Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2024 – 02:37 am BST

PDB ID	:	2XGM
Title	:	Substrate and product analogues as human O-GlcNAc transferase inhibitors.
Authors	:	Dorfmueller, H.C.; Borodkin, V.S.; Blair, D.E.; Pathak, S.; Navratilova, I.; van Aalten, D.M.
Deposited on	:	2010-06-07
Resolution	:	2.55 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:

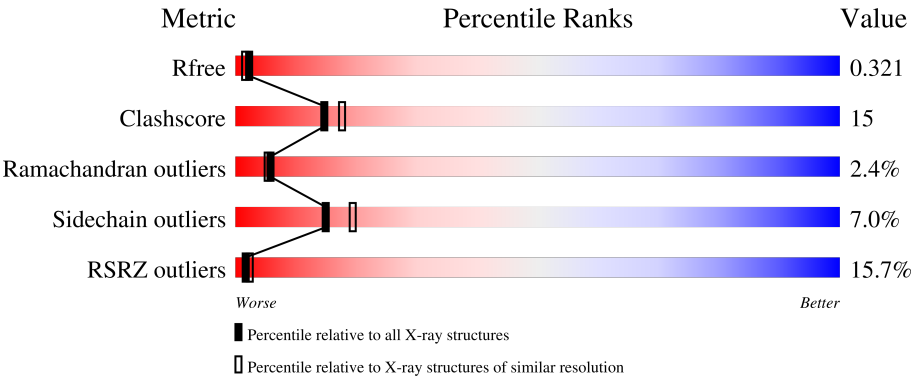
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	568	9% 68% 19% • • 10%
1	B	568	20% 68% 23% • • 5%

2 Entry composition

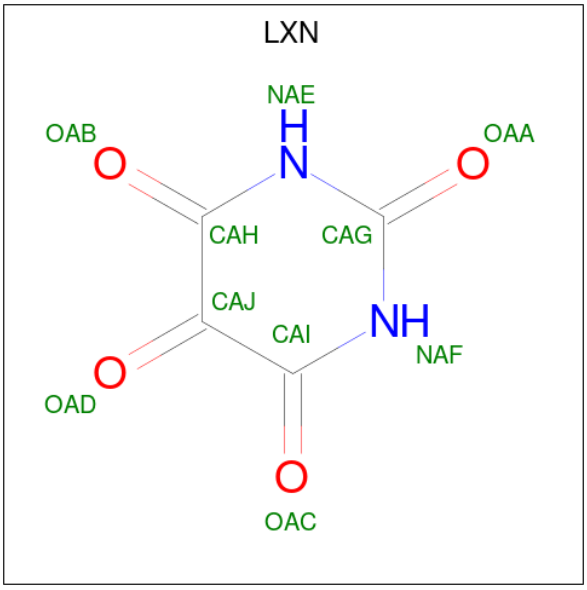
There are 3 unique types of molecules in this entry. The entry contains 8113 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 XCOGT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	512	Total	C	N	O	S	0	2	0
			3923	2480	730	700	13			
1	B	542	Total	C	N	O	S	0	0	0
			4112	2595	761	740	16			

- Molecule 2 is ALLOXAN (three-letter code: LXN) (formula: $C_4H_2N_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	4	2	4		
2	B	1	Total	C	N	O	0	0
			10	4	2	4		

- Molecule 3 is water.

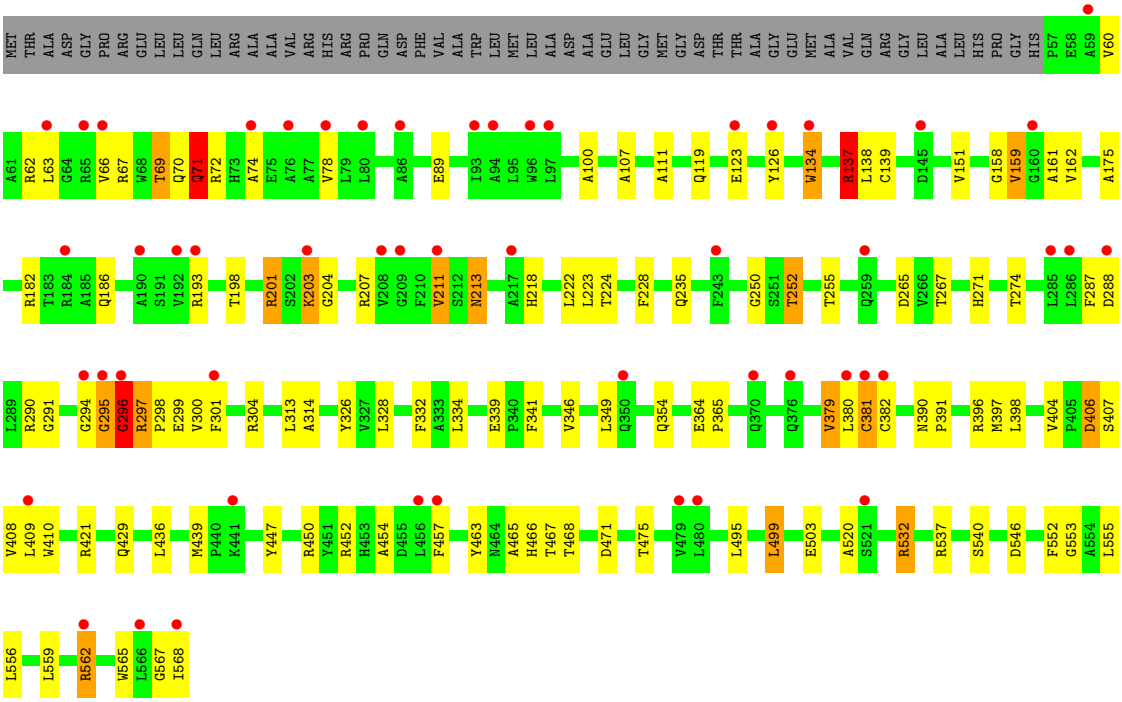
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	21	Total O 21 21	0	0
3	B	37	Total O 37 37	0	0

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.

