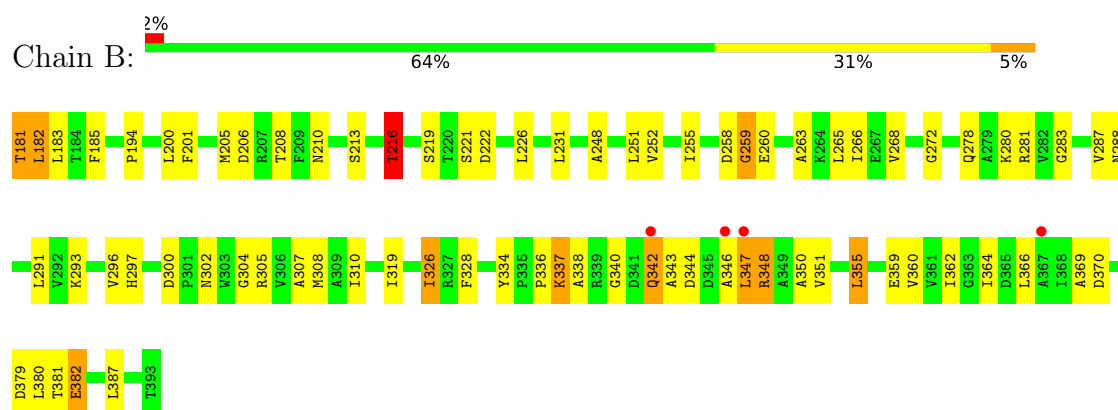
• Molecule 1: GLUTAMATE N-ACETYLTRANSFERASE 2 ALPHA CHAIN



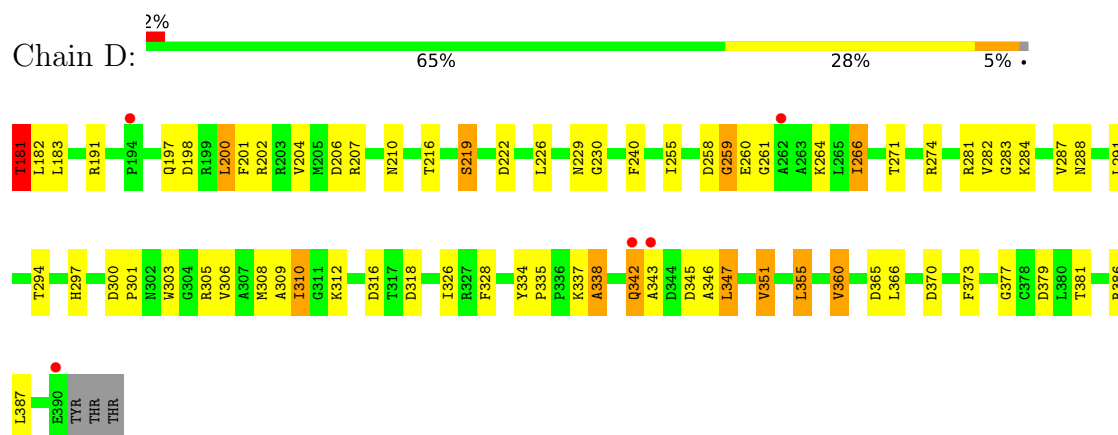
• Molecule 1: GLUTAMATE N-ACETYLTRANSFERASE 2 ALPHA CHAIN



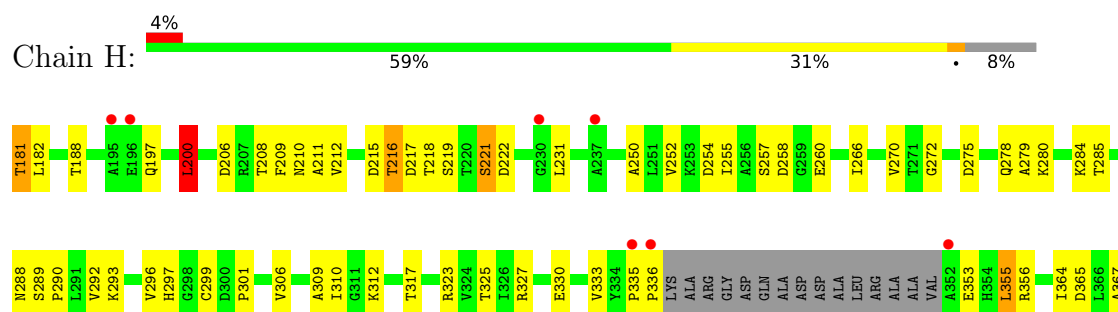
• Molecule 2: GLUTAMATE N-ACETYLTRANSFERASE 2 BETA CHAIN

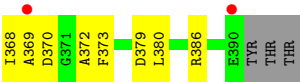


• Molecule 2: GLUTAMATE N-ACETYLTRANSFERASE 2 BETA CHAIN

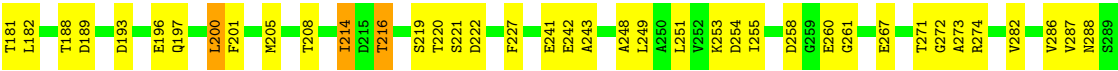


• Molecule 2: GLUTAMATE N-ACETYLTRANSFERASE 2 BETA CHAIN





● Molecule 3: GLUTAMATE N-ACETYLTRANSFERASE 2 BETA CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.22Å 73.42Å 172.33Å 90.00° 93.26° 90.00°	Depositor
Resolution (Å)	61.12 – 2.70 61.12 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.0 (61.12-2.70) 96.1 (61.12-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.65 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.236 0.214 , 0.256	Depositor DCC
R_{free} test set	2120 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	14.4	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	11651	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.72% 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: ACT, TH5

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	0.96	0/1284	1.22	7/1742 (0.4%)
1	C	0.97	0/1284	1.15	4/1742 (0.2%)
1	E	0.88	0/1284	1.13	6/1742 (0.3%)
1	G	0.91	0/1284	1.10	2/1742 (0.1%)
2	B	0.98	1/1616 (0.1%)	1.20	7/2195 (0.3%)
2	D	0.94	1/1589 (0.1%)	1.13	5/2157 (0.2%)
2	H	0.84	0/1480	1.07	3/2009 (0.1%)
3	F	0.89	0/1507	1.11	3/2047 (0.1%)
All	All	0.92	2/11328 (0.0%)	1.14	37/15376 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	216	THR	CA-CB	6.94	1.62	1.54
2	D	351	VAL	CA-CB	5.82	1.61	1.54

