Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 12:51 pm GMT

PDB ID	:	2VZK
Title	:	Structure of the acyl-enzyme complex of an N-terminal nucleophile (Ntn) hydrolase, OAT2
Authors	:	Iqbal, A.; Clifton, I.J.; Schofield, C.J.
Deposited on	:	2008-08-01
Resolution	:	2.33 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 (i) 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 (i)) were used in the production of this report:

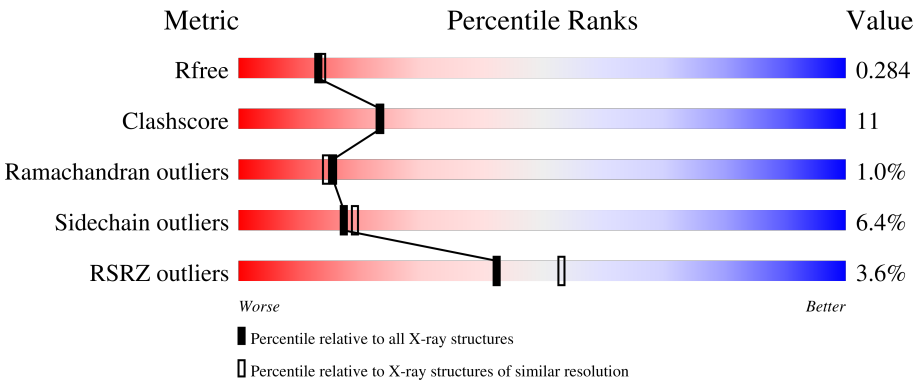
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.33 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}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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 <=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	173	2% 76% 21% •
1	C	173	2% 79% 17% •
1	E	173	3% 74% 23% •
1	G	173	5% 75% 21% •
2	B	213	% 84% 12% • •

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Mol	Chain	Length	Quality of chain
3	D	213	4% 80% 15%
3	F	213	5% 76% 14% 8%
3	H	213	5% 79% 11% 8%

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
5	ACT	G	1181	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11527 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
			Total	C	N	O	S			
1	A	173	1267	783	234	244	6	0	0	0
1	C	173	1267	783	234	244	6	0	0	0
1	E	173	1267	783	234	244	6	0	0	0
1	G	173	1267	783	234	244	6	0	0	0

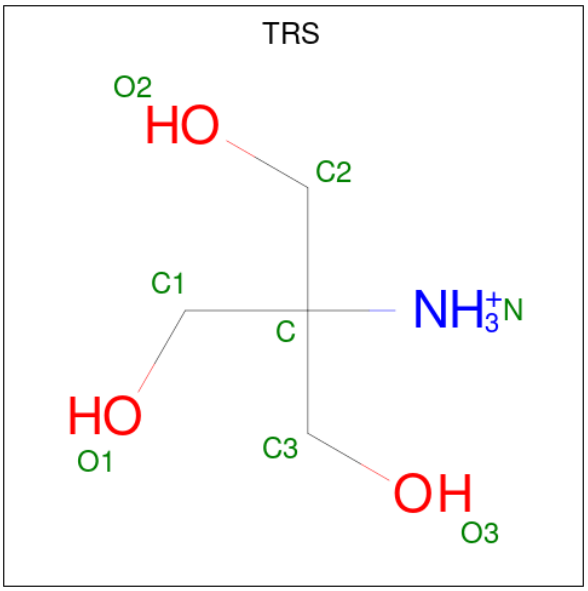
- Molecule 2 is a protein called GLUTAMATE N-ACETYLTRANSFERASE 2 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	213	1603	990	279	329	5	0	0	0

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

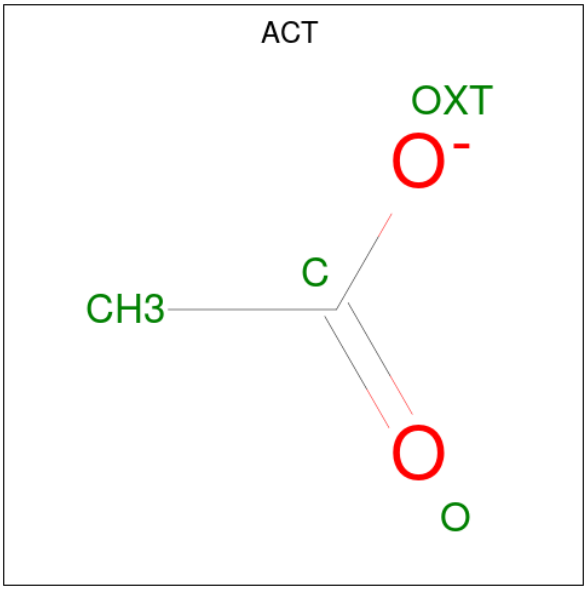
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	210	1579	975	276	323	5	0	0	0
3	F	197	1490	925	255	305	5	0	0	0
3	H	195	1471	912	253	301	5	0	0	0

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	8	4	1	3	0	0
			Total	C	N	O		
4	A	1	8	4	1	3	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is water.

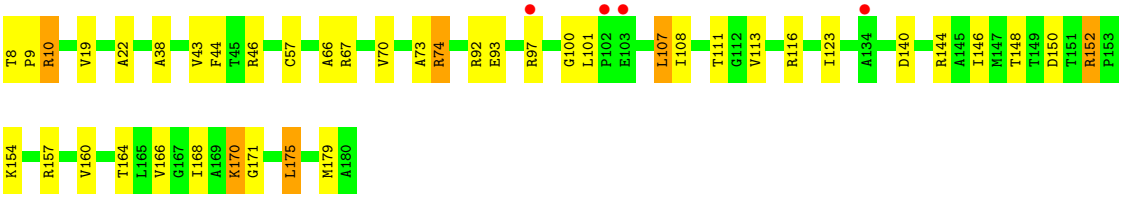
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	36	36	36	0	0
			Total	O		
6	B	48	48	48	0	0
			Total	O		
6	C	34	34	34	0	0
			Total	O		
6	D	41	41	41	0	0
			Total	O		
6	E	32	32	32	0	0
			Total	O		
6	F	37	37	37	0	0
			Total	O		
6	G	34	34	34	0	0
			Total	O		
6	H	30	30	30	0	0

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.