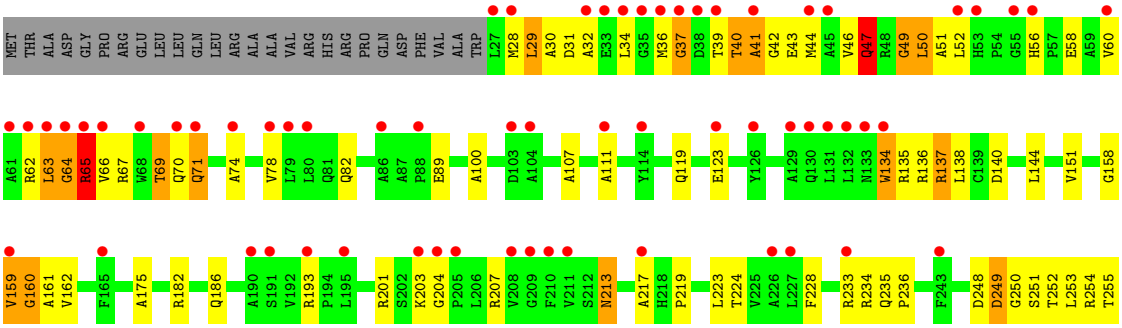
• Molecule 1: XCOGT

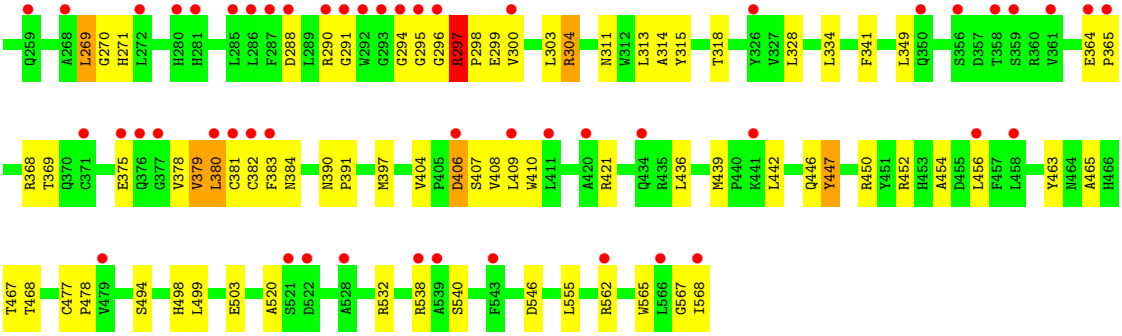
Chain A:



• Molecule 1: XCOGT

Chain B:




Q259
A268
L269
G270
H271
L272
H280
H281
L285
L286
F287
D288
L289
R290
G291
W292
G293
G294
G295
G296
R297
P298
E299
V300
L303
R304
N311
W312
L313
A314
Y315
T318
Y326
V327
L328
L334
F341
L349
Q350
S356
D357
T358
S359
R360
V361
E364
P365
R368
T369
Q370
C371
E375
Q376
G377
V378
V379
L380
C381
C382
F383
N384
N390
P391
M397
V404
P405
D406
S407
V408
L409
W410
L411
A420
R421
Q434
R435
L436
M439
P440
K441
L442
Q446
Y447
R450
Y451
R452
H453
A454
D455
L456
F457
L458
Y463
N464
A465
H466
T467
T468
C477
P478
V479
S494
H498
L499
E503
A520
S521
D522
A528
R532
R538
A539
S540
F543
D546
L555
R562
W565
L566
G567
I568

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.53Å 99.98Å 157.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.55 20.00 – 2.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.55) 97.7 (20.00-2.55)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.94 (at 2.56Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.267 , 0.309 0.278 , 0.321	Depositor DCC
R_{free} test set	1334 reflections (3.13%)	wwPDB-VP
Wilson B-factor (Å^2)	74.6	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 66.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8113	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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

5.1 Standard geometry

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

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	0.78	1/4031 (0.0%)	0.87	8/5501 (0.1%)
1	B	0.64	0/4217	0.83	7/5753 (0.1%)
All	All	0.71	1/8248 (0.0%)	0.85	15/11254 (0.1%)

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	3
1	B	0	5
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	CYS	CB-SG	-5.97	1.72	1.81

