



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:16 AM GMT

PDB ID : 3E0G
Title : Structure of the Leukemia Inhibitory Factor Receptor (LIF-R) domains D1-D5
Authors : Lupardus, P.J.; Garcia, K.C.
Deposited on : 2008-07-31
Resolution : 3.10 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

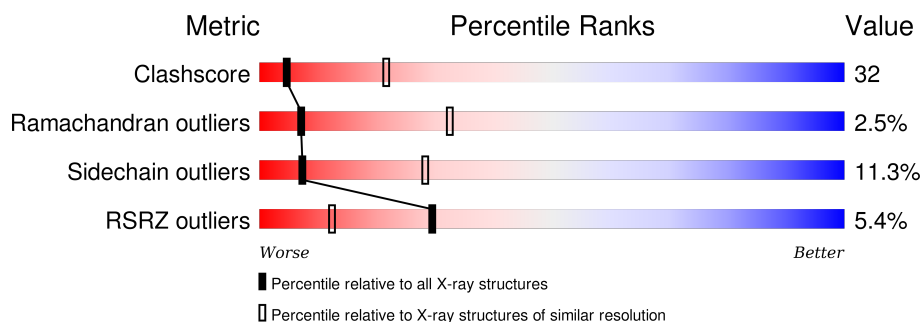
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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))
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	483	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	484	X	-	-	-
2	MAN	A	486	X	-	-	-
2	FUC	A	487	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3987 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 Leukemia inhibitory factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total	C	N	O	S	0	0	0
			3844	2447	652	729	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLN	ASN	ENGINEERED	UNP P42702
A	34	GLN	ASN	ENGINEERED	UNP P42702
A	92	GLN	ASN	ENGINEERED	UNP P42702
A	140	GLN	ASN	ENGINEERED	UNP P42702
A	192	GLN	ASN	ENGINEERED	UNP P42702
A	434	GLN	LYS	ENGINEERED	UNP P42702

- Molecule 2 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		

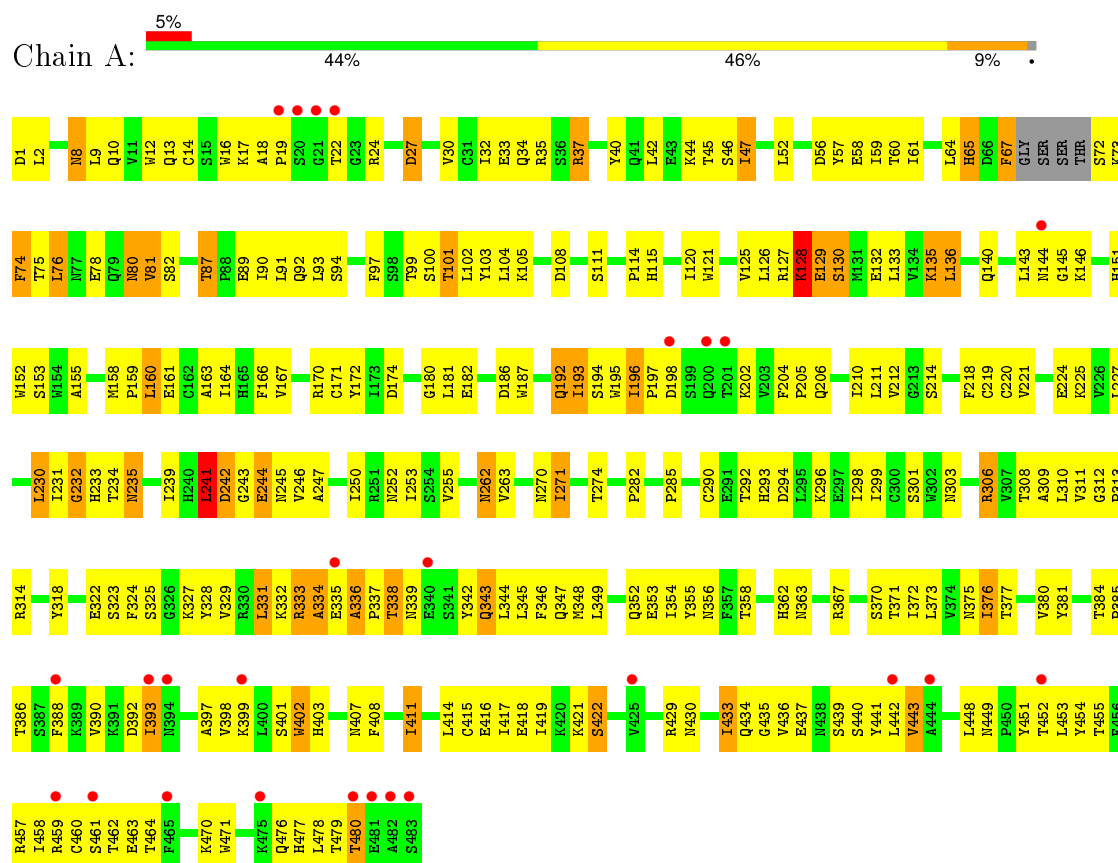
- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			38	22	2	14		