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	348	ARG	N-CA-C	-12.53	95.04	112.45
1	A	148	THR	N-CA-C	12.51	129.59	111.96
3	F	370	ASP	N-CA-C	11.58	126.77	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	MET	CB-CA-C	-11.48	93.03	110.26
2	B	370	ASP	N-CA-C	9.08	123.95	113.15
1	A	147	MET	N-CA-C	8.80	122.52	109.59
2	H	370	ASP	N-CA-C	8.12	122.82	113.15
1	E	160	VAL	CB-CA-C	-8.09	100.47	110.99
1	A	17	ALA	N-CA-C	7.61	114.98	108.13
1	G	76	ALA	N-CA-C	-7.55	103.02	112.90
1	C	160	VAL	CB-CA-C	-7.44	99.09	111.29
2	B	366	LEU	CB-CA-C	7.31	122.04	109.24
2	H	211	ALA	N-CA-C	6.99	120.69	112.72
2	B	308	MET	N-CA-C	-6.28	104.52	111.36
2	B	268	VAL	CB-CA-C	-6.18	103.41	111.25
1	E	74	ARG	N-CA-C	6.13	122.90	113.28
2	D	370	ASP	N-CA-C	6.06	119.72	112.93
1	C	8	THR	CA-C-N	-5.94	114.15	120.03
1	C	8	THR	C-N-CA	-5.94	114.15	120.03
3	F	361	VAL	CB-CA-C	-5.80	103.94	110.96
1	C	46	ARG	N-CA-C	-5.79	104.62	112.26
2	D	255	ILE	CB-CA-C	-5.72	104.54	112.04
2	B	382	GLU	N-CA-C	-5.69	106.50	113.50
2	D	338	ALA	CA-C-O	5.62	121.20	117.94
1	A	149	THR	N-CA-CB	5.54	118.79	110.65
1	E	160	VAL	N-CA-C	5.53	116.07	107.28
1	E	74	ARG	CB-CA-C	-5.36	102.34	110.06
2	H	200	LEU	CA-CB-CG	5.34	134.99	116.30
2	B	319	ILE	CB-CA-C	-5.31	105.56	111.35
1	E	174	MET	N-CA-C	-5.25	104.15	111.39
1	E	19	VAL	N-CA-C	-5.20	108.21	113.20
2	D	310	ILE	N-CA-C	-5.19	104.83	110.23
1	A	46	ARG	N-CA-C	-5.12	104.49	111.56
1	A	68	GLY	N-CA-C	5.08	118.16	110.75
3	F	297	HIS	N-CA-C	5.07	117.46	111.33
2	D	337	LYS	N-CA-C	5.06	117.57	111.40
1	G	130	LEU	CB-CA-C	-5.05	101.60	109.84

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	181	TH5	Mainchain

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	1266	0	1274	65	1
1	C	1266	0	1274	43	0
1	E	1266	0	1274	58	0
1	G	1266	0	1274	59	0
2	B	1605	0	1559	67	0
2	D	1579	0	1536	60	0
2	H	1471	0	1428	55	0
3	F	1487	0	1440	47	0
4	B	9	0	5	6	0
4	C	9	0	5	5	0
5	E	4	0	3	0	0
5	G	4	0	3	0	0
6	A	71	0	0	6	0
6	B	62	0	0	7	1
6	C	58	0	0	4	0
6	D	55	0	0	5	0
6	E	41	0	0	8	0
6	F	50	0	0	2	0
6	G	43	0	0	9	0
6	H	39	0	0	3	0
All	All	11651	0	11075	399	1

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 18.