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	562	ARG	NE-CZ-NH1	-9.71	115.45	120.30
1	A	562	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	B	562	ARG	NE-CZ-NH2	8.28	124.44	120.30
1	A	562	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	A	297	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	A	297	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	B	249	ASP	CB-CG-OD2	7.46	125.02	118.30
1	A	537	ARG	NE-CZ-NH2	-7.45	116.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	421	ARG	NE-CZ-NH1	-7.15	116.72	120.30
1	B	297	ARG	NE-CZ-NH1	-6.56	117.02	120.30
1	B	203	LYS	C-N-CA	5.78	134.43	122.30
1	B	269	LEU	C-N-CA	5.68	134.24	122.30
1	A	137	ARG	NE-CZ-NH2	5.39	123.00	120.30
1	B	297	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	A	396	ARG	NE-CZ-NH2	-5.17	117.72	120.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	203	LYS	Peptide
1	A	296	GLY	Peptide
1	A	406	ASP	Peptide
1	B	160	GLY	Peptide
1	B	296	GLY	Peptide
1	B	406	ASP	Peptide
1	B	63	LEU	Peptide
1	B	64	GLY	Peptide

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	3923	0	3855	116	0
1	B	4112	0	4043	134	0
2	A	10	0	2	0	0
2	B	10	0	2	0	0
3	A	21	0	0	4	0
3	B	37	0	0	10	0
All	All	8113	0	7902	244	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 15.