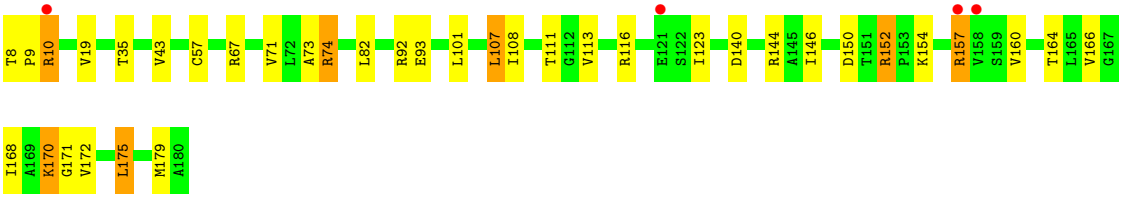
• Molecule 1: GLUTAMATE N-ACETYLTRANSFERASE 2 ALPHA CHAIN

Chain A:



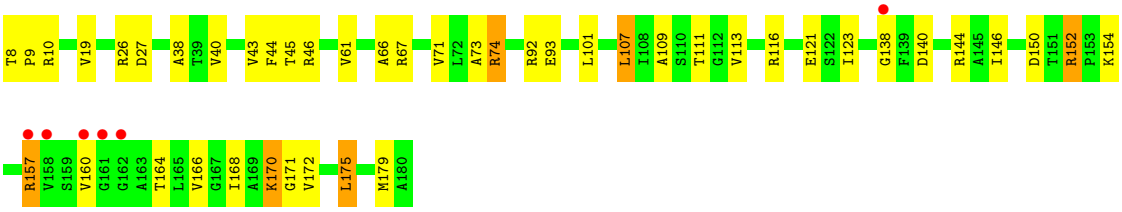
• Molecule 1: GLUTAMATE N-ACETYLTRANSFERASE 2 ALPHA CHAIN

Chain C:



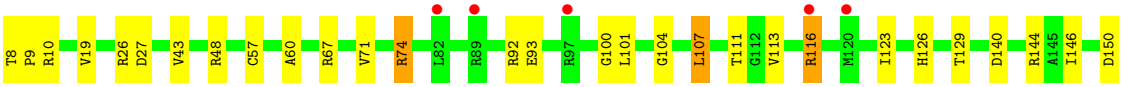
• Molecule 1: GLUTAMATE N-ACETYLTRANSFERASE 2 ALPHA CHAIN

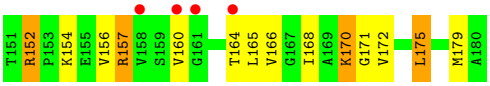
Chain E:



• Molecule 1: GLUTAMATE N-ACETYLTRANSFERASE 2 ALPHA CHAIN

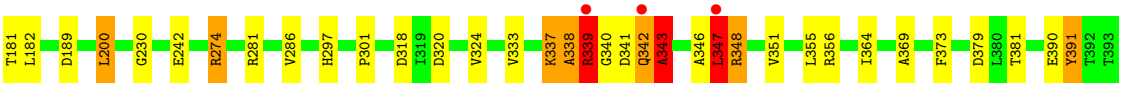
Chain G:





• Molecule 2: GLUTAMATE N-ACETYLTRANSFERASE 2 BETA CHAIN

Chain B:

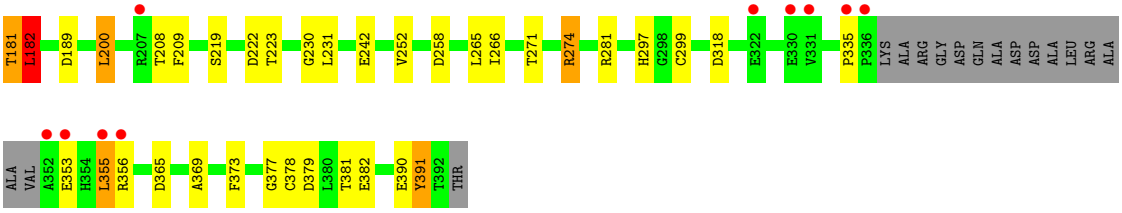


• Molecule 3: GLUTAMATE N-ACETYLTRANSFERASE 2 BETA CHAIN

Chain D:

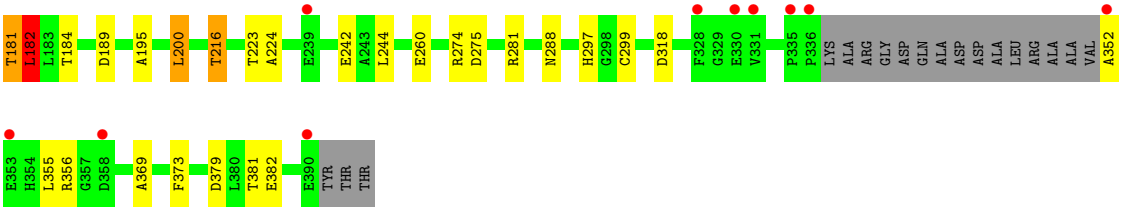
• Molecule 3: GLUTAMATE N-ACETYLTRANSFERASE 2 BETA CHAIN

Chain F:



• Molecule 3: GLUTAMATE N-ACETYLTRANSFERASE 2 BETA CHAIN

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.27Å 73.88Å 172.17Å 90.00° 92.71° 90.00°	Depositor
Resolution (Å)	171.50 – 2.33 37.16 – 2.33	Depositor EDS
% Data completeness (in resolution range)	93.7 (171.50-2.33) 93.7 (37.16-2.33)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.254 , 0.284 0.254 , 0.284	Depositor DCC
R_{free} test set	3048 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	38.2	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 33.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11527	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: TH5, TRS, ACT

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	0.88	0/1285	1.08	5/1742 (0.3%)
1	C	0.89	0/1285	1.06	5/1742 (0.3%)
1	E	0.82	0/1285	1.12	4/1742 (0.2%)
1	G	0.78	1/1285 (0.1%)	1.13	6/1742 (0.3%)
2	B	0.94	0/1624	0.98	9/2205 (0.4%)
3	D	0.90	2/1589 (0.1%)	0.93	4/2157 (0.2%)
3	F	0.88	1/1500 (0.1%)	0.92	9/2037 (0.4%)
3	H	0.89	1/1480 (0.1%)	0.90	5/2009 (0.2%)
All	All	0.87	5/11333 (0.0%)	1.01	47/15376 (0.3%)