3 Residue-property plots

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: Leukemia inhibitory factor receptor



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	90.01Å 143.17Å 80.36Å 90.00° 110.38° 90.00°	Depositor
Resolution (Å)	30.00 – 3.10 19.98 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (30.00-3.10) 98.3 (19.98-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.252 , 0.309 0.255 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	78.2	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 56.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 18720 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3987	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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: FUC, NAG, MAN

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	0.48	0/3940	0.79	15/5363 (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
2	A	3	0

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	LYS	N-CA-C	-11.62	79.63	111.00
1	A	242	ASP	CB-CA-C	-11.05	88.30	110.40
1	A	242	ASP	N-CA-C	10.51	139.39	111.00
1	A	338	THR	CB-CA-C	7.79	132.64	111.60
1	A	128	LYS	CB-CA-C	7.71	125.83	110.40
1	A	393	ILE	CB-CA-C	7.70	126.99	111.60
1	A	334	ALA	CB-CA-C	7.41	121.22	110.10
1	A	232	GLY	N-CA-C	-6.91	95.83	113.10
1	A	338	THR	N-CA-C	-6.76	92.73	111.00
1	A	480	THR	N-CA-C	6.37	128.19	111.00
1	A	130	SER	N-CA-C	6.17	127.67	111.00
1	A	339	ASN	CB-CA-C	5.84	122.08	110.40
1	A	235	ASN	N-CA-C	5.65	126.25	111.00
1	A	241	LEU	N-CA-C	-5.44	96.30	111.00
1	A	480	THR	CB-CA-C	-5.19	97.59	111.60

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	484	NAG	C1
2	A	486	MAN	C1
2	A	487	FUC	C1

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3844	0	3774	249	0
2	A	49	0	43	1	0
3	A	56	0	50	3	0
4	A	38	0	34	3	0
All	All	3987	0	3901	252	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 32.