All (399) 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:A:140:ASP:HB3	6:A:2054:HOH:O	1.45	1.14
1:G:153:PRO:HB2	6:G:2033:HOH:O	1.46	1.13
1:E:60:ALA:O	6:E:2019:HOH:O	1.69	1.09
1:A:26:ARG:NH2	1:A:147:MET:O	1.93	1.01
1:G:74:ARG:HB2	1:G:74:ARG:NH1	1.77	0.99
2:B:347:LEU:C	2:B:347:LEU:HD12	1.89	0.96
1:G:74:ARG:HB2	1:G:74:ARG:HH11	1.31	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:175:LEU:HA	6:G:2040:HOH:O	1.68	0.91
1:A:8:THR:OG1	1:A:157:ARG:NH1	2.03	0.90
2:B:346:ALA:O	2:B:347:LEU:HG	1.73	0.88
1:G:132:TRP:O	6:G:2031:HOH:O	1.93	0.85
6:G:2043:HOH:O	2:H:222:ASP:OD2	1.93	0.85
3:F:282:VAL:O	3:F:286:VAL:HG23	1.76	0.85
2:B:263:ALA:CB	6:B:2028:HOH:O	2.24	0.84
1:G:140:ASP:O	1:G:144:ARG:HG3	1.78	0.83
1:C:74:ARG:HB2	1:C:74:ARG:HH11	1.43	0.83
1:C:19:VAL:HG11	1:C:123:ILE:HD13	1.64	0.80
2:H:310:ILE:HD11	2:H:364:ILE:HD13	1.65	0.79
2:H:306:VAL:O	2:H:310:ILE:HG12	1.84	0.78
1:C:19:VAL:HG12	1:C:19:VAL:O	1.85	0.77
1:A:171:GLY:HA2	4:B:1601:GLU:OE2	1.85	0.76
2:B:347:LEU:C	2:B:347:LEU:CD1	2.58	0.76
2:H:336:PRO:HA	6:H:2038:HOH:O	1.84	0.76
1:E:158:VAL:HG11	3:F:243:ALA:HB1	1.66	0.76
2:H:272:GLY:HA2	2:H:369:ALA:O	1.85	0.75
1:A:20:GLY:O	6:A:2004:HOH:O	2.03	0.75
1:C:179:MET:HE3	2:D:222:ASP:HB3	1.69	0.75
3:F:197:GLN:HA	3:F:200:LEU:HD22	1.69	0.74
1:A:172:VAL:N	4:B:1601:GLU:OE2	2.21	0.74
1:G:172:VAL:HG23	2:H:260:GLU:HG3	1.71	0.73
1:G:157:ARG:HG2	1:G:166:VAL:HG22	1.70	0.73
1:A:144:ARG:HA	1:A:147:MET:HE2	1.69	0.73
1:C:171:GLY:O	1:C:175:LEU:HD13	1.88	0.73
3:F:325:THR:HG21	6:F:2039:HOH:O	1.89	0.73
2:H:310:ILE:CD1	2:H:364:ILE:HD13	2.18	0.73
1:G:45:THR:HB	2:H:222:ASP:HB2	1.70	0.72
2:B:266:ILE:HD11	2:B:296:VAL:HG11	1.70	0.72
3:F:290:PRO:O	3:F:294:THR:HG23	1.89	0.71
1:A:36:ALA:HB2	1:G:35:THR:O	1.92	0.70
2:B:206:ASP:HA	2:B:210:ASN:HB2	1.73	0.70
1:C:172:VAL:HG23	2:D:260:GLU:HG3	1.73	0.70
1:C:157:ARG:HG2	1:C:166:VAL:HG22	1.74	0.70
1:C:148:THR:OG1	4:C:1602:GLU:OE2	2.07	0.69
1:G:19:VAL:HG11	1:G:123:ILE:HG13	1.73	0.69
2:B:263:ALA:HB3	6:B:2028:HOH:O	1.90	0.69
1:A:176:GLU:HG3	2:B:213:SER:HB2	1.73	0.69
2:B:346:ALA:O	2:B:347:LEU:CG	2.40	0.69
2:B:208:THR:HB	2:B:252:VAL:HG21	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:297:HIS:HB2	2:B:379:ASP:HB2	1.75	0.68
2:B:346:ALA:O	2:B:347:LEU:CB	2.41	0.68
1:E:71:VAL:HG22	1:E:109:ALA:HB3	1.74	0.68
2:B:291:LEU:HB3	2:B:305:ARG:HD3	1.75	0.68
2:D:345:ASP:OD2	6:D:2047:HOH:O	2.11	0.68
1:A:144:ARG:HD2	6:A:2056:HOH:O	1.94	0.68
2:H:280:LYS:HD2	2:H:373:PHE:CZ	2.29	0.68
1:E:119:PRO:O	1:E:123:ILE:HG13	1.95	0.67
2:B:343:ALA:O	2:B:347:LEU:HG	1.93	0.67
2:D:343:ALA:O	2:D:347:LEU:HD22	1.96	0.65
2:H:335:PRO:HB2	2:H:336:PRO:HD2	1.76	0.65
1:E:71:VAL:HA	1:E:109:ALA:O	1.95	0.65
1:E:91:VAL:O	1:E:95:VAL:HG23	1.97	0.65
2:B:347:LEU:HD12	2:B:348:ARG:N	2.12	0.64
1:A:140:ASP:CB	6:A:2054:HOH:O	2.22	0.64
3:F:356:ARG:NH1	2:H:323:ARG:HD2	2.12	0.63
2:B:326:ILE:CG1	2:B:334:TYR:HB3	2.29	0.63
2:H:181:TH5:HG22	2:H:221:SER:HB2	1.81	0.62
2:D:283:GLY:HA3	6:D:2021:HOH:O	1.98	0.62
2:B:258:ASP:O	2:B:259:GLY:C	2.42	0.62
2:D:207:ARG:HH12	2:D:373:PHE:HA	1.65	0.62
1:C:111:THR:HB	2:D:183:LEU:HD11	1.82	0.62
1:G:26:ARG:HD2	1:G:27:ASP:O	2.00	0.62
2:B:248:ALA:O	2:B:252:VAL:HG23	2.00	0.62
2:D:291:LEU:HB3	2:D:305:ARG:HD3	1.82	0.62
2:D:274:ARG:HD3	2:D:318:ASP:OD2	2.00	0.61
1:C:73:ALA:O	1:C:74:ARG:HB2	1.99	0.61
1:E:10:ARG:HG3	3:F:189:ASP:OD2	2.00	0.61
1:G:121:GLU:OE1	1:G:121:GLU:HA	2.01	0.60
2:H:280:LYS:HD2	2:H:373:PHE:CE1	2.36	0.60
2:B:326:ILE:HG12	2:B:334:TYR:HB3	1.83	0.60
2:B:347:LEU:HA	2:B:350:ALA:HB3	1.83	0.60
1:E:27:ASP:OD2	6:E:2005:HOH:O	2.16	0.60
3:F:356:ARG:HH12	2:H:323:ARG:HD2	1.67	0.60
1:G:67:ARG:NE	1:G:101:LEU:HD22	2.17	0.60
2:D:266:ILE:CD1	2:D:266:ILE:N	2.64	0.60
2:B:231:LEU:HD22	2:H:231:LEU:HD21	1.85	0.59
2:B:342:GLN:OE1	2:B:342:GLN:N	2.35	0.59
3:F:200:LEU:HD23	3:F:201:PHE:N	2.18	0.59
1:G:70:VAL:HG13	1:G:108:ILE:HG13	1.83	0.59
2:D:197:GLN:HA	2:D:200:LEU:HD22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:263:ALA:O	2:D:274:ARG:HD2	2.02	0.58
2:B:297:HIS:ND1	2:B:381:THR:HG22	2.17	0.58
6:E:2022:HOH:O	3:F:221:SER:HB3	2.03	0.58
2:H:208:THR:HB	2:H:252:VAL:HG21	1.85	0.58
2:D:200:LEU:HD23	2:D:201:PHE:N	2.18	0.58
1:E:23:ASP:O	1:G:48:ARG:NH2	2.37	0.58
4:C:1602:GLU:HG2	2:D:181:TH5:N	2.18	0.58
1:A:97:ARG:HG2	1:A:98:ALA:N	2.19	0.57
1:E:40:VAL:HG21	1:E:66:ALA:HB3	1.86	0.57
2:H:266:ILE:HG12	2:H:296:VAL:HG11	1.86	0.57
1:G:131:GLU:HB2	6:G:2030:HOH:O	2.03	0.57
2:H:289:SER:HB3	2:H:292:VAL:HB	1.86	0.57
1:E:70:VAL:HG13	1:E:108:ILE:HD12	1.85	0.57
3:F:274:ARG:HD3	3:F:318:ASP:OD2	2.03	0.57
2:B:181:TH5:HAA1	2:B:219:SER:HB2	1.87	0.57
1:E:51:GLY:HA3	6:E:2013:HOH:O	2.04	0.57
2:D:297:HIS:HB2	2:D:379:ASP:HB2	1.87	0.57
2:D:259:GLY:O	2:D:260:GLU:C	2.48	0.56
1:A:120:MET:O	1:A:124:ARG:HG3	2.05	0.56
1:G:140:ASP:HB3	6:G:2035:HOH:O	2.04	0.56
1:G:176:GLU:OE1	2:H:216:THR:HA	2.05	0.56
1:A:74:ARG:HH11	1:A:74:ARG:HB2	1.71	0.56
2:B:310:ILE:HD11	2:B:364:ILE:HD13	1.86	0.56
1:C:19:VAL:CG1	1:C:123:ILE:HD13	2.36	0.56
2:D:342:GLN:CD	2:D:342:GLN:H	2.12	0.56
1:C:19:VAL:O	1:C:19:VAL:CG1	2.54	0.56
1:A:46:ARG:NH2	6:A:2013:HOH:O	2.39	0.56
1:C:89:ARG:O	1:C:93:GLU:HB3	2.05	0.55
2:D:281:ARG:NH1	2:D:316:ASP:OD1	2.39	0.55
2:B:344:ASP:O	2:B:348:ARG:HB2	2.06	0.55
2:H:216:THR:HG22	2:H:288:ASN:CG	2.31	0.55
1:A:19:VAL:CG2	1:A:29:PHE:HB2	2.37	0.55
2:B:355:LEU:HD12	2:B:360:VAL:CG2	2.36	0.55
2:H:206:ASP:HA	2:H:210:ASN:HB2	1.87	0.55
1:A:121:GLU:HA	1:A:121:GLU:OE1	2.07	0.55
3:F:297:HIS:HB2	3:F:379:ASP:HB2	1.89	0.55
2:B:293:LYS:HE3	2:B:380:LEU:HB2	1.88	0.55
1:G:179:MET:HE3	2:H:222:ASP:HB3	1.87	0.55
1:A:78:VAL:HB	1:A:114:ILE:HD12	1.88	0.54
1:C:148:THR:OG1	1:C:149:THR:N	2.38	0.54
3:F:216:THR:HG22	3:F:288:ASN:OD1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:325:THR:OG1	2:H:365:ASP:HB3	2.07	0.54