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
1	A	0	1
1	C	0	1
1	E	0	2
1	G	0	1
2	B	2	4
3	D	0	3
3	F	1	1
All	All	3	13

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	182	LEU	N-CA	14.35	1.75	1.46
3	F	182	LEU	N-CA	10.38	1.67	1.46
3	D	182	LEU	N-CA	6.80	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	339	ARG	C-O	6.18	1.35	1.23
1	G	57	CYS	CB-SG	-5.04	1.73	1.81

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	152	ARG	NE-CZ-NH1	-22.60	109.00	120.30
1	E	152	ARG	NE-CZ-NH1	-21.35	109.63	120.30
1	A	152	ARG	NE-CZ-NH2	-19.80	110.40	120.30
1	C	152	ARG	NE-CZ-NH2	-19.13	110.73	120.30
1	G	152	ARG	NE-CZ-NH2	17.08	128.84	120.30
1	E	152	ARG	NE-CZ-NH2	16.85	128.72	120.30
1	C	152	ARG	NE-CZ-NH1	14.04	127.32	120.30
1	A	152	ARG	NE-CZ-NH1	12.95	126.78	120.30
1	A	152	ARG	CD-NE-CZ	10.84	138.78	123.60
1	E	152	ARG	CD-NE-CZ	10.84	138.78	123.60
1	G	152	ARG	CD-NE-CZ	10.82	138.75	123.60
1	C	152	ARG	CD-NE-CZ	10.41	138.18	123.60
2	B	343	ALA	N-CA-CB	8.34	121.78	110.10
3	H	281	ARG	NE-CZ-NH2	-7.46	116.57	120.30
2	B	274	ARG	NE-CZ-NH1	7.38	123.99	120.30
3	F	390	GLU	CA-C-N	7.07	132.76	117.20
3	F	182	LEU	N-CA-CB	6.94	124.28	110.40
2	B	348	ARG	N-CA-CB	6.93	123.08	110.60
2	B	200	LEU	CA-CB-CG	6.89	131.15	115.30
3	H	281	ARG	NE-CZ-NH1	6.86	123.73	120.30
3	H	200	LEU	CA-CB-CG	6.61	130.50	115.30
1	G	48	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	C	10	ARG	NE-CZ-NH2	-6.36	117.12	120.30
3	F	200	LEU	CA-CB-CG	6.30	129.79	115.30
1	A	107	LEU	CA-CB-CG	6.14	129.43	115.30
3	H	182	LEU	N-CA-CB	6.13	122.67	110.40
3	D	281	ARG	NE-CZ-NH2	-6.11	117.25	120.30
2	B	390	GLU	CA-C-N	6.09	130.60	117.20
3	F	390	GLU	C-N-CA	5.89	136.43	121.70
1	C	107	LEU	CA-CB-CG	5.85	128.76	115.30
2	B	390	GLU	N-CA-C	5.84	126.78	111.00
3	F	390	GLU	N-CA-C	5.76	126.54	111.00
1	G	107	LEU	CA-CB-CG	5.73	128.48	115.30
3	F	390	GLU	O-C-N	-5.72	113.54	122.70
3	D	275	ASP	CB-CG-OD1	5.71	123.44	118.30
1	E	107	LEU	CA-CB-CG	5.68	128.38	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	200	LEU	CA-CB-CG	5.59	128.16	115.30
2	B	390	GLU	C-N-CA	5.54	135.54	121.70
3	F	281	ARG	NE-CZ-NH2	-5.54	117.53	120.30
3	F	274	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	G	48	ARG	NE-CZ-NH1	5.51	123.05	120.30
3	F	281	ARG	NE-CZ-NH1	5.18	122.89	120.30
2	B	281	ARG	NE-CZ-NH1	5.17	122.88	120.30
3	D	342	GLN	CB-CA-C	-5.08	100.24	110.40
3	H	275	ASP	CB-CG-OD1	5.06	122.86	118.30
2	B	339	ARG	N-CA-C	5.03	124.57	111.00
1	A	10	ARG	NE-CZ-NH2	-5.02	117.79	120.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	343	ALA	CA
2	B	391	TYR	CA
3	F	391	TYR	CA

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	ARG	Sidechain
2	B	339	ARG	Peptide
2	B	341	ASP	Peptide
2	B	342	GLN	Peptide
2	B	347	LEU	Peptide
1	C	152	ARG	Sidechain
3	D	339	ARG	Peptide
3	D	342	GLN	Peptide
3	D	343	ALA	Peptide
1	E	152	ARG	Sidechain
1	E	45	THR	Peptide
3	F	181	TH5	Peptide
1	G	152	ARG	Sidechain

5.2 Too-close contacts (i)

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	1267	0	1274	38	1
1	C	1267	0	1274	34	0
1	E	1267	0	1274	38	0
1	G	1267	0	1274	31	0
2	B	1603	0	1555	46	0
3	D	1579	0	1536	39	0
3	F	1490	0	1443	29	0
3	H	1471	0	1427	19	0
4	A	16	0	24	9	0
5	E	4	0	3	0	0
5	G	4	0	3	2	0
6	A	36	0	0	7	0
6	B	48	0	0	2	0
6	C	34	0	0	3	0
6	D	41	0	0	3	1
6	E	32	0	0	7	0
6	F	37	0	0	9	0
6	G	34	0	0	7	0
6	H	30	0	0	5	0
All	All	11527	0	11087	253	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 11.