All (244) 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:B:442:LEU:HB3	3:B:2031:HOH:O	1.31	1.26
1:A:67:ARG:HD2	3:A:2001:HOH:O	1.44	1.15
1:B:382:CYS:HB2	1:B:397:MET:HE1	1.24	1.12
1:B:40:THR:HA	1:B:41:ALA:HB3	1.44	0.99
1:B:382:CYS:HB2	1:B:397:MET:CE	1.93	0.98
1:B:382:CYS:CB	1:B:397:MET:HE1	1.92	0.98
1:A:290:ARG:NE	1:A:297:ARG:H	1.62	0.97
1:A:290:ARG:HE	1:A:297:ARG:N	1.63	0.96
1:B:383:PHE:CE1	3:B:2027:HOH:O	2.19	0.95
1:A:290:ARG:HE	1:A:297:ARG:H	0.97	0.95
1:B:446:GLN:HB2	3:B:2031:HOH:O	1.66	0.94
1:A:354:GLN:HE21	1:A:466[A]:HIS:CE1	1.87	0.93
1:B:328:LEU:HD11	1:B:349:LEU:HG	1.52	0.92
1:A:382:CYS:CB	1:A:397:MET:HE1	2.00	0.91
1:A:158:GLY:HA2	1:A:159:VAL:O	1.71	0.90
1:A:406:ASP:HB2	3:A:2015:HOH:O	1.75	0.86
1:A:354:GLN:NE2	1:A:466[A]:HIS:CE1	2.43	0.86
1:A:382:CYS:HB2	1:A:397:MET:CE	2.05	0.86
1:B:43:GLU:C	1:B:47:GLN:HE22	1.79	0.86
1:A:328:LEU:HD11	1:A:349:LEU:HG	1.59	0.84
1:B:223:LEU:HD11	1:B:467:THR:HG22	1.59	0.83
1:A:67:ARG:NH1	1:A:70:GLN:OE1	2.10	0.83
1:B:213:ASN:HD22	1:B:213:ASN:H	1.26	0.83
1:A:223:LEU:HD21	1:A:467:THR:HG22	1.60	0.82
1:A:295:GLY:O	1:A:296:GLY:O	2.00	0.80
1:A:354:GLN:NE2	1:A:466[A]:HIS:ND1	2.30	0.79
1:A:382:CYS:HB2	1:A:397:MET:HE1	1.60	0.78
1:B:151:VAL:HG13	1:B:162:VAL:HG22	1.65	0.78
1:A:382:CYS:SG	1:A:397:MET:HE1	2.25	0.76
1:B:378:VAL:HB	3:B:2025:HOH:O	1.84	0.76
1:B:151:VAL:HG13	1:B:162:VAL:CG2	2.16	0.75
1:A:159:VAL:O	1:A:159:VAL:HG23	1.86	0.74
1:A:213:ASN:H	1:A:213:ASN:HD22	1.37	0.73
1:B:290:ARG:HH11	1:B:297:ARG:H	1.38	0.72
1:B:381:CYS:HB2	3:B:2027:HOH:O	1.89	0.72
1:A:159:VAL:O	1:A:159:VAL:CG2	2.38	0.71
1:B:158:GLY:HA2	1:B:159:VAL:O	1.90	0.71
1:A:290:ARG:HH11	1:A:298:PRO:HD3	1.56	0.70
1:A:568:ILE:HG22	1:A:568:ILE:O	1.90	0.70
1:A:252:THR:HA	1:B:252:THR:HG22	1.73	0.70
1:B:368:ARG:HB3	3:B:2024:HOH:O	1.92	0.69
1:B:288:ASP:CG	1:B:290:ARG:HH21	1.96	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:LEU:O	1:B:66:VAL:HB	1.93	0.68
1:B:40:THR:HG21	1:B:70:GLN:HE21	1.59	0.68
1:B:40:THR:CA	1:B:41:ALA:HB3	2.22	0.67
1:B:111:ALA:HB2	1:B:134:TRP:HD1	1.58	0.67
1:A:235:GLN:HE21	1:A:235:GLN:HA	1.59	0.67
1:A:288:ASP:CG	1:A:290:ARG:HH21	1.97	0.67
1:B:46:VAL:N	1:B:47:GLN:O	2.28	0.66
1:B:290:ARG:HH11	1:B:298:PRO:HD3	1.60	0.66
1:B:56:HIS:HD2	1:B:58:GLU:H	1.44	0.65
1:B:297:ARG:H	1:B:298:PRO:HD3	1.63	0.64
1:B:288:ASP:OD2	1:B:290:ARG:NH2	2.31	0.63
1:A:382:CYS:HB2	1:A:397:MET:HE2	1.79	0.63
1:B:201:ARG:NH1	1:B:207:ARG:HE	1.96	0.63
1:B:313:LEU:O	1:B:313:LEU:HG	1.97	0.63
1:A:182:ARG:HH21	1:A:186:GLN:HE22	1.47	0.63
1:A:111:ALA:HB2	1:A:134:TRP:HD1	1.63	0.62
1:B:568:ILE:O	1:B:568:ILE:HG22	2.01	0.61
1:B:67:ARG:HA	1:B:67:ARG:HE	1.65	0.60
1:A:290:ARG:NH1	1:A:298:PRO:HD3	2.15	0.60
1:B:56:HIS:CD2	1:B:58:GLU:HB2	2.36	0.60
1:B:43:GLU:HA	1:B:47:GLN:OE1	2.01	0.60
1:A:252:THR:HG22	1:B:252:THR:HA	1.82	0.59
1:A:158:GLY:HA2	1:A:159:VAL:C	2.19	0.59
1:A:298:PRO:HD2	1:A:299:GLU:OE1	2.03	0.59
1:B:503:GLU:OE2	1:B:532:ARG:NH1	2.33	0.58
1:B:297:ARG:H	1:B:298:PRO:CD	2.17	0.58
1:B:290:ARG:HB2	1:B:290:ARG:CZ	2.33	0.58
1:A:439:MET:CE	1:A:447:TYR:HD1	2.17	0.57
1:B:204:GLY:O	1:B:565:TRP:HZ2	1.86	0.57
1:A:235:GLN:HA	1:A:235:GLN:NE2	2.19	0.57
1:B:47:GLN:O	1:B:47:GLN:CD	2.42	0.57
1:A:204:GLY:O	1:A:565:TRP:HZ2	1.87	0.57
1:A:290:ARG:CZ	1:A:297:ARG:H	2.17	0.57
1:B:235:GLN:HE21	1:B:235:GLN:HA	1.70	0.56
1:B:47:GLN:O	1:B:47:GLN:NE2	2.39	0.56
1:A:288:ASP:OD2	1:A:290:ARG:NH2	2.39	0.56
1:B:43:GLU:HA	1:B:47:GLN:NE2	2.20	0.56
1:B:43:GLU:HG3	1:B:47:GLN:NE2	2.21	0.56
1:B:379:VAL:HG22	1:B:454:ALA:HA	1.88	0.56
1:B:43:GLU:CA	1:B:47:GLN:HE22	2.18	0.55