1:G:171:GLY:C	1:G:175:LEU:HD13	2.32	0.54
2:D:387:LEU:HD23	2:D:387:LEU:O	2.08	0.54
1:C:69:VAL:HG23	1:C:107:LEU:HB2	1.89	0.53
1:E:165:LEU:HD12	3:F:188:THR:HB	1.90	0.53
2:H:212:VAL:HB	2:H:252:VAL:HG13	1.89	0.53
1:E:76:ALA:O	1:E:78:VAL:HG23	2.08	0.53
1:A:174:MET:SD	2:B:181:TH5:HAA1	2.47	0.53
2:B:272:GLY:HA2	2:B:369:ALA:O	2.08	0.53
1:E:111:THR:OG1	3:F:181:THR:HB	2.08	0.53
1:E:151:THR:OG1	3:F:258:ASP:OD1	2.19	0.53
2:B:340:GLY:HA3	6:B:2051:HOH:O	2.08	0.53
1:G:8:THR:HB	1:G:164:THR:HG21	1.91	0.53
1:E:140:ASP:HB3	6:E:2034:HOH:O	2.08	0.52
1:A:63:ASP:CG	1:A:65:GLN:HB3	2.35	0.52
1:A:19:VAL:HG21	1:A:29:PHE:HB2	1.91	0.52
2:B:182:LEU:HD22	2:B:183:LEU:N	2.25	0.52
2:D:266:ILE:N	2:D:266:ILE:HD13	2.25	0.52
1:E:26:ARG:O	6:E:2002:HOH:O	2.19	0.52
1:E:179:MET:HE3	3:F:222:ASP:HB3	1.92	0.52
1:C:21:LEU:HD11	1:C:72:LEU:HD23	1.91	0.51
3:F:249:LEU:HD11	3:F:253:LYS:HE3	1.92	0.51
1:A:168:ILE:HD11	2:B:185:PHE:HD2	1.75	0.51
1:G:12:PHE:HE2	2:H:188:THR:O	1.93	0.51
1:E:175:LEU:HD22	3:F:255:ILE:HG21	1.91	0.51
1:A:71:VAL:HA	1:A:109:ALA:O	2.11	0.51
2:H:197:GLN:HA	2:H:200:LEU:HD13	1.93	0.51
1:E:41:SER:OG	3:F:197:GLN:HG2	2.11	0.51
1:A:14:VAL:HG22	1:A:32:LEU:HD12	1.92	0.51
1:A:174:MET:SD	2:B:181:TH5:CAA	2.99	0.51
1:E:142:ALA:O	1:E:146:ILE:HG23	2.10	0.51
2:H:310:ILE:HD11	2:H:364:ILE:CD1	2.38	0.51
1:A:171:GLY:C	1:A:175:LEU:CD1	2.84	0.51
2:H:270:VAL:O	2:H:372:ALA:HA	2.11	0.50
1:A:171:GLY:O	2:B:255:ILE:HD12	2.10	0.50
2:B:280:LYS:HA	6:B:2024:HOH:O	2.11	0.50
3:F:219:SER:OG	3:F:222:ASP:OD1	2.28	0.50
1:A:171:GLY:C	1:A:175:LEU:HD13	2.36	0.50
2:B:201:PHE:CE1	2:B:205:MET:HE3	2.47	0.50
1:G:170:LYS:NZ	2:H:181:TH5:O	2.39	0.50
1:A:170:LYS:C	1:A:170:LYS:HD3	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:43:VAL:O	1:G:179:MET:HE2	2.12	0.50
1:A:8:THR:HG1	1:A:157:ARG:HH11	1.54	0.49
1:A:148:THR:OG1	4:B:1601:GLU:OE1	2.30	0.49
3:F:208:THR:HG21	3:F:248:ALA:HB3	1.93	0.49
3:F:273:ALA:HB3	3:F:371:GLY:HA3	1.94	0.49
2:H:250:ALA:O	2:H:254:ASP:HB2	2.12	0.49
1:C:35:THR:HB	1:E:67:ARG:NH1	2.26	0.49
1:A:78:VAL:HG12	1:A:114:ILE:HG23	1.93	0.49
1:G:154:LYS:HE2	2:H:255:ILE:HA	1.95	0.49
1:C:170:LYS:NZ	2:D:181:TH5:O	2.40	0.49
2:H:215:ASP:OD1	2:H:215:ASP:N	2.43	0.49
1:A:24:ASP:OD2	1:A:74:ARG:NH2	2.46	0.49
1:E:21:LEU:HD22	1:E:75:ASN:HB3	1.95	0.49
1:A:37:PRO:HA	1:A:67:ARG:HD2	1.93	0.49
1:G:74:ARG:HB2	1:G:74:ARG:CZ	2.42	0.49
2:B:182:LEU:O	2:B:222:ASP:HA	2.12	0.49
1:G:70:VAL:HG21	1:G:95:VAL:HG21	1.94	0.49
3:F:271:THR:O	3:F:365:ASP:HA	2.13	0.49
1:G:138:GLY:HA3	1:G:141:ARG:HH21	1.78	0.49
1:E:104:GLY:O	6:E:2019:HOH:O	2.20	0.48
1:E:169:ALA:HB2	3:F:251:LEU:HD13	1.94	0.48
3:F:316:ASP:C	3:F:318:ASP:H	2.21	0.48
2:B:355:LEU:HD12	2:B:360:VAL:HG21	1.95	0.48
2:D:197:GLN:O	2:D:200:LEU:CD2	2.62	0.48
1:G:12:PHE:CE2	2:H:188:THR:O	2.66	0.48
1:G:28:ASP:CB	1:G:74:ARG:HH12	2.26	0.48
2:H:309:ALA:HA	2:H:312:LYS:HG3	1.95	0.48
2:B:181:TH5:N	4:B:1601:GLU:HB2	2.28	0.48
1:E:21:LEU:HD11	1:E:72:LEU:HB3	1.95	0.48
1:G:74:ARG:HG3	6:G:2016:HOH:O	2.13	0.48
2:H:272:GLY:CA	2:H:369:ALA:O	2.59	0.48
2:D:334:TYR:CD1	2:D:335:PRO:HA	2.48	0.48
2:H:284:LYS:O	2:H:285:THR:C	2.53	0.48
1:C:71:VAL:HA	1:C:109:ALA:O	2.12	0.48
2:D:300:ASP:OD1	2:D:301:PRO:HD2	2.13	0.48
1:E:41:SER:HG	3:F:197:GLN:HG2	1.78	0.48
1:A:22:ALA:H	1:A:74:ARG:HH12	1.62	0.48
3:F:267:GLU:HG3	3:F:376:TYR:CE2	2.49	0.48
2:B:337:LYS:H	2:B:337:LYS:HD2	1.78	0.48
1:C:26:ARG:HB3	1:C:74:ARG:HH21	1.79	0.48
2:H:327:ARG:HG2	6:H:2033:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:ARG:N	1:E:111:THR:O	2.47	0.47
1:A:149:THR:N	4:B:1601:GLU:OE1	2.35	0.47
2:D:200:LEU:O	2:D:204:VAL:HG23	2.14	0.47
1:E:123:ILE:HG22	1:E:127:LEU:HD11	1.96	0.47
2:H:217:ASP:O	2:H:218:THR:C	2.58	0.47
2:B:265:LEU:HB3	2:B:359:GLU:HG2	1.95	0.47
1:C:170:LYS:HZ3	4:C:1602:GLU:CD	2.22	0.47
3:F:272:GLY:C	3:F:369:ALA:O	2.58	0.47
2:H:297:HIS:HB2	2:H:379:ASP:HB2	1.96	0.47
2:H:335:PRO:HG3	6:H:2032:HOH:O	2.14	0.47
1:A:12:PHE:O	1:A:136:GLU:HB3	2.15	0.47
1:C:179:MET:HE3	2:D:222:ASP:C	2.40	0.47
1:G:69:VAL:HB	1:G:107:LEU:HB2	1.97	0.47
2:B:342:GLN:N	2:B:342:GLN:CD	2.73	0.47
1:C:175:LEU:HA	6:C:2055:HOH:O	2.14	0.47
2:D:346:ALA:HB1	6:D:2048:HOH:O	2.15	0.47
1:A:111:THR:OG1	2:B:181:TH5:HB	2.15	0.47
1:G:12:PHE:CE1	1:G:34:SER:HB2	2.50	0.47
2:H:278:GLN:O	2:H:279:ALA:C	2.58	0.47
2:B:326:ILE:HG13	2:B:334:TYR:HB3	1.96	0.46
2:D:338:ALA:N	6:D:2045:HOH:O	2.47	0.46
2:H:299:CYS:SG	2:H:356:ARG:HD3	2.54	0.46
2:B:304:GLY:O	2:B:307:ALA:HB3	2.15	0.46
3:F:272:GLY:HA2	3:F:369:ALA:O	2.15	0.46
1:G:111:THR:OG1	1:G:170:LYS:HE3	2.14	0.46
1:G:111:THR:HG21	1:G:170:LYS:HE3	1.97	0.46
2:D:284:LYS:O	2:D:288:ASN:HB2	2.15	0.46
1:E:83:GLU:HB3	1:E:117:GLN:HE22	1.80	0.46
1:G:52:PRO:HB3	1:G:85:GLU:HG2	1.96	0.46
2:H:288:ASN:O	2:H:290:PRO:HD3	2.16	0.46
1:A:120:MET:O	1:A:124:ARG:CG	2.63	0.46
1:C:15:HIS:O	1:C:30:THR:HA	2.16	0.46
2:H:272:GLY:O	2:H:368:ILE:HB	2.16	0.46
1:C:174:MET:HG2	2:D:219:SER:HB2	1.98	0.46
1:E:8:THR:HB	1:E:164:THR:HG21	1.98	0.46
3:F:188:THR:HG22	3:F:227:PHE:O	2.16	0.46
1:G:57:CYS:O	1:G:58:ARG:C	2.59	0.46
2:H:293:LYS:HE3	2:H:380:LEU:HB2	1.98	0.46
1:E:60:ALA:HB3	1:E:107:LEU:CD2	2.46	0.45
1:A:11:GLY:O	1:A:34:SER:HA	2.17	0.45
1:A:171:GLY:CA	4:B:1601:GLU:OE2	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:GLU:OE2	1:C:157:ARG:NH1	2.49	0.45
4:C:1602:GLU:CG	2:D:181:TH5:N	2.79	0.45
3:F:214:ILE:N	3:F:214:ILE:CD1	2.79	0.45
2:H:258:ASP:CG	2:H:258:ASP:O	2.58	0.45
1:A:30:THR:O	1:A:70:VAL:HA	2.16	0.45
1:C:13:VAL:HG12	1:C:136:GLU:HA	1.98	0.45
6:G:2043:HOH:O	2:H:222:ASP:CB	2.64	0.45
1:E:34:SER:OG	1:E:36:ALA:O	2.27	0.45
1:E:48:ARG:HA	1:E:48:ARG:NE	2.32	0.45
2:H:323:ARG:HB3	2:H:367:ALA:HB3	1.98	0.45
1:A:15:HIS:HB3	1:A:31:VAL:HB	1.97	0.45
1:A:39:THR:HG21	2:B:194:PRO:HG3	1.98	0.45
2:B:251:LEU:O	2:B:255:ILE:HG12	2.17	0.45