All (253) 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)
3:H:182:LEU:CA	3:H:182:LEU:N	1.75	1.50
2:B:342:GLN:HB3	2:B:343:ALA:CB	1.44	1.47
2:B:342:GLN:CB	2:B:343:ALA:HB3	1.59	1.32
1:E:40:VAL:HG11	6:E:2007:HOH:O	1.09	1.27
2:B:339:ARG:CB	2:B:342:GLN:HE22	1.51	1.21
2:B:347:LEU:HD12	2:B:348:ARG:N	1.53	1.21
3:F:265:LEU:HA	6:F:2035:HOH:O	1.42	1.18
3:D:339:ARG:HB3	3:D:340:GLY:HA3	1.18	1.16
3:D:343:ALA:CB	3:D:346:ALA:HB3	1.75	1.15
2:B:339:ARG:HB3	2:B:342:GLN:HE22	1.02	1.15
2:B:342:GLN:HB3	2:B:343:ALA:CA	1.76	1.15
2:B:339:ARG:HB3	2:B:340:GLY:HA3	1.31	1.13
2:B:339:ARG:CB	2:B:342:GLN:NE2	2.13	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:378:CYS:HA	6:F:2035:HOH:O	1.48	1.09
3:D:343:ALA:HB1	3:D:346:ALA:HB3	1.17	1.08
2:B:339:ARG:HB3	2:B:342:GLN:NE2	1.67	1.07
3:D:346:ALA:O	3:D:347:LEU:HB2	1.47	1.06
3:D:339:ARG:HB3	3:D:340:GLY:CA	1.90	1.01
4:A:1181:TRS:H12	2:B:181:THR:N	1.78	0.98
2:B:347:LEU:HD12	2:B:347:LEU:C	1.84	0.96
3:D:339:ARG:CB	3:D:340:GLY:HA3	1.98	0.92
1:G:140:ASP:HB3	6:G:2030:HOH:O	1.71	0.90
2:B:342:GLN:HB3	2:B:343:ALA:HB3	0.91	0.89
2:B:339:ARG:HB3	2:B:340:GLY:CA	2.03	0.89
1:A:100:GLY:O	1:G:100:GLY:HA2	1.73	0.88
2:B:342:GLN:CG	2:B:343:ALA:HB3	2.03	0.88
1:E:8:THR:HG21	6:E:2001:HOH:O	1.76	0.86
3:D:343:ALA:HA	3:D:346:ALA:N	1.91	0.85
2:B:337:LYS:O	2:B:338:ALA:HB3	1.73	0.85
1:A:146:ILE:HG21	6:A:2030:HOH:O	1.77	0.85
2:B:347:LEU:HD12	2:B:348:ARG:H	1.42	0.84
3:D:346:ALA:O	3:D:347:LEU:CB	2.27	0.83
3:H:299:CYS:O	6:H:2020:HOH:O	1.97	0.81
1:C:10:ARG:CZ	3:F:231:LEU:HD23	2.11	0.81
2:B:342:GLN:CB	2:B:343:ALA:CA	2.58	0.80
2:B:339:ARG:CB	2:B:340:GLY:HA3	2.09	0.80
1:C:10:ARG:NH2	3:F:231:LEU:HD23	1.96	0.80
1:C:157:ARG:HG2	1:C:166:VAL:HG22	1.63	0.80
2:B:343:ALA:O	2:B:347:LEU:HG	1.83	0.79
2:B:339:ARG:HB2	2:B:342:GLN:NE2	1.98	0.78
1:E:157:ARG:HG2	1:E:166:VAL:HG22	1.65	0.77
2:B:347:LEU:C	2:B:347:LEU:CD1	2.54	0.76
3:D:314:SER:OG	6:D:2029:HOH:O	2.03	0.76
1:A:157:ARG:HG2	1:A:166:VAL:HG22	1.67	0.75
1:G:116:ARG:HB3	6:G:2022:HOH:O	1.86	0.75
5:G:1181:ACT:H1	3:H:181:TH5:N	2.02	0.74
2:B:342:GLN:CB	2:B:343:ALA:CB	2.36	0.73
1:G:60:ALA:O	6:G:2009:HOH:O	2.07	0.73
2:B:346:ALA:O	2:B:347:LEU:HG	1.88	0.73
1:A:19:VAL:HG12	1:A:19:VAL:O	1.86	0.73
1:G:157:ARG:HG2	1:G:166:VAL:HG22	1.71	0.73
2:B:346:ALA:O	2:B:347:LEU:CB	2.35	0.73
1:A:146:ILE:CG2	6:A:2030:HOH:O	2.36	0.72
1:G:126:HIS:CE1	6:G:2025:HOH:O	2.44	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:343:ALA:HB2	3:D:346:ALA:HB3	1.71	0.71
2:B:337:LYS:O	2:B:338:ALA:CB	2.37	0.70
1:E:8:THR:HB	1:E:164:THR:HG21	1.73	0.70
1:G:19:VAL:HG12	1:G:19:VAL:O	1.90	0.70
1:C:10:ARG:CZ	3:F:231:LEU:HA	2.22	0.70
2:B:339:ARG:CA	2:B:342:GLN:HE22	2.04	0.69
2:B:342:GLN:HG2	2:B:343:ALA:HB3	1.73	0.69
3:D:280:LYS:HE2	6:D:2020:HOH:O	1.92	0.69
1:E:121:GLU:OE1	6:E:2021:HOH:O	2.11	0.69
2:B:346:ALA:O	2:B:347:LEU:CG	2.41	0.68
1:E:19:VAL:HG12	1:E:19:VAL:O	1.94	0.68
3:F:266:ILE:N	6:F:2035:HOH:O	2.27	0.67
1:G:10:ARG:HG3	3:H:189:ASP:OD2	1.94	0.67
1:G:104:GLY:O	6:G:2009:HOH:O	2.13	0.67
1:G:129:THR:HG22	6:G:2024:HOH:O	1.95	0.66
3:F:382:GLU:HG3	6:F:2020:HOH:O	1.94	0.66
1:G:8:THR:HB	1:G:164:THR:HG21	1.78	0.66
3:D:339:ARG:CB	3:D:342:GLN:OE1	2.44	0.66
1:A:8:THR:HB	1:A:164:THR:HG21	1.77	0.66
3:F:377:GLY:O	6:F:2035:HOH:O	2.13	0.66
1:C:8:THR:HG21	6:C:2001:HOH:O	1.96	0.65
1:A:111:THR:HG21	1:A:170:LYS:HE2	1.79	0.65
3:D:343:ALA:CB	3:D:346:ALA:CB	2.65	0.65
1:C:111:THR:HG21	1:C:170:LYS:HE2	1.79	0.64
1:C:8:THR:HB	1:C:164:THR:HG21	1.79	0.64
3:D:339:ARG:HB2	3:D:342:GLN:OE1	1.98	0.64
1:C:10:ARG:NH1	3:F:231:LEU:HA	2.13	0.63
1:A:97:ARG:NH1	6:A:2017:HOH:O	2.31	0.62
1:E:111:THR:HG21	1:E:170:LYS:HE2	1.82	0.62
1:C:10:ARG:NH2	3:F:231:LEU:HA	2.16	0.61