1:A:67:ARG:HE	1:A:67:ARG:HA	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:VAL:N	1:B:47:GLN:C	2.60	0.55
1:A:204:GLY:O	1:A:565:TRP:CZ2	2.60	0.55
1:B:134:TRP:CZ3	1:B:137:ARG:HD2	2.41	0.55
1:A:406:ASP:CB	3:A:2015:HOH:O	2.45	0.54
1:A:290:ARG:CZ	1:A:290:ARG:HB2	2.37	0.54
1:B:288:ASP:CG	1:B:290:ARG:NH2	2.61	0.54
1:A:379:VAL:HG22	1:A:454:ALA:HA	1.89	0.54
1:A:175:ALA:HB2	1:A:341:PHE:CE1	2.43	0.53
1:A:218:HIS:O	1:A:222:LEU:HB3	2.08	0.53
1:A:288:ASP:HB2	1:A:301:PHE:CZ	2.43	0.53
1:A:354:GLN:HE21	1:A:466[A]:HIS:HE1	1.46	0.53
1:B:56:HIS:CD2	1:B:58:GLU:H	2.25	0.53
1:B:269:LEU:O	1:B:297:ARG:NH1	2.37	0.53
1:B:298:PRO:HD2	1:B:299:GLU:OE1	2.08	0.53
1:B:43:GLU:HA	1:B:47:GLN:CD	2.29	0.52
1:A:74:ALA:O	1:A:78:VAL:HG23	2.09	0.52
1:A:365:PRO:HG3	1:A:452:ARG:HB2	1.90	0.52
1:B:56:HIS:HD2	1:B:58:GLU:HB2	1.74	0.52
1:B:204:GLY:O	1:B:565:TRP:CZ2	2.61	0.52
1:A:201:ARG:NH1	1:A:207:ARG:HE	2.07	0.52
1:B:67:ARG:NH1	1:B:70:GLN:OE1	2.39	0.52
1:B:288:ASP:OD1	1:B:290:ARG:NH2	2.38	0.52
1:A:213:ASN:H	1:A:213:ASN:ND2	2.05	0.52
1:A:62:ARG:O	1:A:66:VAL:HG23	2.09	0.51
1:A:398:LEU:HD12	1:A:429:GLN:HG3	1.92	0.51
1:B:158:GLY:HA2	1:B:159:VAL:C	2.29	0.51
1:B:36:MET:H	1:B:37:GLY:CA	2.23	0.51
1:B:410:TRP:C	3:B:2027:HOH:O	2.48	0.51
1:A:126:TYR:HA	1:A:161:ALA:HB1	1.91	0.51
1:A:568:ILE:O	1:A:568:ILE:CG2	2.59	0.51
1:A:555:LEU:HD23	1:A:555:LEU:C	2.31	0.51
1:B:40:THR:HA	1:B:41:ALA:CB	2.22	0.51
1:A:151:VAL:HG13	1:A:162:VAL:HG22	1.93	0.51
1:B:74:ALA:O	1:B:78:VAL:HG23	2.11	0.51
1:B:62:ARG:O	1:B:65:ARG:HB3	2.11	0.51
1:A:67:ARG:HH11	1:A:70:GLN:CD	2.11	0.50
1:B:297:ARG:N	1:B:298:PRO:CD	2.73	0.50
1:B:160:GLY:HA2	1:B:161:ALA:HB3	1.93	0.50
1:A:439:MET:HE3	1:A:447:TYR:HD1	1.77	0.50
1:B:151:VAL:HG13	1:B:162:VAL:HG21	1.92	0.50
1:B:313:LEU:O	1:B:313:LEU:CG	2.56	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:ARG:O	1:B:538:ARG:HG2	2.12	0.50
1:A:213:ASN:HD22	1:A:213:ASN:N	2.01	0.50
1:B:369:THR:OG1	1:B:375:GLU:OE2	2.28	0.49
1:A:439:MET:SD	1:A:450:ARG:HG3	2.53	0.49
1:A:252:THR:HG21	1:B:255:THR:OG1	2.12	0.49
1:B:365:PRO:HG3	1:B:452:ARG:HB2	1.94	0.49
1:A:404:VAL:HG11	1:A:520:ALA:HB1	1.94	0.49
1:A:409:LEU:HD23	1:A:436:LEU:HD22	1.94	0.49
1:A:290:ARG:NH1	1:A:298:PRO:CD	2.76	0.49
1:B:290:ARG:NH1	1:B:298:PRO:HD3	2.25	0.49
1:A:203:LYS:HD3	3:A:2021:HOH:O	2.13	0.49
1:B:175:ALA:HB2	1:B:341:PHE:CE1	2.47	0.49
1:B:271:HIS:ND1	1:B:299:GLU:HG3	2.28	0.49
1:B:271:HIS:CE1	1:B:299:GLU:HG3	2.48	0.48
1:B:439:MET:SD	1:B:450:ARG:HG3	2.53	0.48
1:B:290:ARG:HE	1:B:297:ARG:N	2.12	0.48
1:B:390:ASN:HB2	1:B:391:PRO:HD2	1.94	0.48
1:A:471:ASP:O	1:A:475:THR:HG23	2.13	0.48
1:B:439:MET:CE	1:B:447:TYR:HD1	2.27	0.48
1:A:274:THR:OG1	1:A:297:ARG:NH2	2.43	0.48
1:A:252:THR:HG23	1:B:250:GLY:O	2.14	0.48
1:A:503:GLU:OE2	1:A:532:ARG:NH1	2.39	0.48
1:B:50:LEU:HB3	3:B:2001:HOH:O	2.14	0.48
1:A:63:LEU:O	1:A:66:VAL:HB	2.13	0.48
1:B:136:ARG:HH12	1:B:144:LEU:HD21	1.79	0.48
1:B:46:VAL:HB	1:B:47:GLN:HG3	1.94	0.48
1:B:235:GLN:HA	1:B:235:GLN:NE2	2.28	0.48
1:A:290:ARG:NH1	1:A:291:GLY:O	2.47	0.47
1:A:313:LEU:HG	1:A:313:LEU:O	2.14	0.47
1:B:248:ASP:OD1	1:B:254:ARG:HG2	2.14	0.47
1:B:555:LEU:C	1:B:555:LEU:HD23	2.35	0.47
1:A:297:ARG:O	1:A:300:VAL:HB	2.14	0.47
1:A:134:TRP:CZ3	1:A:137:ARG:HD2	2.50	0.47
1:B:304:ARG:HE	1:B:304:ARG:HB3	1.41	0.47
1:B:404:VAL:HG11	1:B:520:ALA:HB1	1.96	0.47
1:A:235:GLN:HG3	1:A:553:GLY:HA3	1.95	0.47
1:A:70:GLN:O	1:A:72:ARG:N	2.48	0.47
1:B:62:ARG:O	1:B:66:VAL:HG23	2.15	0.47
1:B:234:ARG:O	1:B:236:PRO:HD3	2.15	0.47
1:B:290:ARG:NH1	1:B:291:GLY:O	2.48	0.47