2:D:305:ARG:O	2:D:308:MET:HB3	2.17	0.45
2:D:198:ASP:O	2:D:202:ARG:HG3	2.17	0.45
2:D:297:HIS:ND1	2:D:381:THR:HG22	2.32	0.45
3:F:200:LEU:HD12	3:F:241:GLU:HB2	1.98	0.45
1:C:81:GLY:HA2	6:C:2032:HOH:O	2.17	0.44
2:D:342:GLN:OE1	2:D:342:GLN:N	2.45	0.44
1:G:80:THR:OG1	1:G:84:GLY:HA3	2.17	0.44
1:A:19:VAL:CG2	1:A:29:PHE:CB	2.96	0.44
1:A:22:ALA:H	1:A:74:ARG:NH1	2.14	0.44
2:D:258:ASP:O	2:D:259:GLY:C	2.59	0.44
1:A:46:ARG:HD3	1:A:180:ALA:HB3	2.00	0.44
1:A:157:ARG:HG2	1:A:166:VAL:HG22	1.99	0.44
1:E:146:ILE:O	1:E:170:LYS:HG3	2.17	0.44
1:G:19:VAL:CG1	1:G:123:ILE:HG13	2.43	0.44
2:B:382:GLU:OE1	6:B:2060:HOH:O	2.21	0.44
1:A:15:HIS:O	1:A:30:THR:HA	2.18	0.44
2:B:297:HIS:CE1	2:B:381:THR:HG22	2.53	0.44
1:E:165:LEU:CD1	3:F:188:THR:HB	2.47	0.44
3:F:216:THR:HG22	3:F:288:ASN:CG	2.43	0.44
1:A:31:VAL:HG11	1:A:99:LEU:HD11	1.99	0.44
1:A:8:THR:HB	1:A:164:THR:HG21	1.99	0.43
2:B:208:THR:HB	2:B:252:VAL:CG2	2.47	0.43
1:E:63:ASP:OD1	1:E:65:GLN:HB3	2.18	0.43
1:A:35:THR:HB	1:G:67:ARG:HH12	1.82	0.43
1:A:173:GLY:HA3	2:B:260:GLU:CD	2.43	0.43
2:B:342:GLN:CD	2:B:342:GLN:H	2.26	0.43
1:C:15:HIS:HE1	6:C:2044:HOH:O	2.02	0.43
1:E:44:PHE:O	1:E:179:MET:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:287:VAL:HG22	6:F:2008:HOH:O	2.18	0.43
1:G:15:HIS:O	1:G:30:THR:HA	2.17	0.43
1:G:41:SER:OG	2:H:197:GLN:HG2	2.17	0.43
1:A:138:GLY:O	1:A:141:ARG:N	2.51	0.43
2:B:300:ASP:O	2:B:302:ASN:N	2.44	0.43
1:A:168:ILE:CD1	2:B:185:PHE:HD2	2.30	0.43
1:C:52:PRO:HD2	1:C:77:ASN:O	2.18	0.43
1:G:130:LEU:HG	1:G:131:GLU:N	2.27	0.43
2:B:336:PRO:HB3	6:B:2048:HOH:O	2.18	0.43
1:A:109:ALA:HB1	2:B:183:LEU:HD22	2.00	0.43
1:E:49:PHE:O	3:F:220:THR:HB	2.18	0.43
2:D:306:VAL:HG12	2:D:326:ILE:HD12	2.00	0.43
1:C:69:VAL:HG23	1:C:107:LEU:CB	2.48	0.43
1:A:19:VAL:HG21	1:A:29:PHE:CB	2.48	0.43
1:A:94:ALA:HB3	1:A:127:LEU:HD13	2.01	0.43
1:C:176:GLU:OE1	2:D:216:THR:HA	2.19	0.43
2:D:261:GLY:O	2:D:381:THR:HG21	2.19	0.43
2:B:283:GLY:HA3	6:B:2024:HOH:O	2.18	0.42
1:E:42:ALA:HB1	1:E:44:PHE:CZ	2.54	0.42
2:B:355:LEU:HD12	2:B:360:VAL:HG22	2.01	0.42
1:E:40:VAL:CG1	1:E:41:SER:N	2.82	0.42
1:E:69:VAL:HA	1:E:107:LEU:O	2.18	0.42
3:F:201:PHE:O	3:F:205:MET:HG2	2.20	0.42
1:E:75:ASN:OD1	1:E:75:ASN:C	2.63	0.42
1:G:19:VAL:CG1	1:G:19:VAL:O	2.67	0.42
1:G:28:ASP:HB2	1:G:74:ARG:HH12	1.83	0.42
1:G:89:ARG:O	1:G:93:GLU:HB3	2.18	0.42
2:D:309:ALA:HA	2:D:312:LYS:HG3	1.99	0.42
1:E:172:VAL:HG23	3:F:260:GLU:HG3	2.01	0.42
1:G:140:ASP:O	1:G:144:ARG:CG	2.61	0.42
1:G:144:ARG:HA	1:G:147:MET:HE2	2.00	0.42
1:G:170:LYS:HG2	1:G:171:GLY:N	2.34	0.42
1:G:172:VAL:O	2:H:260:GLU:HG3	2.19	0.42
2:B:181:TH5:HG22	2:B:221:SER:HB2	2.00	0.42
1:C:11:GLY:O	1:C:34:SER:HA	2.19	0.42
2:D:191:ARG:HB2	2:D:230:GLY:HA3	2.02	0.42
2:D:355:LEU:HD12	2:D:360:VAL:HG11	2.01	0.42
2:H:208:THR:OG1	2:H:209:PHE:N	2.53	0.42
1:C:76:ALA:O	1:C:110:SER:HB3	2.20	0.42
1:E:171:GLY:O	3:F:255:ILE:HG23	2.20	0.42
1:E:8:THR:N	1:E:9:PRO:CD	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:155:GLU:HG2	1:G:156:VAL:N	2.35	0.42
1:A:26:ARG:HB3	1:A:74:ARG:NH2	2.35	0.42
1:A:172:VAL:HG11	2:B:258:ASP:HB3	2.02	0.42
2:D:282:VAL:HG21	2:D:366:LEU:HD11	2.02	0.42
3:F:292:VAL:O	3:F:296:VAL:HG23	2.19	0.42
1:C:125:GLU:O	1:C:128:LYS:HB2	2.20	0.42
2:D:229:ASN:OD1	2:D:229:ASN:O	2.38	0.42
1:E:155:GLU:OE1	1:E:157:ARG:NH1	2.53	0.42
1:C:171:GLY:C	1:C:175:LEU:HD13	2.45	0.42
2:D:200:LEU:HD11	2:D:240:PHE:HD2	1.85	0.42
1:G:36:ALA:O	1:G:37:PRO:C	2.59	0.42
2:H:289:SER:HB3	2:H:292:VAL:CG2	2.50	0.42
1:A:70:VAL:HG21	1:A:95:VAL:HG21	2.01	0.41
1:A:144:ARG:CA	1:A:147:MET:HE2	2.45	0.41
2:B:278:GLN:HA	2:B:281:ARG:NH1	2.35	0.41
2:B:328:PHE:HB2	2:B:351:VAL:HG22	2.01	0.41
1:C:26:ARG:HB3	1:C:74:ARG:NH2	2.35	0.41
2:D:379:ASP:OD1	2:D:379:ASP:N	2.53	0.41
1:A:21:LEU:HD12	1:A:28:ASP:CG	2.46	0.41
2:B:216:THR:HG22	2:B:288:ASN:CG	2.45	0.41
1:E:14:VAL:HG11	1:E:142:ALA:HB2	2.01	0.41
1:E:24:ASP:C	1:E:24:ASP:OD1	2.63	0.41
1:E:77:ASN:HB2	1:E:118:TYR:CE1	2.56	0.41
1:G:67:ARG:CZ	1:G:101:LEU:HD22	2.51	0.41
2:B:337:LYS:O	2:B:338:ALA:HB3	2.20	0.41
1:C:170:LYS:HD3	1:C:170:LYS:C	2.44	0.41
2:D:197:GLN:O	2:D:200:LEU:HD23	2.19	0.41
2:D:271:THR:O	2:D:365:ASP:HA	2.21	0.41
2:D:347:LEU:HD12	2:D:347:LEU:HA	1.93	0.41
1:A:176:GLU:OE1	2:B:216:THR:HA	2.19	0.41
2:D:309:ALA:O	2:D:310:ILE:C	2.64	0.41
1:C:8:THR:HG22	1:C:8:THR:O	2.20	0.41
2:D:206:ASP:HA	2:D:210:ASN:HB2	2.03	0.41
1:E:19:VAL:CG1	1:E:123:ILE:HG12	2.50	0.41
1:E:21:LEU:CD1	1:E:72:LEU:HB3	2.50	0.41
2:H:301:PRO:HB3	2:H:355:LEU:HD13	2.03	0.41
1:A:135:GLY:HA2	6:A:2052:HOH:O	2.21	0.41
1:E:158:VAL:CG1	3:F:243:ALA:HB1	2.43	0.41
3:F:300:ASP:O	3:F:302:ASN:N	2.52	0.41
1:G:138:GLY:O	1:G:141:ARG:N	2.49	0.41
1:G:179:MET:HE3	2:H:222:ASP:C	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:291:LEU:HD12	3:F:308:MET:HE2	2.03	0.41
1:C:41:SER:OG	2:D:197:GLN:HG2	2.21	0.40
2:D:264:LYS:HG3	6:D:2016:HOH:O	2.21	0.40
2:D:287:VAL:CG2	2:D:377:GLY:HA3	2.51	0.40
3:F:309:ALA:O	3:F:312:LYS:HG3	2.21	0.40
1:G:144:ARG:NH1	1:G:153:PRO:HG3	2.36	0.40
1:E:57:CYS:HA	1:E:107:LEU:CD2	2.51	0.40
1:E:60:ALA:HB3	1:E:107:LEU:HD23	2.02	0.40
1:C:157:ARG:NH2	6:C:2047:HOH:O	2.55	0.40
1:C:180:ALA:O	2:D:202:ARG:NH2	2.52	0.40
1:E:16:THR:HG21	1:E:141:ARG:HB3	2.04	0.40
1:G:98:ALA:HB1	1:G:130:LEU:O	2.21	0.40
2:H:335:PRO:HB2	2:H:336:PRO:CD	2.44	0.40
2:D:216:THR:HG22	2:D:288:ASN:CG	2.46	0.40
2:D:328:PHE:HB2	2:D:351:VAL:HG22	2.03	0.40
1:E:58:ARG:NE	6:E:2016:HOH:O	2.43	0.40
3:F:309:ALA:HA	3:F:312:LYS:HG3	2.02	0.40
1:C:78:VAL:HB	1:C:114:ILE:HD12	2.04	0.40
4:C:1602:GLU:N	2:D:181:TH5:HN1	2.20	0.40
2:D:303:TRP:O	2:D:306:VAL:HB	2.21	0.40
2:D:343:ALA:O	2:D:347:LEU:CD2	2.67	0.40
3:F:193:ASP:HB3	3:F:196:GLU:HB2	2.03	0.40
1:G:74:ARG:HA	6:G:2016:HOH:O	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ARG:NH1	6:B:2060:HOH:O[2_544]	1.88	0.32