3:D:274:ARG:HD3	3:D:318:ASP:OD2	2.01	0.61
2:B:339:ARG:HA	2:B:339:ARG:NE	2.15	0.60
1:C:19:VAL:HG12	1:C:19:VAL:O	2.01	0.60
1:G:19:VAL:HG11	1:G:123:ILE:HG12	1.83	0.60
1:A:150:ASP:OD2	1:A:154:LYS:NZ	2.32	0.60
2:B:274:ARG:HD3	2:B:318:ASP:OD2	2.01	0.59
3:D:342:GLN:O	3:D:343:ALA:HB2	2.03	0.59
1:E:61:VAL:HA	6:E:2007:HOH:O	2.04	0.58
1:C:10:ARG:HH22	3:F:230:GLY:C	2.07	0.58
1:C:82:LEU:CD1	6:C:2012:HOH:O	2.52	0.58
1:A:74:ARG:HG3	4:A:1182:TRS:H22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:343:ALA:HB1	3:D:346:ALA:CB	2.11	0.58
1:A:57:CYS:SG	1:A:108:ILE:O	2.62	0.57
3:F:265:LEU:CA	6:F:2035:HOH:O	2.19	0.57
1:E:19:VAL:HG11	1:E:123:ILE:HG12	1.86	0.57
1:A:19:VAL:HG11	1:A:123:ILE:HG12	1.87	0.57
2:B:301:PRO:HB3	2:B:351:VAL:HG12	1.86	0.57
3:H:274:ARG:HD3	3:H:318:ASP:OD2	2.04	0.56
1:C:19:VAL:HG11	1:C:123:ILE:HG12	1.87	0.56
3:F:274:ARG:HD3	3:F:318:ASP:OD2	2.05	0.56
3:H:195:ALA:HB3	6:H:2002:HOH:O	2.05	0.56
1:E:67:ARG:CZ	1:E:101:LEU:CD2	2.84	0.56
2:B:333:VAL:HG11	2:B:351:VAL:HG21	1.88	0.55
4:A:1181:TRS:C1	2:B:181:THR:N	2.64	0.55
3:H:297:HIS:ND1	3:H:381:THR:HG22	2.21	0.55
2:B:342:GLN:HB2	6:B:2036:HOH:O	2.07	0.54
1:E:43:VAL:O	1:E:179:MET:HE1	2.07	0.54
1:E:150:ASP:OD2	1:E:154:LYS:NZ	2.38	0.54
3:D:342:GLN:O	3:D:343:ALA:CB	2.56	0.54
1:G:150:ASP:OD2	1:G:154:LYS:NZ	2.38	0.54
1:A:140:ASP:OD1	1:A:144:ARG:NH1	2.41	0.54
1:C:150:ASP:OD2	1:C:154:LYS:NZ	2.41	0.54
2:B:297:HIS:HB2	2:B:379:ASP:HB2	1.91	0.53
2:B:297:HIS:ND1	2:B:381:THR:HG22	2.23	0.53
1:E:38:ALA:HB3	1:E:66:ALA:O	2.09	0.53
4:A:1181:TRS:O1	4:A:1181:TRS:O3	2.20	0.53
1:E:67:ARG:CZ	1:E:101:LEU:HD21	2.39	0.53
1:C:35:THR:HB	1:E:67:ARG:NH1	2.24	0.53
3:F:353:GLU:HB2	6:F:2030:HOH:O	2.09	0.53
1:A:74:ARG:HG3	4:A:1182:TRS:C2	2.39	0.52
1:C:43:VAL:O	1:C:179:MET:HE1	2.10	0.52
1:G:111:THR:HG21	1:G:170:LYS:HE2	1.92	0.52
3:F:297:HIS:ND1	3:F:381:THR:HG22	2.24	0.52
1:E:71:VAL:HG11	1:E:146:ILE:HG22	1.92	0.52
1:E:40:VAL:CG1	6:E:2007:HOH:O	1.96	0.52
3:H:352:ALA:HB1	6:H:2020:HOH:O	2.10	0.51
1:G:129:THR:HA	6:G:2024:HOH:O	2.11	0.50
1:C:8:THR:N	1:C:9:PRO:HD2	2.27	0.50
1:C:140:ASP:OD1	1:C:144:ARG:NH1	2.44	0.50
3:D:343:ALA:CA	3:D:346:ALA:O	2.60	0.49
3:D:292:VAL:O	3:D:296:VAL:HG23	2.11	0.49
3:H:352:ALA:CB	6:H:2020:HOH:O	2.58	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:LEU:HD12	6:C:2012:HOH:O	2.12	0.49
1:E:71:VAL:HA	1:E:109:ALA:O	2.12	0.49
2:B:297:HIS:CE1	2:B:381:THR:HG22	2.47	0.49
1:G:171:GLY:O	1:G:175:LEU:HD13	2.11	0.49
1:G:19:VAL:HG11	1:G:123:ILE:HA	1.95	0.49
1:A:144:ARG:HD2	6:A:2028:HOH:O	2.13	0.49
3:F:381:THR:HB	6:F:2036:HOH:O	2.12	0.49
1:A:8:THR:N	1:A:9:PRO:HD2	2.27	0.49
1:A:74:ARG:HG2	4:A:1182:TRS:H12	1.95	0.49
1:G:140:ASP:OD1	1:G:144:ARG:NH1	2.46	0.49
3:D:208:THR:HB	3:D:252:VAL:HG21	1.94	0.48
1:A:168:ILE:CD1	6:A:2030:HOH:O	2.60	0.48
3:D:343:ALA:O	3:D:346:ALA:O	2.31	0.48
1:A:74:ARG:HH11	1:A:74:ARG:HB2	1.78	0.48
1:C:10:ARG:CZ	3:F:231:LEU:CD2	2.89	0.48
3:D:297:HIS:ND1	3:D:381:THR:HG22	2.27	0.48
1:G:71:VAL:HG11	1:G:146:ILE:HG22	1.94	0.48
1:G:19:VAL:O	1:G:19:VAL:CG1	2.60	0.48
1:A:111:THR:HG21	1:A:170:LYS:CE	2.43	0.48
1:C:74:ARG:HB2	1:C:74:ARG:HH11	1.79	0.48
1:C:164:THR:O	3:D:188:THR:HA	2.13	0.48
3:D:297:HIS:CE1	3:D:381:THR:HG22	2.49	0.48
1:E:8:THR:N	1:E:9:PRO:HD2	2.28	0.48
3:D:280:LYS:CE	6:D:2020:HOH:O	2.58	0.48
3:H:297:HIS:HB2	3:H:379:ASP:HB2	1.96	0.48
1:E:172:VAL:HG11	3:F:258:ASP:HB3	1.96	0.47
1:G:8:THR:N	1:G:9:PRO:HD2	2.30	0.47
3:H:297:HIS:CE1	3:H:381:THR:HG22	2.49	0.47
1:C:146:ILE:HD13	1:C:168:ILE:HD12	1.96	0.47
1:A:148:THR:HA	4:A:1182:TRS:H21	1.96	0.47
2:B:333:VAL:HG12	2:B:347:LEU:HD13	1.95	0.47
1:C:111:THR:HG21	1:C:170:LYS:CE	2.43	0.47
2:B:301:PRO:HB3	2:B:351:VAL:CG1	2.45	0.47
