Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:32 AM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

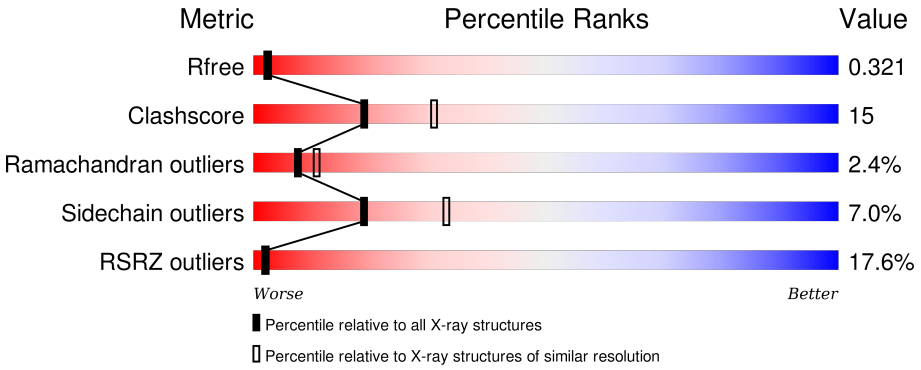
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	10% 68% 19% • • 10%
1	B	568	22% 68% 23% • • 5%

2 Entry composition

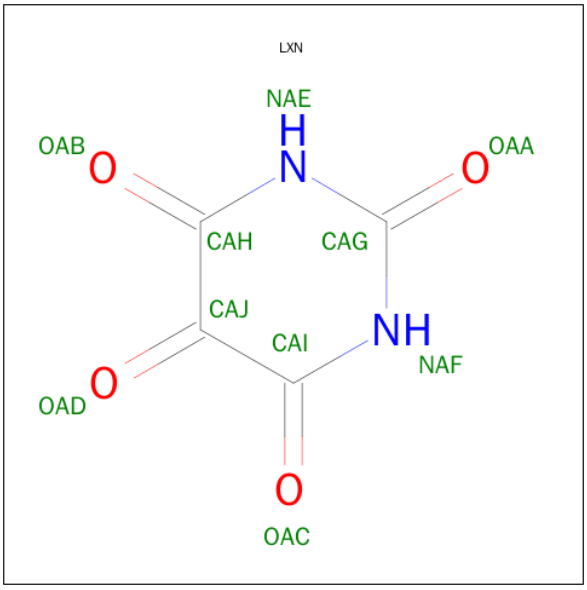
There are 3 unique types of molecules in this entry. The entry contains 8113 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

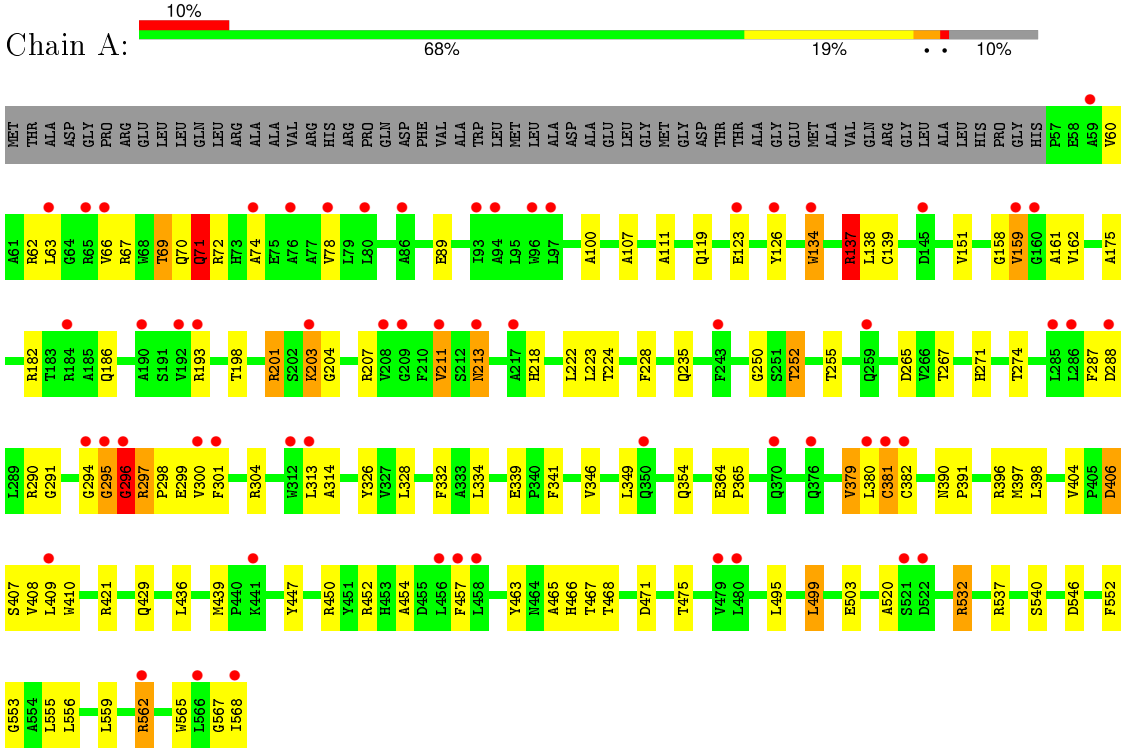
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	21	Total O 21 21	0	0
3	B	37	Total O 37 37	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