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	171/180 (95%)	159 (93%)	11 (6%)	1 (1%)	21	44
1	C	171/180 (95%)	160 (94%)	11 (6%)	0	100	100
1	E	171/180 (95%)	163 (95%)	8 (5%)	0	100	100
1	G	171/180 (95%)	155 (91%)	16 (9%)	0	100	100
2	B	211/213 (99%)	196 (93%)	14 (7%)	1 (0%)	24	48
2	D	208/213 (98%)	192 (92%)	15 (7%)	1 (0%)	24	48
2	H	191/213 (90%)	176 (92%)	15 (8%)	0	100	100
3	F	193/213 (91%)	181 (94%)	11 (6%)	1 (0%)	24	48
All	All	1487/1572 (95%)	1382 (93%)	101 (7%)	4 (0%)	36	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	259	GLY
1	A	172	VAL
2	D	259	GLY
3	F	261	GLY

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	128/135 (95%)	112 (88%)	16 (12%)	4	11
1	C	128/135 (95%)	117 (91%)	11 (9%)	10	25
1	E	128/135 (95%)	115 (90%)	13 (10%)	7	18
1	G	128/135 (95%)	111 (87%)	17 (13%)	4	10
2	B	165/165 (100%)	153 (93%)	12 (7%)	13	32
2	D	162/165 (98%)	151 (93%)	11 (7%)	14	35
2	H	153/165 (93%)	140 (92%)	13 (8%)	10	25
3	F	156/166 (94%)	146 (94%)	10 (6%)	16	38
All	All	1148/1201 (96%)	1045 (91%)	103 (9%)	9	23