3:D:333:VAL:HG11	3:D:351:VAL:HG21	1.97	0.47
1:E:26:ARG:HD2	1:E:27:ASP:O	2.14	0.47
1:E:140:ASP:OD1	1:E:144:ARG:NH1	2.47	0.46
1:A:171:GLY:O	1:A:175:LEU:HD13	2.15	0.46
1:E:10:ARG:HG3	3:F:189:ASP:OD2	2.14	0.46
1:C:19:VAL:HG11	1:C:123:ILE:HA	1.97	0.46
1:E:138:GLY:HA2	6:E:2025:HOH:O	2.16	0.46
1:A:168:ILE:HD11	6:A:2030:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:VAL:O	1:A:19:VAL:CG1	2.58	0.46
1:A:97:ARG:CZ	6:A:2017:HOH:O	2.62	0.46
3:F:297:HIS:HB2	3:F:379:ASP:HB2	1.98	0.46
3:D:297:HIS:HB2	3:D:379:ASP:HB2	1.97	0.46
5:G:1181:ACT:H1	3:H:181:TH5:HN1	1.80	0.46
1:C:67:ARG:CZ	1:C:101:LEU:HD21	2.46	0.45
1:C:171:GLY:O	1:C:175:LEU:HD13	2.16	0.45
2:B:286:VAL:HG21	2:B:364:ILE:CD1	2.46	0.45
3:H:184:THR:O	3:H:224:ALA:HA	2.16	0.45
2:B:339:ARG:CG	2:B:340:GLY:HA3	2.45	0.45
1:G:74:ARG:HH11	1:G:74:ARG:HB2	1.81	0.45
1:G:146:ILE:HD13	1:G:168:ILE:HD12	1.98	0.45
1:E:44:PHE:CE2	3:F:223:THR:HG23	2.51	0.45
2:B:230:GLY:HA3	6:B:2002:HOH:O	2.16	0.45
1:G:165:LEU:HD21	3:H:244:LEU:HA	1.98	0.45
1:C:57:CYS:SG	1:C:108:ILE:O	2.75	0.45
1:E:8:THR:CG2	6:E:2001:HOH:O	2.50	0.45
2:B:320:ASP:O	2:B:324:VAL:HG23	2.17	0.44
1:A:148:THR:OG1	4:A:1181:TRS:H32	2.18	0.44
3:D:343:ALA:HA	3:D:345:ASP:C	2.37	0.44
2:B:343:ALA:O	2:B:346:ALA:O	2.35	0.44
3:F:208:THR:HB	3:F:252:VAL:HG21	1.99	0.44
1:G:171:GLY:C	1:G:175:LEU:HD13	2.36	0.44
1:G:67:ARG:CZ	1:G:101:LEU:CD2	2.96	0.44
3:D:343:ALA:HA	3:D:346:ALA:H	1.80	0.44
3:D:181:TH5:HG22	3:D:221:SER:HB2	1.99	0.43
3:F:297:HIS:CE1	3:F:381:THR:HG22	2.52	0.43
1:A:67:ARG:CZ	1:A:101:LEU:CD2	2.96	0.43
1:C:35:THR:HB	1:E:67:ARG:HH12	1.83	0.43
1:C:71:VAL:HG11	1:C:146:ILE:HG22	1.99	0.43
1:A:10:ARG:HG3	2:B:189:ASP:OD2	2.18	0.43
3:D:341:ASP:O	3:D:343:ALA:N	2.47	0.43
1:G:26:ARG:HD2	1:G:27:ASP:O	2.19	0.43
3:H:182:LEU:N	3:H:182:LEU:C	2.62	0.43
1:A:73:ALA:C	1:A:74:ARG:HD3	2.39	0.43
3:F:271:THR:O	3:F:365:ASP:HA	2.18	0.43
1:C:73:ALA:C	1:C:74:ARG:HD3	2.39	0.43
1:E:19:VAL:HG11	1:E:123:ILE:HA	2.01	0.43
1:E:146:ILE:HD13	1:E:168:ILE:HD12	2.00	0.43
1:A:43:VAL:O	1:A:179:MET:HE1	2.19	0.43
1:A:171:GLY:C	1:A:175:LEU:HD13	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:ARG:HH11	1:E:74:ARG:HB2	1.84	0.43
2:B:339:ARG:CB	2:B:340:GLY:CA	2.77	0.42
1:C:19:VAL:O	1:C:19:VAL:CG1	2.68	0.42
1:E:19:VAL:O	1:E:19:VAL:CG1	2.65	0.42
1:A:38:ALA:HB3	1:A:66:ALA:O	2.19	0.42
1:A:70:VAL:HG13	1:A:108:ILE:HG13	2.01	0.42
1:G:172:VAL:HG23	3:H:260:GLU:HG3	2.02	0.42
3:H:382:GLU:HG3	6:H:2019:HOH:O	2.20	0.42
3:D:343:ALA:CA	3:D:345:ASP:N	2.83	0.41
1:G:43:VAL:O	1:G:179:MET:HE1	2.20	0.41
1:A:19:VAL:HG11	1:A:123:ILE:HA	2.01	0.41
1:A:22:ALA:H	1:A:74:ARG:HH12	1.67	0.41
3:D:200:LEU:C	3:D:200:LEU:HD23	2.40	0.41
3:F:299:CYS:C	3:F:355:LEU:HD23	2.40	0.41
1:A:44:PHE:O	1:A:179:MET:HA	2.20	0.41
1:C:10:ARG:HG3	3:D:189:ASP:OD2	2.19	0.41
1:A:67:ARG:CZ	1:A:101:LEU:HD21	2.50	0.41
1:A:74:ARG:CG	4:A:1182:TRS:H22	2.49	0.41
3:D:343:ALA:HA	3:D:346:ALA:O	2.21	0.41
1:C:172:VAL:HG23	3:D:260:GLU:HG3	2.03	0.41
1:E:73:ALA:O	1:E:74:ARG:HD3	2.21	0.41
1:E:171:GLY:O	1:E:175:LEU:HD13	2.21	0.41
3:F:182:LEU:O	3:F:222:ASP:HA	2.21	0.41
3:H:216:THR:HG22	3:H:288:ASN:CG	2.41	0.41
3:D:320:ASP:O	3:D:324:VAL:HG23	2.21	0.41
1:E:179:MET:HE3	3:F:223:THR:N	2.36	0.41
1:G:156:VAL:HG22	1:G:157:ARG:N	2.35	0.40
1:E:67:ARG:NH1	1:E:101:LEU:CD2	2.85	0.40
1:G:179:MET:HE3	3:H:223:THR:N	2.36	0.40
1:E:73:ALA:C	1:E:74:ARG:HD3	2.41	0.40
3:F:182:LEU:HD11	3:F:209:PHE:CD1	2.56	0.40
3:F:335:PRO:HG3	6:F:2028:HOH:O	2.22	0.40
3:D:343:ALA:CA	3:D:344:ASP:C	2.90	0.40
1:E:9:PRO:HD3	1:E:166:VAL:HG23	2.02	0.40
1:E:44:PHE:O	1:E:179:MET:HA	2.22	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:NH2	6:D:2029:HOH:O[2_544]	2.18	0.02