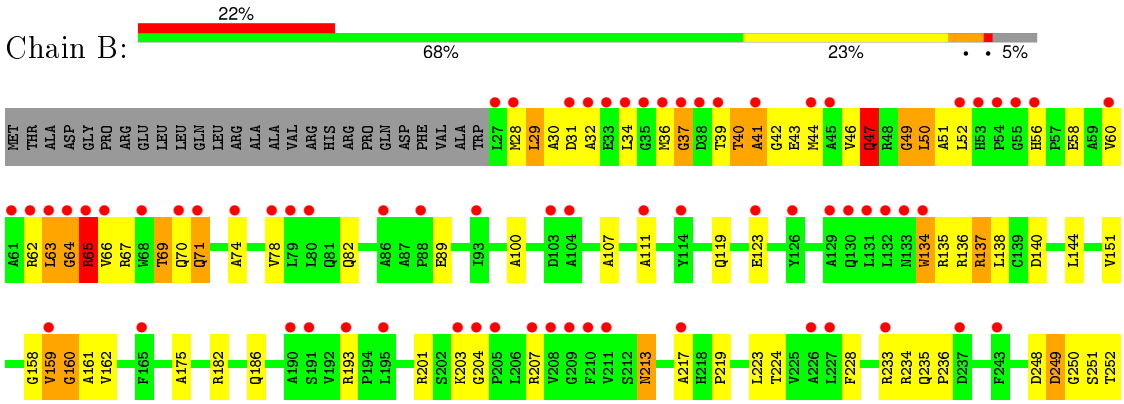
- Molecule 1: XCOGT

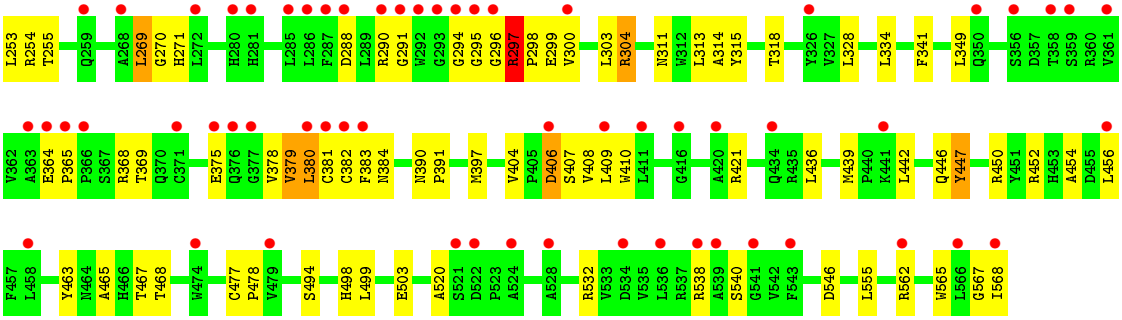
Chain A:



- Molecule 1: XCOGT

Chain B:




L253 R254 T255 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
V362 A363 E364 P365 P366 S367 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 G416 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 W474 C477 P478 V479 S494 H498 L499 E503 A520 S521 D522 P523 A524 A528 R532 V533 D534 V535 L536 R537 R538 A539 S540 G541 V542 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 (3.23%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 42601 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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:H	1:B:213:ASN:HD22	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:HG23	1:A:159:VAL:O	1.86	0.74
1:A:213:ASN:HD22	1:A:213:ASN:H	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:288:ASP:CG	1:A:290:ARG:HH21	1.97	0.67
1:A:235:GLN:HA	1:A:235:GLN:HE21	1.59	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:HG	1:B:313:LEU:O	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:HE	1:B:67:ARG:HA	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:CZ	1:B:290:ARG:HB2	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:B:47:GLN:O	1:B:47:GLN:CD	2.42	0.57
1:A:235:GLN:HA	1:A:235:GLN:NE2	2.19	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:HA	1:B:235:GLN:HE21	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:HA	1:A:67:ARG:HE	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:269:LEU:O	1:B:297:ARG:NH1	2.37	0.53
1:B:56:HIS:CD2	1:B:58:GLU:H	2.25	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:B:56:HIS:HD2	1:B:58:GLU:HB2	1.74	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:204:GLY:O	1:B:565:TRP:CZ2	2.61	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:201:ARG:NH1	1:A:207:ARG:HE	2.07	0.52
1:A:213:ASN:ND2	1:A:213:ASN:H	2.05	0.52
1:B:158:GLY:HA2	1:B:159:VAL:C	2.29	0.51
1:A:398:LEU:HD12	1:A:429:GLN:HG3	1.92	0.51
1:A:62:ARG:O	1:A:66:VAL:HG23	2.09	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:568:ILE:O	1:A:568:ILE:CG2	2.59	0.51
1:A:126:TYR:HA	1:A:161:ALA:HB1	1.91	0.51
1:B:40:THR:HA	1:B:41:ALA:CB	2.22	0.51
1:A:555:LEU:C	1:A:555:LEU:HD23	2.31	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:B:151:VAL:HG13	1:B:162:VAL:HG21	1.92	0.50
1:A:439:MET:HE3	1:A:447:TYR:HD1	1.77	0.50
1:B:313:LEU:CG	1:B:313:LEU:O	2.56	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:ARG:HG2	1:B:538:ARG:O	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:271:HIS:ND1	1:B:299:GLU:HG3	2.28	0.49
1:B:175:ALA:HB2	1:B:341:PHE:CE1	2.47	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:B:439:MET:CE	1:B:447:TYR:HD1	2.27	0.48
1:A:471:ASP:O	1:A:475:THR:HG23	2.13	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:NE2	1:B:235:GLN:HA	2.28	0.48
1:A:290:ARG:NH1	1:A:291:GLY:O	2.47	0.47
1:B:248:ASP:OD1	1:B:254:ARG:HG2	2.14	0.47
1:A:313:LEU:HG	1:A:313:LEU:O	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:410:TRP:HB3	3:B:2027:HOH:O	2.14	0.47
1:B:290:ARG:NH1	1:B:291:GLY:O	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

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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:B:213:ASN:N	1:B:213:ASN:HD22	2.00	0.46
1:A:223:LEU:HD11	1:A:467:THR:CG2	2.45	0.46
1:B:290:ARG:HB2	1:B:290:ARG:NH2	2.30	0.46
1:A:465:ALA:HB1	1:A:468:THR:OG1	2.15	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:B:303:LEU:O	1:B:304:ARG:C	2.54	0.46
1:A:552:PHE:CE2	1:A:556:LEU:HD11	2.50	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:409:LEU:HD23	1:B:436:LEU:HD22	1.98	0.45
1:B:380:LEU:HA	1:B:456:LEU:O	2.16	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:B:538:ARG:NH2	1:B:538:ARG:HB3	2.31	0.45
1:A:495:LEU:O	1:A:499:LEU:HB2	2.17	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:B:67:ARG:NE	1:B:67:ARG:HA	2.32	0.44
1:A:158:GLY:CA	1:A:159:VAL:C	2.86	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:B:62:ARG:C	1:B:64:GLY:HA3	2.39	0.43
1:A:332:PHE:C	1:A:332:PHE:CD2	2.92	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:B:43:GLU:HA	1:B:47:GLN:HE22	1.81	0.43
1:A:364:GLU:OE2	1:A:365:PRO:HD2	2.18	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:CG	1:A:313:LEU:O	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:O	1:A:222:LEU:HD12	2.19	0.42
1:B:290:ARG:HB2	1:B:291:GLY:HA2	2.02	0.42
1:B:138:LEU:O	1:B:421:ARG:NH2	2.51	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:255:THR:OG1	1:B:252:THR:HG21	2.20	0.41
1:A:66:VAL:O	1:A:69:THR:N	2.53	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:B:213:ASN:H	1:B:213:ASN:ND2	2.05	0.41
1:A:326:TYR:CE2	1:A:559:LEU:HD11	2.56	0.41
1:A:211:VAL:HG22	1:A:290:ARG:HD2	2.01	0.41
1:B:382:CYS:CB	1:B:397:MET:CE	2.72	0.41
1:A:271:HIS:HD2	1:A:297:ARG:HG2	1.84	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%)	12 20
1	B	540/568 (95%)	490 (91%)	33 (6%)	17 (3%)	5 6
All	All	1052/1136 (93%)	962 (91%)	65 (6%)	25 (2%)	7 11