All (252) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:VAL:HG12	1:A:82:SER:H	0.98	1.14
1:A:133:LEU:N	1:A:133:LEU:HD22	1.82	0.94
1:A:81:VAL:HG12	1:A:82:SER:N	1.78	0.93
1:A:81:VAL:CG1	1:A:82:SER:H	1.83	0.91
1:A:451:TYR:CD2	1:A:479:THR:O	2.24	0.90
1:A:231:ILE:HD12	1:A:263:VAL:HG22	1.53	0.89
1:A:384:THR:HB	1:A:470:LYS:HB2	1.52	0.88
1:A:293:HIS:HA	1:A:381:TYR:O	1.74	0.87
1:A:417:ILE:HG22	1:A:458:ILE:HG22	1.56	0.87
1:A:204:PHE:HB2	1:A:219:CYS:HB2	1.58	0.85
1:A:80:ASN:H	1:A:80:ASN:HD22	1.24	0.84
1:A:18:ALA:HB1	1:A:19:PRO:HD2	1.60	0.84
1:A:127:ARG:O	1:A:164:ILE:O	1.96	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:THR:HG23	1:A:371:THR:HG22	1.58	0.84
1:A:57:TYR:HB2	1:A:78:GLU:HB2	1.58	0.84
1:A:459:ARG:HD2	1:A:471:TRP:HE1	1.41	0.82
1:A:349:LEU:HB2	1:A:352:GLN:HG3	1.61	0.82
1:A:451:TYR:CE2	1:A:479:THR:O	2.31	0.81
1:A:27:ASP:HB2	1:A:64:LEU:HD22	1.62	0.81
1:A:323:SER:HB2	1:A:356:ASN:HD22	1.46	0.81
1:A:101:THR:HB	1:A:155:ALA:HA	1.62	0.81
1:A:111:SER:HA	1:A:145:GLY:O	1.83	0.79
1:A:392:ASP:OD1	1:A:393:ILE:O	2.00	0.79
1:A:210:ILE:HD13	1:A:253:ILE:HG21	1.65	0.76
1:A:429:ARG:HH22	1:A:448:LEU:HD21	1.48	0.76
1:A:166:PHE:CD2	1:A:192:GLN:HB3	2.21	0.75
1:A:455:THR:HG22	1:A:476:GLN:HB3	1.67	0.75
1:A:333:ARG:HD3	1:A:333:ARG:H	1.50	0.74
1:A:451:TYR:HD2	1:A:479:THR:O	1.71	0.74
1:A:61:ILE:HB	1:A:74:PHE:HB3	1.69	0.74
1:A:323:SER:HA	2:A:484:NAG:H82	1.69	0.74
1:A:127:ARG:NH1	1:A:158:MET:HB3	2.03	0.74
1:A:415:CYS:HA	1:A:460:CYS:HA	1.69	0.73
1:A:2:LEU:HA	1:A:16:TRP:HA	1.70	0.73
1:A:67:PHE:HB3	1:A:72:SER:N	2.03	0.73
1:A:282:PRO:HD3	1:A:363:ASN:HB3	1.71	0.73
1:A:81:VAL:HA	3:A:493:NAG:O7	1.89	0.72
1:A:90:ILE:HD13	1:A:104:LEU:HD11	1.71	0.72
1:A:225:LYS:HA	1:A:244:GLU:HG2	1.71	0.72
1:A:239:ILE:HB	1:A:247:ALA:HB3	1.71	0.72
1:A:14:CYS:HB2	1:A:47:ILE:HD13	1.72	0.71
1:A:174:ASP:HA	1:A:182:GLU:OE2	1.91	0.71
1:A:214:SER:H	1:A:253:ILE:HG22	1.56	0.70
1:A:59:ILE:HD11	1:A:76:LEU:HB2	1.74	0.69
1:A:323:SER:CB	1:A:356:ASN:HD22	2.05	0.69
1:A:333:ARG:HD3	1:A:333:ARG:N	2.07	0.69
1:A:327:LYS:HD2	1:A:346:PHE:CZ	2.28	0.69
1:A:80:ASN:N	1:A:80:ASN:HD22	1.90	0.68
1:A:1:ASP:H1	1:A:17:LYS:HD3	1.58	0.68
1:A:42:LEU:HD11	1:A:47:ILE:HG23	1.76	0.67
1:A:323:SER:HB3	1:A:356:ASN:HB3	1.76	0.67
1:A:296:LYS:O	1:A:348:MET:HB2	1.94	0.67