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	171/173 (99%)	163 (95%)	8 (5%)	0	100	100
1	C	171/173 (99%)	163 (95%)	8 (5%)	0	100	100
1	E	171/173 (99%)	164 (96%)	7 (4%)	0	100	100
1	G	171/173 (99%)	164 (96%)	7 (4%)	0	100	100
2	B	211/213 (99%)	197 (93%)	9 (4%)	5 (2%)	6	3
3	D	208/213 (98%)	196 (94%)	6 (3%)	6 (3%)	4	2
3	F	193/213 (91%)	185 (96%)	5 (3%)	3 (2%)	9	7
3	H	191/213 (90%)	186 (97%)	4 (2%)	1 (0%)	29	31
All	All	1487/1544 (96%)	1418 (95%)	54 (4%)	15 (1%)	15	14

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	391	TYR
3	D	339	ARG
3	D	342	GLN
3	D	343	ALA
3	D	347	LEU
3	F	391	TYR
2	B	338	ALA
2	B	339	ARG
2	B	343	ALA
3	F	182	LEU
3	D	345	ASP
3	D	369	ALA
3	H	369	ALA
2	B	369	ALA
3	F	369	ALA

5.3.2 Protein sidechains (i)

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	128/128 (100%)	119 (93%)	9 (7%)	15	16
1	C	128/128 (100%)	118 (92%)	10 (8%)	12	12
1	E	128/128 (100%)	117 (91%)	11 (9%)	10	10
1	G	128/128 (100%)	118 (92%)	10 (8%)	12	12
2	B	166/166 (100%)	156 (94%)	10 (6%)	19	22
3	D	162/165 (98%)	153 (94%)	9 (6%)	21	24
3	F	155/165 (94%)	147 (95%)	8 (5%)	23	28
3	H	153/165 (93%)	146 (95%)	7 (5%)	27	33
All	All	1148/1173 (98%)	1074 (94%)	74 (6%)	17	19

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ARG
1	A	92	ARG
1	A	93	GLU
1	A	107	LEU
1	A	113	VAL
1	A	116	ARG
1	A	160	VAL
1	A	170	LYS
1	A	175	LEU
2	B	182	LEU
2	B	200	LEU
2	B	242	GLU
2	B	337	LYS
2	B	339	ARG
2	B	347	LEU
2	B	355	LEU
2	B	356	ARG
2	B	373	PHE
2	B	391	TYR

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Mol	Chain	Res	Type
1	C	74	ARG
1	C	92	ARG
1	C	93	GLU
1	C	107	LEU
1	C	113	VAL
1	C	116	ARG
1	C	157	ARG
1	C	160	VAL
1	C	170	LYS
1	C	175	LEU
3	D	182	LEU
3	D	200	LEU
3	D	242	GLU
3	D	339	ARG
3	D	342	GLN
3	D	348	ARG
3	D	355	LEU
3	D	356	ARG
3	D	373	PHE
1	E	46	ARG
1	E	74	ARG
1	E	92	ARG
1	E	93	GLU
1	E	107	LEU
1	E	113	VAL
1	E	116	ARG
1	E	157	ARG
1	E	160	VAL
1	E	170	LYS
1	E	175	LEU
3	F	182	LEU
3	F	200	LEU
3	F	219	SER
3	F	242	GLU
3	F	355	LEU
3	F	356	ARG
3	F	373	PHE
3	F	391	TYR
1	G	74	ARG
1	G	92	ARG
1	G	93	GLU
1	G	107	LEU

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Mol	Chain	Res	Type
1	G	113	VAL
1	G	116	ARG
1	G	157	ARG
1	G	160	VAL
1	G	170	LYS
1	G	175	LEU
3	H	182	LEU
3	H	200	LEU
3	H	216	THR
3	H	242	GLU
3	H	355	LEU
3	H	356	ARG
3	H	373	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	342	GLN
1	C	65	GLN
1	E	65	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	$\#\|Z\| > 2$
3	TH5	F	181	3	8,9,10	0.95	1 (12%)	9,11,13	2.74	4 (44%)
3	TH5	D	181	3	8,9,10	1.98	4 (50%)	9,11,13	2.17	2 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	TH5	H	181	3	8,9,10	1.32	1 (12%)	9,11,13	3.21	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
3	TH5	F	181	3	-	1/8/10/12	-
3	TH5	D	181	3	-	0/8/10/12	-
3	TH5	H	181	3	-	0/8/10/12	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	181	TH5	OG1-CAH	3.17	1.42	1.35
3	D	181	TH5	OG1-CB	-3.02	1.41	1.46
3	D	181	TH5	CG2-CB	2.47	1.57	1.51
3	F	181	TH5	CG2-CB	2.16	1.56	1.51
3	H	181	TH5	CG2-CB	2.12	1.56	1.51
3	D	181	TH5	O-C	2.08	1.28	1.19