1:B:410:TRP:HB3	3:B:2027:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:THR:HB	1:B:40:THR:HB	1.97	0.47
1:A:223:LEU:HD11	1:A:467:THR:CG2	2.45	0.46
1:B:213:ASN:HD22	1:B:213:ASN:N	2.00	0.46
1:A:465:ALA:HB1	1:A:468:THR:OG1	2.15	0.46
1:B:290:ARG:NH2	1:B:290:ARG:HB2	2.30	0.46
1:B:565:TRP:CZ3	1:B:567:GLY:HA2	2.51	0.46
1:A:250:GLY:O	1:B:252:THR:HG23	2.14	0.46
1:A:552:PHE:CE2	1:A:556:LEU:HD11	2.50	0.46
1:B:303:LEU:O	1:B:304:ARG:C	2.54	0.46
1:A:201:ARG:O	1:A:565:TRP:HD1	1.98	0.46
1:A:390:ASN:HB2	1:A:391:PRO:HD2	1.98	0.46
1:B:364:GLU:OE2	1:B:365:PRO:HD2	2.16	0.46
1:A:218:HIS:O	1:A:222:LEU:CB	2.63	0.45
1:B:182:ARG:HH21	1:B:186:GLN:HE22	1.63	0.45
1:B:380:LEU:HA	1:B:456:LEU:O	2.16	0.45
1:B:409:LEU:HD23	1:B:436:LEU:HD22	1.98	0.45
1:A:137:ARG:HG2	1:A:137:ARG:HH21	1.82	0.45
1:B:43:GLU:CA	1:B:47:GLN:NE2	2.79	0.45
1:B:135:ARG:HB3	1:B:140:ASP:O	2.17	0.45
1:A:69:THR:O	1:A:71:GLN:NE2	2.50	0.45
1:A:495:LEU:O	1:A:499:LEU:HB2	2.17	0.45
1:B:538:ARG:HB3	1:B:538:ARG:NH2	2.31	0.45
1:A:224:THR:HB	1:A:228:PHE:CE2	2.51	0.44
1:B:270:GLY:O	1:B:271:HIS:C	2.55	0.44
1:A:158:GLY:CA	1:A:159:VAL:C	2.86	0.44
1:B:67:ARG:HA	1:B:67:ARG:NE	2.32	0.44
1:A:67:ARG:HA	1:A:67:ARG:NE	2.32	0.44
1:B:40:THR:CA	1:B:41:ALA:CB	2.91	0.44
1:B:297:ARG:O	1:B:300:VAL:HB	2.18	0.44
1:A:364:GLU:OE2	1:A:364:GLU:HA	2.17	0.44
1:A:265:ASP:OD1	1:A:267:THR:HB	2.17	0.44
1:B:36:MET:H	1:B:37:GLY:HA2	1.83	0.44
1:B:439:MET:HE1	1:B:447:TYR:HD1	1.82	0.43
1:A:271:HIS:CD2	1:A:297:ARG:HG2	2.53	0.43
1:B:36:MET:N	1:B:37:GLY:CA	2.81	0.43
1:A:288:ASP:CG	1:A:290:ARG:NH2	2.69	0.43
1:A:290:ARG:HH11	1:A:297:ARG:N	2.16	0.43
1:A:332:PHE:CD2	1:A:332:PHE:C	2.92	0.43
1:B:62:ARG:C	1:B:64:GLY:HA3	2.39	0.43
1:B:494:SER:O	1:B:498:HIS:ND1	2.50	0.43
1:A:151:VAL:HG13	1:A:162:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:MET:C	1:B:30:ALA:H	2.22	0.43
1:A:364:GLU:OE2	1:A:365:PRO:HD2	2.18	0.43
1:B:43:GLU:HA	1:B:47:GLN:HE22	1.81	0.43
1:B:217:ALA:HA	1:B:253:LEU:HD12	2.00	0.43
1:A:297:ARG:HB3	1:A:300:VAL:CG2	2.48	0.43
1:B:465:ALA:HB1	1:B:468:THR:OG1	2.19	0.43
1:A:313:LEU:O	1:A:313:LEU:CG	2.63	0.43
1:A:381:CYS:HB2	1:A:410:TRP:HB3	2.00	0.43
1:A:107:ALA:HB1	1:A:138:LEU:HD21	2.00	0.42
1:A:339:GLU:HG2	1:A:346:VAL:HG21	2.02	0.42
1:B:34:LEU:HD23	1:B:69:THR:HG21	2.01	0.42
1:B:42:GLY:C	1:B:44:MET:H	2.23	0.42
1:B:49:GLY:O	1:B:51:ALA:N	2.52	0.42
1:A:222:LEU:HD12	1:A:222:LEU:O	2.19	0.42
1:B:138:LEU:O	1:B:421:ARG:NH2	2.51	0.42
1:B:290:ARG:HB2	1:B:291:GLY:HA2	2.02	0.42
1:B:219:PRO:HB3	1:B:467:THR:HG21	2.00	0.42
1:A:287:PHE:CZ	1:A:556:LEU:HD21	2.55	0.42
1:B:201:ARG:O	1:B:565:TRP:HD1	2.02	0.42
1:B:249:ASP:OD2	1:B:251:SER:OG	2.30	0.42
1:A:565:TRP:CH2	1:A:567:GLY:HA2	2.55	0.41
1:A:288:ASP:HB2	1:A:301:PHE:CE2	2.54	0.41
1:A:271:HIS:CE1	1:A:299:GLU:HG3	2.55	0.41
1:A:379:VAL:HG22	1:A:379:VAL:O	2.20	0.41
1:A:66:VAL:O	1:A:69:THR:N	2.53	0.41
1:A:255:THR:OG1	1:B:252:THR:HG21	2.20	0.41
1:B:477:CYS:HA	1:B:478:PRO:HD2	1.94	0.41
1:A:439:MET:HE1	1:A:447:TYR:HD1	1.85	0.41
1:B:315:TYR:HE2	1:B:318:THR:O	2.02	0.41
1:A:326:TYR:CE2	1:A:559:LEU:HD11	2.56	0.41
1:B:213:ASN:H	1:B:213:ASN:ND2	2.05	0.41
1:A:211:VAL:HG22	1:A:290:ARG:HD2	2.01	0.41
1:A:271:HIS:HD2	1:A:297:ARG:HG2	1.84	0.41
1:B:382:CYS:CB	1:B:397:MET:CE	2.72	0.41
1:A:223:LEU:CD2	1:A:467:THR:HG22	2.40	0.41
1:B:82:GLN:NE2	3:B:2005:HOH:O	2.54	0.40
1:A:457:PHE:C	1:A:457:PHE:CD2	2.94	0.40
1:B:224:THR:HB	1:B:228:PHE:CE2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	512/568 (90%)	472 (92%)	32 (6%)	8 (2%)	9 12
1	B	540/568 (95%)	490 (91%)	33 (6%)	17 (3%)	4 3
All	All	1052/1136 (93%)	962 (91%)	65 (6%)	25 (2%)	6 5