1:A:390:VAL:HB	1:A:477:HIS:HB3	1.77	0.67
1:A:127:ARG:HH12	1:A:158:MET:CB	2.08	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ILE:HG22	1:A:234:THR:HB	1.77	0.66
1:A:225:LYS:HA	1:A:244:GLU:CG	2.25	0.66
1:A:335:GLU:C	1:A:337:PRO:HD3	2.15	0.66
1:A:449:ASN:HB2	1:A:454:TYR:HE2	1.59	0.66
4:A:490:NAG:H62	4:A:491:NAG:O7	1.94	0.66
1:A:37:ARG:NE	1:A:37:ARG:O	2.30	0.65
1:A:196:ILE:HD12	1:A:196:ILE:H	1.62	0.65
1:A:205:PRO:HD2	1:A:218:PHE:CD1	2.33	0.64
1:A:459:ARG:HD2	1:A:471:TRP:NE1	2.13	0.64
1:A:419:ILE:HG12	1:A:429:ARG:HH21	1.62	0.64
1:A:127:ARG:HH12	1:A:158:MET:HB3	1.61	0.63
1:A:282:PRO:HD3	1:A:363:ASN:CB	2.29	0.62
1:A:454:TYR:H	1:A:478:LEU:HD21	1.64	0.62
1:A:349:LEU:CB	1:A:352:GLN:HG3	2.29	0.62
1:A:230:LEU:HB3	1:A:235:ASN:H	1.64	0.62
1:A:143:LEU:HD23	1:A:146:LYS:HB2	1.82	0.61
1:A:18:ALA:HB1	1:A:19:PRO:CD	2.29	0.61
1:A:323:SER:CB	1:A:356:ASN:HB3	2.29	0.61
1:A:429:ARG:NH2	1:A:448:LEU:HD21	2.14	0.61
1:A:34:GLN:HG3	1:A:52:LEU:HD21	1.82	0.61
1:A:128:LYS:HE3	1:A:128:LYS:HA	1.83	0.61
1:A:230:LEU:HD23	1:A:230:LEU:N	2.16	0.60
1:A:457:ARG:HE	1:A:471:TRP:HB3	1.67	0.60
1:A:299:ILE:CD1	1:A:345:LEU:HG	2.32	0.60
1:A:421:LYS:HG2	1:A:422:SER:H	1.67	0.60
1:A:1:ASP:N	1:A:17:LYS:HD3	2.17	0.59
1:A:377:THR:HB	1:A:464:THR:HG21	1.84	0.59
1:A:221:VAL:HA	1:A:245:ASN:OD1	2.03	0.59
1:A:125:VAL:HG22	1:A:167:VAL:HG22	1.85	0.59
1:A:384:THR:HB	1:A:470:LYS:HE3	1.84	0.58
1:A:436:VAL:HG22	1:A:441:TYR:CZ	2.38	0.58
1:A:220:CYS:HB3	1:A:246:VAL:HG23	1.85	0.58
1:A:166:PHE:CD2	1:A:192:GLN:CB	2.86	0.58
1:A:12:TRP:CD2	1:A:81:VAL:HG21	2.38	0.58
1:A:336:ALA:N	1:A:337:PRO:HD3	2.19	0.58
1:A:12:TRP:CE2	1:A:81:VAL:HG21	2.38	0.57
1:A:37:ARG:O	1:A:37:ARG:CD	2.52	0.57
1:A:429:ARG:HH22	1:A:448:LEU:HD11	1.68	0.57
1:A:419:ILE:CD1	1:A:429:ARG:HE	2.17	0.57
1:A:353:GLU:O	1:A:353:GLU:HG2	2.05	0.57
1:A:285:PRO:HG2	1:A:370:SER:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:LEU:HG	1:A:152:TRP:CZ2	2.40	0.57
1:A:133:LEU:N	1:A:133:LEU:CD2	2.57	0.57
1:A:312:GLY:C	1:A:314:ARG:H	2.08	0.57
1:A:306:ARG:HD3	1:A:306:ARG:N	2.19	0.57
1:A:164:ILE:HD11	1:A:192:GLN:HG3	1.86	0.57
1:A:459:ARG:HB3	1:A:471:TRP:CD1	2.40	0.56
1:A:127:ARG:NH1	1:A:158:MET:CB	2.69	0.56
1:A:392:ASP:HA	1:A:399:LYS:HE3	1.88	0.56
1:A:91:LEU:HB3	1:A:105:LYS:O	2.05	0.56