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	181	TH5	OG1-CAH-CAA	6.91	123.80	111.09
3	F	181	TH5	OG1-CAH-CAA	6.83	123.65	111.09
3	D	181	TH5	OG1-CAH-CAA	5.19	120.65	111.09
3	H	181	TH5	OG1-CB-CA	-3.47	98.01	105.89
3	H	181	TH5	OG1-CAH-OAD	-3.15	116.70	122.96
3	H	181	TH5	OG1-CB-CG2	2.92	114.01	108.21
3	H	181	TH5	CG2-CB-CA	-2.91	107.43	113.16
3	F	181	TH5	OG1-CAH-OAD	-2.80	117.41	122.96
3	F	181	TH5	O-C-CA	-2.22	118.96	124.78
3	D	181	TH5	OG1-CB-CA	-2.19	100.93	105.89
3	F	181	TH5	CB-OG1-CAH	-2.09	113.86	117.81

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	181	TH5	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	181	TH5	1	0
3	H	181	TH5	2	0

5.5 Carbohydrates (i)

There are no monosaccharides 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	$\#\|Z\| > 2$
5	ACT	E	1181	-	3,3,3	0.71	0	3,3,3	1.16	0
4	TRS	A	1181	-	7,7,7	1.16	1 (14%)	9,9,9	1.45	1 (11%)
5	ACT	G	1181	-	3,3,3	0.95	0	3,3,3	0.59	0
4	TRS	A	1182	-	7,7,7	1.15	0	9,9,9	1.64	3 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TRS	A	1181	-	-	7/9/9/9	-
4	TRS	A	1182	-	-	6/9/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1181	TRS	C-N	-2.60	1.40	1.49

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1181	TRS	O3-C3-C	-3.48	99.96	111.00
4	A	1182	TRS	O1-C1-C	2.60	119.23	111.00
4	A	1182	TRS	C2-C-N	-2.57	100.31	107.98
4	A	1182	TRS	C3-C-C1	2.43	118.34	110.81

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1181	TRS	C2-C-C1-O1
4	A	1181	TRS	C3-C-C1-O1
4	A	1181	TRS	N-C-C1-O1
4	A	1181	TRS	N-C-C3-O3
4	A	1182	TRS	C3-C-C2-O2
4	A	1182	TRS	C1-C-C3-O3
4	A	1182	TRS	C2-C-C3-O3
4	A	1182	TRS	N-C-C3-O3
4	A	1181	TRS	C3-C-C2-O2
4	A	1181	TRS	N-C-C2-O2
4	A	1182	TRS	C1-C-C2-O2
4	A	1182	TRS	N-C-C2-O2
4	A	1181	TRS	C1-C-C2-O2

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1181	TRS	4	0
5	G	1181	ACT	2	0
4	A	1182	TRS	5	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	173/173 (100%)	0.24	4 (2%)	60	69	28, 36, 50, 55	0
1	C	173/173 (100%)	0.30	4 (2%)	60	69	28, 37, 50, 53	0
1	E	173/173 (100%)	0.20	6 (3%)	44	54	30, 38, 49, 54	0
1	G	173/173 (100%)	0.37	9 (5%)	27	38	32, 40, 50, 57	0
2	B	213/213 (100%)	0.11	3 (1%)	75	82	24, 35, 46, 52	0
3	D	209/213 (98%)	0.22	8 (3%)	40	51	25, 36, 48, 54	0
3	F	196/213 (92%)	0.40	10 (5%)	28	39	28, 38, 50, 61	0
3	H	194/213 (91%)	0.30	10 (5%)	27	38	27, 39, 53, 66	0
All	All	1504/1544 (97%)	0.27	54 (3%)	42	53	24, 37, 50, 66	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	352	ALA	14.2
3	F	336	PRO	12.2
3	H	352	ALA	6.8
3	H	390	GLU	4.8
3	H	336	PRO	4.7
3	F	335	PRO	4.7
1	C	157	ARG	4.4
1	G	82	LEU	4.3
1	C	10	ARG	4.3
3	D	343	ALA	4.1
3	D	259	GLY	4.1
3	D	262	ALA	4.0
3	F	331	VAL	3.8
1	G	160	VAL	3.7
3	H	331	VAL	3.6
1	E	161	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	103	GLU	3.0
1	G	161	GLY	3.0
1	A	102	PRO	2.9
1	A	97	ARG	2.9
3	H	330	GLU	2.9
3	F	355	LEU	2.9
3	H	353	GLU	2.9
1	E	158	VAL	2.8
1	C	158	VAL	2.8
2	B	339	ARG	2.8
3	H	239	GLU	2.7
1	E	162	GLY	2.7
3	D	260	GLU	2.6
3	H	358	ASP	2.6
1	A	134	ALA	2.5
1	G	97	ARG	2.4
2	B	342	GLN	2.4
1	G	116	ARG	2.4
3	H	328	PHE	2.4
1	G	89	ARG	2.3
3	D	339	ARG	2.3
3	D	263	ALA	2.3
3	F	322	GLU	2.2
3	F	356	ARG	2.2
1	G	158	VAL	2.2
3	D	242	GLU	2.2
1	E	157	ARG	2.2
1	E	160	VAL	2.2
3	F	353	GLU	2.2
3	H	335	PRO	2.2
1	G	164	THR	2.1
3	D	261	GLY	2.1
3	F	207	ARG	2.1
3	F	330	GLU	2.0
2	B	347	LEU	2.0
1	G	120	MET	2.0
1	E	138	GLY	2.0
1	C	121	GLU	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
3	TH5	H	181	10/11	0.92	0.18	18,28,31,32	0
3	TH5	D	181	10/11	0.95	0.13	16,25,26,27	0
3	TH5	F	181	10/11	0.96	0.16	21,27,29,29	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ACT	G	1181	4/4	0.75	0.29	48,49,49,49	0
4	TRS	A	1182	8/8	0.79	0.30	38,39,40,41	0
4	TRS	A	1181	8/8	0.84	0.26	35,35,39,40	0
5	ACT	E	1181	4/4	0.93	0.32	46,47,47,47	0

6.5 Other polymers (i)

There are no such residues in this entry.