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	159	VAL
1	A	296	GLY
1	B	49	GLY
1	B	65	ARG
1	B	297	ARG
1	A	60	VAL
1	A	314	ALA
1	B	50	LEU
1	B	71	GLN
1	A	100	ALA
1	B	32	ALA
1	B	41	ALA
1	B	314	ALA
1	A	295	GLY
1	B	29	LEU
1	B	100	ALA
1	B	107	ALA
1	B	159	VAL
1	B	294	GLY
1	B	295	GLY
1	A	294	GLY
1	B	47	GLN
1	B	37	GLY
1	B	60	VAL

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	390/429 (91%)	364 (93%)	26 (7%)	16	21
1	B	407/429 (95%)	377 (93%)	30 (7%)	13	18
All	All	797/858 (93%)	741 (93%)	56 (7%)	15	19

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	THR
1	A	71	GLN
1	A	89	GLU
1	A	119	GLN
1	A	123	GLU
1	A	134	TRP
1	A	137	ARG
1	A	193	ARG
1	A	198	THR
1	A	201	ARG
1	A	211	VAL
1	A	213	ASN
1	A	252	THR
1	A	304	ARG
1	A	334	LEU
1	A	379	VAL
1	A	380	LEU
1	A	381	CYS
1	A	407	SER
1	A	408	VAL
1	A	463	TYR
1	A	499	LEU
1	A	532	ARG
1	A	540	SER
1	A	546	ASP
1	A	562	ARG
1	B	29	LEU

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Mol	Chain	Res	Type
1	B	31	ASP
1	B	40	THR
1	B	47	GLN
1	B	52	LEU
1	B	65	ARG
1	B	69	THR
1	B	71	GLN
1	B	89	GLU
1	B	119	GLN
1	B	123	GLU
1	B	134	TRP
1	B	137	ARG
1	B	193	ARG
1	B	213	ASN
1	B	233	ARG
1	B	304	ARG
1	B	311	ASN
1	B	334	LEU
1	B	379	VAL
1	B	380	LEU
1	B	384	ASN
1	B	406	ASP
1	B	407	SER
1	B	408	VAL
1	B	447	TYR
1	B	463	TYR
1	B	499	LEU
1	B	540	SER
1	B	546	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	177	GLN
1	A	186	GLN
1	A	213	ASN
1	A	259	GLN
1	A	271	HIS
1	A	277	HIS
1	A	281	HIS
1	A	354	GLN

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Mol	Chain	Res	Type
1	A	385	ASN
1	A	392	GLN
1	B	47	GLN
1	B	56	HIS
1	B	71	GLN
1	B	82	GLN
1	B	118	HIS
1	B	157	GLN
1	B	177	GLN
1	B	213	ASN
1	B	235	GLN
1	B	259	GLN
1	B	350	GLN
1	B	370	GLN
1	B	392	GLN
1	B	434	GLN
1	B	557	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

2 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	$\#\|Z\|>2$
2	LXN	B	1569	-	10,10,10	6.52	3 (30%)	14,14,14	2.28	3 (21%)
2	LXN	A	1569	-	10,10,10	6.52	2 (20%)	14,14,14	2.25	5 (35%)