1:A:299:ILE:HD13	1:A:345:LEU:HG	1.88	0.56
1:A:451:TYR:HE2	1:A:479:THR:O	1.87	0.55
1:A:429:ARG:NH2	1:A:448:LEU:HD11	2.22	0.55
1:A:80:ASN:HB2	1:A:180:GLY:HA2	1.88	0.55
1:A:128:LYS:HG2	1:A:242:ASP:OD2	2.07	0.55
1:A:214:SER:N	1:A:253:ILE:HG22	2.22	0.55
1:A:80:ASN:H	1:A:80:ASN:ND2	1.98	0.55
1:A:306:ARG:H	1:A:306:ARG:HD3	1.70	0.55
1:A:386:THR:O	1:A:403:HIS:HB3	2.06	0.55
1:A:230:LEU:CB	1:A:235:ASN:H	2.19	0.55
1:A:331:LEU:HB3	1:A:344:LEU:HD22	1.89	0.55
1:A:416:GLU:HG2	1:A:430:ASN:HB3	1.88	0.55
1:A:8:ASN:C	1:A:10:GLN:H	2.10	0.55
1:A:301:SER:HB3	1:A:343:GLN:HB3	1.89	0.55
1:A:105:LYS:HG2	1:A:151:HIS:ND1	2.21	0.54
1:A:290:CYS:HA	1:A:299:ILE:O	2.07	0.54
1:A:327:LYS:HD2	1:A:346:PHE:CE2	2.41	0.54
1:A:312:GLY:O	1:A:314:ARG:N	2.40	0.54
1:A:33:GLU:HB3	1:A:58:GLU:HB3	1.89	0.54
1:A:332:LYS:HD3	1:A:333:ARG:NH1	2.22	0.54
1:A:202:LYS:O	1:A:220:CYS:HA	2.08	0.53
1:A:127:ARG:C	1:A:164:ILE:O	2.45	0.53
1:A:402:TRP:CD1	1:A:441:TYR:HB2	2.44	0.53
1:A:231:ILE:HG23	1:A:232:GLY:H	1.72	0.53
1:A:93:LEU:HD12	1:A:103:TYR:O	2.09	0.53
1:A:19:PRO:HB2	1:A:22:THR:O	2.08	0.52
1:A:480:THR:HG23	1:A:480:THR:O	2.08	0.52
1:A:78:GLU:HA	3:A:493:NAG:H61	1.91	0.52
1:A:429:ARG:HH22	1:A:448:LEU:CD2	2.21	0.52
1:A:414:LEU:HB3	1:A:461:SER:HB3	1.91	0.52
1:A:132:GLU:C	1:A:133:LEU:HD22	2.28	0.52
1:A:80:ASN:HB2	1:A:180:GLY:CA	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:GLU:O	1:A:439:SER:N	2.42	0.51
1:A:164:ILE:HG13	1:A:194:SER:HB2	1.92	0.51
1:A:231:ILE:HD13	1:A:250:ILE:HD13	1.93	0.51
1:A:436:VAL:HG23	1:A:437:GLU:O	2.10	0.51
1:A:270:ASN:CG	1:A:271:ILE:H	2.14	0.51
1:A:457:ARG:NE	1:A:471:TRP:HB3	2.26	0.51
1:A:64:LEU:O	1:A:65:HIS:HB2	2.11	0.50
1:A:454:TYR:N	1:A:478:LEU:HD21	2.26	0.50
1:A:392:ASP:OD2	1:A:398:VAL:HG12	2.12	0.50
1:A:323:SER:HB2	1:A:356:ASN:ND2	2.21	0.49
1:A:336:ALA:N	1:A:337:PRO:CD	2.75	0.49
1:A:61:ILE:HB	1:A:74:PHE:CB	2.40	0.49
1:A:384:THR:CB	1:A:470:LYS:HB2	2.33	0.49
1:A:311:VAL:O	1:A:314:ARG:HG2	2.13	0.48
1:A:433:ILE:HD13	1:A:433:ILE:H	1.77	0.48
1:A:437:GLU:OE1	1:A:437:GLU:HA	2.13	0.48
1:A:397:ALA:HB1	1:A:448:LEU:HD23	1.96	0.48
1:A:158:MET:HE3	1:A:163:ALA:HB3	1.95	0.48
1:A:397:ALA:CB	1:A:448:LEU:HD23	2.44	0.48
1:A:419:ILE:N	1:A:419:ILE:HD12	2.28	0.48
1:A:32:ILE:HG22	1:A:59:ILE:HG22	1.95	0.48
1:A:308:THR:O	1:A:310:LEU:HG	2.14	0.47