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	19	VAL
1	A	26	ARG
1	A	74	ARG
1	A	82	LEU
1	A	92	ARG
1	A	93	GLU
1	A	97	ARG
1	A	105	GLU
1	A	107	LEU
1	A	113	VAL
1	A	121	GLU
1	A	158	VAL
1	A	160	VAL
1	A	165	LEU
1	A	175	LEU
2	B	182	LEU
2	B	200	LEU
2	B	216	THR
2	B	226	LEU
2	B	287	VAL
2	B	326	ILE
2	B	337	LYS
2	B	342	GLN
2	B	347	LEU
2	B	355	LEU
2	B	362	ILE
2	B	387	LEU
1	C	10	ARG
1	C	21	LEU
1	C	41	SER
1	C	74	ARG
1	C	92	ARG
1	C	93	GLU
1	C	121	GLU
1	C	123	ILE
1	C	160	VAL
1	C	170	LYS
1	C	175	LEU
2	D	182	LEU
2	D	200	LEU
2	D	219	SER

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Mol	Chain	Res	Type
2	D	226	LEU
2	D	266	ILE
2	D	294	THR
2	D	342	GLN
2	D	347	LEU
2	D	355	LEU
2	D	360	VAL
2	D	386	ARG
1	E	13	VAL
1	E	19	VAL
1	E	41	SER
1	E	74	ARG
1	E	75	ASN
1	E	80	THR
1	E	92	ARG
1	E	108	ILE
1	E	113	VAL
1	E	121	GLU
1	E	158	VAL
1	E	160	VAL
1	E	175	LEU
3	F	182	LEU
3	F	200	LEU
3	F	214	ILE
3	F	216	THR
3	F	242	GLU
3	F	254	ASP
3	F	310	ILE
3	F	333	VAL
3	F	355	LEU
3	F	392	THR
1	G	8	THR
1	G	19	VAL
1	G	39	THR
1	G	69	VAL
1	G	74	ARG
1	G	92	ARG
1	G	93	GLU
1	G	107	LEU
1	G	113	VAL
1	G	125	GLU
1	G	129	THR