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	LXN	B	1569	-	-	-	0/1/1/1
2	LXN	A	1569	-	-	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1569	LXN	CAI-CAJ	-15.20	1.39	1.54
2	B	1569	LXN	CAI-CAJ	-14.56	1.39	1.54
2	B	1569	LXN	CAH-CAJ	-14.06	1.40	1.54
2	A	1569	LXN	CAH-CAJ	-13.72	1.40	1.54
2	B	1569	LXN	CAG-NAE	2.44	1.41	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1569	LXN	CAH-NAE-CAG	-5.31	118.69	126.34
2	A	1569	LXN	CAI-NAF-CAG	-4.55	119.78	126.34
2	B	1569	LXN	CAI-NAF-CAG	-4.52	119.83	126.34
2	A	1569	LXN	CAH-NAE-CAG	-4.30	120.14	126.34
2	B	1569	LXN	NAE-CAG-NAF	2.95	120.54	115.80
2	A	1569	LXN	OAB-CAH-CAJ	2.90	122.60	119.65
2	A	1569	LXN	NAE-CAG-NAF	2.78	120.27	115.80
2	A	1569	LXN	OAD-CAJ-CAH	2.03	121.31	116.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	512/568 (90%)	0.45	52 (10%) 6 8	35, 38, 42, 74	0
1	B	542/568 (95%)	1.16	114 (21%) 1 0	35, 38, 52, 74	0
All	All	1054/1136 (92%)	0.81	166 (15%) 2 2	35, 38, 48, 74	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	39	THR	13.8
1	B	44	MET	8.7
1	B	285	LEU	7.8
1	B	293	GLY	7.3
1	B	52	LEU	7.1
1	B	292	TRP	7.1
1	B	204	GLY	6.7
1	B	36	MET	6.7
1	B	55	GLY	6.2
1	B	568	ILE	6.1
1	B	294	GLY	6.1
1	B	32	ALA	6.1
1	B	295	GLY	5.9
1	B	64	GLY	5.8
1	B	208	VAL	5.7
1	A	295	GLY	5.5
1	A	568	ILE	5.5
1	B	205	PRO	5.3
1	B	78	VAL	5.2
1	B	33	GLU	5.1
1	B	287	PHE	5.1
1	B	375	GLU	5.0
1	B	159	VAL	5.0
1	B	286	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	281	HIS	4.9
1	B	209	GLY	4.8
1	B	38	ASP	4.8
1	A	294	GLY	4.8
1	B	74	ALA	4.5
1	A	211	VAL	4.4
1	B	296	GLY	4.4
1	A	286	LEU	4.4
1	B	210	PHE	4.4
1	B	300	VAL	4.3
1	A	203	LYS	4.3
1	B	41	ALA	4.3
1	B	35	GLY	4.2
1	B	365	PRO	4.1
1	B	562	ARG	4.1
1	B	86	ALA	4.1
1	A	59	ALA	3.9
1	B	380	LEU	3.9
1	B	411	LEU	3.9
1	B	56	HIS	3.9
1	B	358	THR	3.8
1	B	456	LEU	3.8
1	B	458	LEU	3.8
1	B	126	TYR	3.8
1	A	80	LEU	3.8
1	B	381	CYS	3.8
1	B	190	ALA	3.7
1	B	191	SER	3.7
1	A	126	TYR	3.7
1	B	65	ARG	3.6
1	B	68	TRP	3.6
1	B	566	LEU	3.6
1	B	361	VAL	3.6
1	B	434	GLN	3.6
1	B	280	HIS	3.5
1	A	94	ALA	3.5
1	B	71	GLN	3.5
1	B	382	CYS	3.5
1	B	539	ALA	3.5
1	B	62	ARG	3.4
1	A	193	ARG	3.4
1	A	217	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	93	ILE	3.3
1	A	134	TRP	3.3
1	B	291	GLY	3.2
1	B	211	VAL	3.2
1	A	376	GLN	3.2
1	B	45	ALA	3.2
1	B	376	GLN	3.2
1	B	409	LEU	3.2
1	A	192	VAL	3.1
1	B	61	ALA	3.1
1	A	97	LEU	3.1
1	A	76	ALA	3.0
1	B	528	ALA	3.0
1	A	479	VAL	3.0
1	B	359	SER	3.0
1	B	104	ALA	3.0
1	B	193	ARG	3.0
1	B	364	GLU	3.0
1	A	456	LEU	3.0
1	B	538	ARG	3.0
1	A	123	GLU	3.0
1	A	566	LEU	2.9
1	B	111	ALA	2.9
1	B	53	HIS	2.9
1	A	160	GLY	2.9
1	B	420	ALA	2.9
1	B	103	ASP	2.9
1	A	562	ARG	2.9
1	A	209	GLY	2.9
1	A	190	ALA	2.9
1	A	66	VAL	2.8
1	A	301	PHE	2.8
1	A	381	CYS	2.7
1	B	114	TYR	2.7
1	B	377	GLY	2.7
1	B	28	MET	2.7
1	B	80	LEU	2.6
1	B	132	LEU	2.6
1	A	65	ARG	2.6
1	A	285	LEU	2.6
1	B	37	GLY	2.6
1	A	480	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	350	GLN	2.6
1	A	457	PHE	2.6
1	B	203	LYS	2.5
1	A	74	ALA	2.5
1	A	350	GLN	2.5
1	A	259	GLN	2.5
1	B	123	GLU	2.5
1	A	409	LEU	2.4
1	A	380	LEU	2.4
1	A	96	TRP	2.4
1	B	217	ALA	2.4
1	B	79	LEU	2.4
1	B	66	VAL	2.4
1	B	88	PRO	2.4
1	B	70	GLN	2.4
1	B	356	SER	2.3
1	B	131	LEU	2.3
1	B	259	GLN	2.3
1	B	130	GLN	2.3
1	B	60	VAL	2.3
1	A	521	SER	2.3
1	A	78	VAL	2.3
1	B	63	LEU	2.3
1	A	184	ARG	2.2
1	B	165	PHE	2.2
1	B	383	PHE	2.2
1	B	272	LEU	2.2
1	B	441	LYS	2.2
1	B	406	ASP	2.2
1	B	543	PHE	2.2
1	A	370	GLN	2.2
1	B	27	LEU	2.2
1	B	522	ASP	2.2
1	B	134	TRP	2.2
1	A	441	LYS	2.2
1	B	226	ALA	2.2
1	A	288	ASP	2.2
1	A	382	CYS	2.2
1	B	243	PHE	2.1
1	B	133	ASN	2.1
1	B	195	LEU	2.1
1	B	227	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	243	PHE	2.1
1	A	63	LEU	2.1
1	B	233	ARG	2.1
1	B	268	ALA	2.1
1	B	326	TYR	2.1
1	B	34	LEU	2.1
1	B	371	CYS	2.1
1	A	145	ASP	2.0
1	B	479	VAL	2.0
1	B	521	SER	2.0
1	B	290	ARG	2.0
1	A	86	ALA	2.0
1	B	129	ALA	2.0
1	A	208	VAL	2.0
1	A	296	GLY	2.0
1	B	288	ASP	2.0

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 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, 95^{th} 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	LXN	A	1569	10/10	0.89	0.21	23,26,27,29	0
2	LXN	B	1569	10/10	0.90	0.21	52,54,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.