1:A:127:ARG:HG2	1:A:133:LEU:HD21	1.95	0.47
1:A:8:ASN:OD1	1:A:10:GLN:HB2	2.14	0.47
1:A:37:ARG:O	1:A:37:ARG:HD2	2.14	0.47
1:A:132:GLU:OE2	1:A:135:LYS:HG3	2.14	0.47
1:A:436:VAL:HG22	1:A:441:TYR:CE2	2.50	0.47
1:A:102:LEU:O	1:A:153:SER:HA	2.15	0.47
1:A:108:ASP:HB3	1:A:121:TRP:CZ2	2.50	0.47
1:A:1:ASP:HB3	1:A:17:LYS:HB3	1.97	0.47
1:A:358:THR:HA	1:A:371:THR:HA	1.97	0.47
1:A:422:SER:HB3	1:A:453:LEU:HB2	1.96	0.47
1:A:30:VAL:O	1:A:40:TYR:N	2.44	0.47
1:A:16:TRP:O	1:A:45:THR:HG21	2.14	0.46
1:A:97:PHE:HE2	1:A:195:TRP:HB2	1.81	0.46
1:A:30:VAL:HA	1:A:60:THR:O	2.16	0.46
1:A:292:THR:HB	1:A:376:ILE:HD11	1.97	0.46
1:A:37:ARG:C	1:A:37:ARG:HE	2.19	0.46
1:A:419:ILE:HG12	1:A:429:ARG:NH2	2.28	0.46
1:A:34:GLN:NE2	1:A:35:ARG:HG2	2.30	0.46
1:A:128:LYS:CE	1:A:129:GLU:H	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ALA:HB3	1:A:337:PRO:HD2	1.99	0.45
1:A:34:GLN:HG3	1:A:52:LEU:CD2	2.46	0.45
1:A:127:ARG:HH12	1:A:158:MET:HB2	1.78	0.45
1:A:42:LEU:HD13	1:A:46:SER:O	2.15	0.45
1:A:80:ASN:ND2	1:A:80:ASN:N	2.59	0.45
1:A:419:ILE:HD11	1:A:429:ARG:HE	1.82	0.45
1:A:14:CYS:O	1:A:47:ILE:HD12	2.16	0.45
1:A:298:ILE:HG12	1:A:376:ILE:HD13	1.99	0.45
1:A:8:ASN:O	1:A:10:GLN:N	2.49	0.45
1:A:322:GLU:OE1	1:A:325:SER:N	2.49	0.45
1:A:292:THR:OG1	1:A:294:ASP:O	2.35	0.45
1:A:243:GLY:H	1:A:245:ASN:HD22	1.65	0.44
1:A:241:LEU:HB3	1:A:242:ASP:H	1.66	0.44
1:A:101:THR:HB	1:A:155:ALA:CA	2.40	0.44
1:A:73:LYS:NZ	1:A:75:THR:HG22	2.32	0.44
1:A:451:TYR:HA	1:A:478:LEU:HB3	1.99	0.44
1:A:402:TRP:HE3	1:A:458:ILE:HD12	1.83	0.44
1:A:392:ASP:HB3	1:A:399:LYS:H	1.82	0.44
1:A:133:LEU:H	1:A:133:LEU:HD22	1.76	0.44
1:A:333:ARG:CD	1:A:333:ARG:H	2.23	0.44
1:A:196:ILE:O	1:A:198:ASP:OD2	2.36	0.44
1:A:97:PHE:HD2	1:A:161:GLU:HG3	1.83	0.44
1:A:459:ARG:HB3	1:A:471:TRP:HD1	1.83	0.43
1:A:308:THR:O	1:A:309:ALA:HB3	2.18	0.43
1:A:362:HIS:HA	1:A:367:ARG:HG2	2.00	0.43
4:A:490:NAG:HO3	4:A:491:NAG:C1	2.31	0.43
1:A:100:SER:C	1:A:160:LEU:HD22	2.39	0.43
3:A:489:NAG:O3	3:A:489:NAG:H83	2.18	0.43
1:A:12:TRP:CG	1:A:81:VAL:HG21	2.53	0.43
1:A:462:THR:HG22	1:A:463:GLU:N	2.34	0.43
1:A:436:VAL:HG21	1:A:440:SER:O	2.19	0.43
1:A:231:ILE:HG23	1:A:232:GLY:N	2.33	0.43
1:A:327:LYS:HG2	1:A:328:TYR:N	2.32	0.43
1:A:99:THR:OG1	1:A:101:THR:HG23	2.19	0.42
1:A:225:LYS:CA	1:A:244:GLU:HG2	2.43	0.42