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%)	20 35
1	B	407/429 (95%)	377 (93%)	30 (7%)	17 30
All	All	797/858 (93%)	741 (93%)	56 (7%)	19 33

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

Some 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 carbohydrates 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	A	1569	-	10,10,10	5.77	3 (30%)	14,14,14	2.14	4 (28%)
2	LXN	B	1569	-	10,10,10	5.79	4 (40%)	14,14,14	2.20	3 (21%)

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	A	1569	-	-	0/0/16/16	0/1/1/1
2	LXN	B	1569	-	-	0/0/16/16	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1569	LXN	CAI-CAJ	-13.41	1.39	1.54
2	B	1569	LXN	CAI-CAJ	-12.85	1.39	1.54
2	B	1569	LXN	CAH-CAJ	-12.40	1.40	1.54
2	A	1569	LXN	CAH-CAJ	-12.10	1.40	1.54
2	A	1569	LXN	CAG-NAF	2.00	1.40	1.37
2	B	1569	LXN	CAG-NAF	2.03	1.40	1.37
2	B	1569	LXN	CAG-NAE	2.55	1.41	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1569	LXN	CAH-NAE-CAG	-5.13	118.69	126.33
2	A	1569	LXN	CAI-NAF-CAG	-4.40	119.78	126.33
2	B	1569	LXN	CAI-NAF-CAG	-4.37	119.83	126.33
2	A	1569	LXN	CAH-NAE-CAG	-4.15	120.14	126.33
2	A	1569	LXN	OAB-CAH-CAJ	2.61	122.60	119.75
2	A	1569	LXN	NAE-CAG-NAF	2.75	120.27	115.82
2	B	1569	LXN	NAE-CAG-NAF	2.92	120.54	115.82

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

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, 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%)	0.52	59 (11%) 6 7	35, 38, 42, 74	0
1	B	542/568 (95%)	1.25	127 (23%) 1 1	35, 38, 52, 74	0
All	All	1054/1136 (92%)	0.90	186 (17%) 2 2	35, 38, 48, 74	0