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Mol	Chain	Res	Type
1	G	160	VAL
1	G	164	THR
1	G	166	VAL
1	G	170	LYS
1	G	172	VAL
1	G	175	LEU
2	H	182	LEU
2	H	200	LEU
2	H	216	THR
2	H	219	SER
2	H	221	SER
2	H	257	SER
2	H	275	ASP
2	H	317	THR
2	H	330	GLU
2	H	333	VAL
2	H	353	GLU
2	H	355	LEU
2	H	386	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	245	HIS
3	F	388	ASN
1	G	87	ASN
2	H	229	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	TH5	H	181	2	8,9,10	2.56	2 (25%)	9,11,13	3.64	4 (44%)
2	TH5	B	181	2	8,9,10	1.04	1 (12%)	9,11,13	3.42	5 (55%)
2	TH5	D	181	2	8,9,10	1.50	1 (12%)	9,11,13	2.93	5 (55%)

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	TH5	H	181	2	-	1/8/10/12	-
2	TH5	B	181	2	-	0/8/10/12	-
2	TH5	D	181	2	-	3/8/10/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	181	TH5	OG1-CB	-6.79	1.36	1.46
2	D	181	TH5	OG1-CB	-3.10	1.41	1.46
2	B	181	TH5	OG1-CB	-2.50	1.42	1.46
2	H	181	TH5	CB-CA	-2.14	1.49	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	181	TH5	CG2-CB-CA	-7.45	98.75	113.26
2	B	181	TH5	OG1-CB-CA	-6.77	90.93	105.80
2	H	181	TH5	OG1-CAH-CAA	5.66	121.18	111.09
2	D	181	TH5	OG1-CAH-CAA	5.64	121.16	111.09
2	B	181	TH5	OG1-CAH-CAA	4.72	119.50	111.09
2	B	181	TH5	CB-OG1-CAH	4.34	125.81	117.83
2	H	181	TH5	OG1-CB-CA	-3.94	97.14	105.80
2	D	181	TH5	CB-OG1-CAH	-3.72	110.98	117.83
2	B	181	TH5	OG1-CB-CG2	3.27	114.75	108.20
2	D	181	TH5	OG1-CB-CG2	-3.11	101.97	108.20
2	D	181	TH5	O-C-CA	-2.80	117.57	124.77
2	H	181	TH5	OG1-CAH-OAD	-2.50	118.16	122.99
2	D	181	TH5	CG2-CB-CA	2.31	117.77	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	181	TH5	OAD-CAH-CAA	-2.19	117.03	124.77

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	181	TH5	O-C-CA-CB
2	D	181	TH5	C-CA-CB-OG1
2	D	181	TH5	C-CA-CB-CG2
2	H	181	TH5	O-C-CA-CB

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	181	TH5	2	0
2	B	181	TH5	6	0
2	D	181	TH5	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
4	GLU	C	1602	-	7,8,9	1.66	2 (28%)	4,9,11	1.26	0
5	ACT	G	1181	-	3,3,3	0.78	0	3,3,3	1.18	0
5	ACT	E	1181	-	3,3,3	1.11	0	3,3,3	0.96	0
4	GLU	B	1601	-	7,8,9	1.50	0	4,9,11	1.17	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
4	GLU	C	1602	-	-	3/6/7/9	-
4	GLU	B	1601	-	-	6/6/7/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1602	GLU	CG-CD	2.73	1.56	1.50
4	C	1602	GLU	O-C	2.12	1.28	1.20

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1601	GLU	O-C-CA-CB
4	B	1601	GLU	C-CA-CB-CG
4	C	1602	GLU	CA-CB-CG-CD
4	B	1601	GLU	N-CA-CB-CG
4	B	1601	GLU	CA-CB-CG-CD
4	B	1601	GLU	OE2-CD-CG-CB
4	B	1601	GLU	OE1-CD-CG-CB
4	C	1602	GLU	OE2-CD-CG-CB
4	C	1602	GLU	OE1-CD-CG-CB

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1602	GLU	5	0
4	B	1601	GLU	6	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	173/180 (96%)	0.22	5 (2%) 53 50	1, 9, 22, 29	0
1	C	173/180 (96%)	0.19	2 (1%) 76 75	1, 7, 20, 24	0
1	E	173/180 (96%)	0.44	4 (2%) 61 58	4, 15, 25, 28	0
1	G	173/180 (96%)	0.59	4 (2%) 61 58	6, 16, 29, 33	0
2	B	212/213 (99%)	0.22	4 (1%) 66 63	1, 6, 19, 28	0
2	D	209/213 (98%)	0.20	5 (2%) 59 56	1, 7, 20, 29	0
2	H	194/213 (91%)	0.57	9 (4%) 37 34	6, 17, 32, 40	0
3	F	197/213 (92%)	0.37	4 (2%) 65 62	2, 14, 25, 31	0
All	All	1504/1572 (95%)	0.35	37 (2%) 58 55	1, 11, 25, 40	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	336	PRO	4.6
2	B	342	GLN	4.5
2	H	352	ALA	4.2
3	F	352	ALA	3.5
1	G	22	ALA	3.1
2	B	347	LEU	2.9
1	C	134	ALA	2.8
1	E	46	ARG	2.8
2	H	230	GLY	2.6
1	G	134	ALA	2.6
3	F	353	GLU	2.5
1	A	134	ALA	2.5
2	D	262	ALA	2.5
2	H	237	ALA	2.5
1	E	180	ALA	2.5
2	D	390	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	194	PRO	2.4
2	H	196	GLU	2.4
1	G	89	ARG	2.4
1	A	93	GLU	2.4
1	A	135	GLY	2.4
3	F	356	ARG	2.3
2	H	335	PRO	2.3
2	B	367	ALA	2.2
2	H	195	ALA	2.2
1	A	103	GLU	2.2
1	E	161	GLY	2.2
1	A	65	GLN	2.2
1	G	8	THR	2.2
3	F	391	TYR	2.2
1	E	96	ALA	2.1
2	B	346	ALA	2.1
2	D	342	GLN	2.1
2	H	390	GLU	2.1
2	H	369	ALA	2.1
1	C	10	ARG	2.1
2	D	343	ALA	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	TH5	D	181	10/11	0.88	0.13	5,8,13,13	0
2	TH5	B	181	10/11	0.92	0.11	1,3,7,7	0
2	TH5	H	181	10/11	0.93	0.10	9,13,14,15	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GLU	C	1602	9/10	0.70	0.21	26,28,31,31	0
4	GLU	B	1601	9/10	0.81	0.19	13,15,19,21	0
5	ACT	E	1181	4/4	0.88	0.14	16,17,17,17	0
5	ACT	G	1181	4/4	0.90	0.13	15,16,16,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.