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	39	THR	13.9
1	B	44	MET	9.2
1	B	285	LEU	8.2
1	B	293	GLY	7.7
1	B	52	LEU	7.4
1	B	292	TRP	7.3
1	B	36	MET	7.1
1	B	204	GLY	7.0
1	B	32	ALA	6.5
1	B	55	GLY	6.5
1	B	294	GLY	6.4
1	B	568	ILE	6.4
1	B	64	GLY	6.2
1	B	295	GLY	6.2
1	B	208	VAL	6.0
1	A	568	ILE	5.7
1	A	295	GLY	5.7
1	B	78	VAL	5.5
1	B	205	PRO	5.5
1	B	287	PHE	5.2
1	B	286	LEU	5.2
1	B	159	VAL	5.2
1	B	209	GLY	5.1
1	B	33	GLU	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	281	HIS	5.0
1	B	38	ASP	5.0
1	A	294	GLY	5.0
1	B	375	GLU	5.0
1	B	74	ALA	4.9
1	A	211	VAL	4.7
1	B	300	VAL	4.6
1	B	210	PHE	4.5
1	B	41	ALA	4.5
1	A	286	LEU	4.5
1	B	296	GLY	4.4
1	B	35	GLY	4.4
1	A	203	LYS	4.4
1	B	365	PRO	4.3
1	B	86	ALA	4.3
1	B	562	ARG	4.2
1	A	59	ALA	4.2
1	B	380	LEU	4.1
1	B	411	LEU	4.1
1	B	56	HIS	4.0
1	B	381	CYS	4.0
1	B	458	LEU	4.0
1	A	80	LEU	3.9
1	B	456	LEU	3.9
1	B	358	THR	3.9
1	B	190	ALA	3.9
1	B	126	TYR	3.9
1	B	68	TRP	3.8
1	B	191	SER	3.8
1	A	126	TYR	3.8
1	B	65	ARG	3.8
1	B	361	VAL	3.7
1	B	566	LEU	3.7
1	B	382	CYS	3.7
1	B	434	GLN	3.7
1	B	280	HIS	3.7
1	A	94	ALA	3.6
1	B	539	ALA	3.6
1	B	71	GLN	3.6
1	B	62	ARG	3.6
1	A	193	ARG	3.5
1	A	93	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	291	GLY	3.4
1	A	134	TRP	3.4
1	A	217	ALA	3.4
1	A	192	VAL	3.3
1	B	211	VAL	3.3
1	B	376	GLN	3.3
1	B	409	LEU	3.3
1	B	45	ALA	3.3
1	A	97	LEU	3.3
1	A	376	GLN	3.2
1	A	76	ALA	3.2
1	A	479	VAL	3.2
1	B	111	ALA	3.2
1	B	359	SER	3.2
1	B	528	ALA	3.2
1	B	538	ARG	3.1
1	A	123	GLU	3.1
1	A	190	ALA	3.1
1	B	193	ARG	3.1
1	B	104	ALA	3.1
1	B	364	GLU	3.1
1	B	420	ALA	3.1
1	B	61	ALA	3.1
1	A	209	GLY	3.1
1	B	377	GLY	3.1
1	A	456	LEU	3.0
1	A	566	LEU	3.0
1	B	103	ASP	3.0
1	A	381	CYS	3.0
1	A	66	VAL	3.0
1	A	160	GLY	3.0
1	A	562	ARG	2.9
1	B	53	HIS	2.9
1	B	37	GLY	2.9
1	B	114	TYR	2.9
1	A	301	PHE	2.9
1	B	132	LEU	2.8
1	A	480	LEU	2.8
1	A	285	LEU	2.8
1	B	80	LEU	2.8
1	A	65	ARG	2.8
1	B	28	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	74	ALA	2.8
1	B	350	GLN	2.7
1	B	203	LYS	2.7
1	A	457	PHE	2.6
1	A	259	GLN	2.6
1	B	123	GLU	2.6
1	A	350	GLN	2.6
1	A	380	LEU	2.6
1	A	409	LEU	2.5
1	B	66	VAL	2.5
1	B	259	GLN	2.5
1	B	356	SER	2.5
1	B	79	LEU	2.5
1	B	217	ALA	2.5
1	B	88	PRO	2.4
1	A	96	TRP	2.4
1	B	70	GLN	2.4
1	B	131	LEU	2.4
1	A	521	SER	2.4
1	B	130	GLN	2.4
1	A	78	VAL	2.4
1	B	60	VAL	2.4
1	B	272	LEU	2.4
1	B	441	LYS	2.4
1	B	383	PHE	2.4
1	B	522	ASP	2.4
1	A	184	ARG	2.3
1	A	382	CYS	2.3
1	B	63	LEU	2.3
1	A	370	GLN	2.3
1	B	406	ASP	2.3
1	B	195	LEU	2.3
1	B	165	PHE	2.3
1	B	543	PHE	2.3
1	B	134	TRP	2.3
1	B	371	CYS	2.3
1	B	27	LEU	2.3
1	A	288	ASP	2.3
1	A	441	LYS	2.3
1	B	226	ALA	2.3
1	B	233	ARG	2.3
1	B	243	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	133	ASN	2.2
1	B	227	LEU	2.2
1	B	326	TYR	2.2
1	A	86	ALA	2.2
1	B	129	ALA	2.2
1	B	237	ASP	2.2
1	A	243	PHE	2.2
1	B	524	ALA	2.2
1	B	536	LEU	2.2
1	A	145	ASP	2.2
1	B	290	ARG	2.1
1	B	416	GLY	2.1
1	B	268	ALA	2.1
1	B	479	VAL	2.1
1	A	522	ASP	2.1
1	A	63	LEU	2.1
1	A	208	VAL	2.1
1	B	288	ASP	2.1
1	A	312	TRP	2.1
1	B	34	LEU	2.1
1	B	363	ALA	2.1
1	B	474	TRP	2.1
1	B	93	ILE	2.1
1	A	296	GLY	2.1
1	B	541	GLY	2.1
1	B	31	ASP	2.1
1	B	534	ASP	2.1
1	B	54	PRO	2.1
1	A	159	VAL	2.0
1	A	458	LEU	2.0
1	B	207	ARG	2.0
1	A	300	VAL	2.0
1	B	366	PRO	2.0
1	B	521	SER	2.0
1	A	313	LEU	2.0
1	A	213	ASN	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	LXN	A	1569	10/10	0.89	0.20	0.49	23,26,27,29	0
2	LXN	B	1569	10/10	0.91	0.20	0.01	52,54,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.