1:A:292:THR:CG2	1:A:380:VAL:HA	2.49	0.42
1:A:452:THR:HG22	1:A:452:THR:O	2.19	0.42
1:A:353:GLU:HA	1:A:376:ILE:HG22	1.99	0.42
1:A:8:ASN:C	1:A:10:GLN:N	2.72	0.42
1:A:231:ILE:O	1:A:262:ASN:O	2.37	0.42
1:A:418:GLU:CG	1:A:457:ARG:HB3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LYS:HB3	1:A:45:THR:H	1.70	0.42
1:A:94:SER:OG	1:A:103:TYR:HB2	2.20	0.42
1:A:1:ASP:CB	1:A:17:LYS:HB3	2.49	0.42
1:A:193:ILE:HG13	1:A:193:ILE:O	2.20	0.42
1:A:206:GLN:HA	1:A:274:THR:OG1	2.20	0.42
1:A:373:LEU:C	1:A:373:LEU:HD23	2.40	0.41
1:A:384:THR:HA	1:A:385:PRO:HD3	1.93	0.41
1:A:402:TRP:CZ2	1:A:443:VAL:HG11	2.54	0.41
1:A:120:ILE:O	1:A:171:CYS:HA	2.20	0.41
1:A:312:GLY:C	1:A:314:ARG:N	2.73	0.41
1:A:2:LEU:HD13	1:A:76:LEU:HD22	2.03	0.41
1:A:336:ALA:O	1:A:338:THR:O	2.38	0.41
1:A:252:ASN:CG	4:A:490:NAG:HN2	2.23	0.41
1:A:388:PHE:HB2	1:A:401:SER:O	2.21	0.41
1:A:411:ILE:HD13	1:A:411:ILE:H	1.86	0.41
1:A:218:PHE:CE2	1:A:263:VAL:HG21	2.55	0.41
1:A:211:LEU:O	1:A:212:VAL:C	2.59	0.41
1:A:232:GLY:O	1:A:233:HIS:C	2.58	0.41
1:A:220:CYS:HB3	1:A:246:VAL:CG2	2.51	0.41
1:A:87:THR:HB	1:A:186:ASP:HB2	2.02	0.41
1:A:358:THR:CG2	1:A:371:THR:HG22	2.40	0.41
1:A:408:PHE:O	1:A:435:GLY:HA3	2.20	0.40
1:A:170:ARG:HG2	1:A:187:TRP:CZ3	2.56	0.40
1:A:158:MET:HG3	1:A:159:PRO:HD2	2.02	0.40
1:A:205:PRO:HD2	1:A:218:PHE:CE1	2.55	0.40
1:A:449:ASN:HB2	1:A:454:TYR:CE2	2.45	0.40
1:A:120:ILE:HB	1:A:172:TYR:HB3	2.03	0.40
1:A:323:SER:HB2	1:A:356:ASN:HB3	2.01	0.40
1:A:348:MET:HG2	1:A:355:TYR:OH	2.21	0.40
1:A:318:TYR:HB2	1:A:331:LEU:HD22	2.03	0.40
1:A:93:LEU:HG	1:A:193:ILE:HG21	2.02	0.40
1:A:227:LEU:HD23	1:A:227:LEU:HA	1.91	0.40
1:A:354:ILE:HD12	1:A:354:ILE:O	2.22	0.40
1:A:372:ILE:HG23	1:A:372:ILE:O	2.21	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	475/483 (98%)	380 (80%)	83 (18%)	12 (2%)	7	32

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	336	ALA
1	A	81	VAL
1	A	197	PRO
1	A	422	SER
1	A	65	HIS
1	A	144	ASN
1	A	313	PRO
1	A	329	VAL
1	A	9	LEU
1	A	376	ILE
1	A	114	PRO
1	A	443	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	442/445 (99%)	392 (89%)	50 (11%)	7	28

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	13	GLN
1	A	24	ARG
1	A	27	ASP
1	A	37	ARG
1	A	47	ILE
1	A	56	ASP
1	A	67	PHE
1	A	74	PHE
1	A	76	LEU
1	A	80	ASN
1	A	87	THR
1	A	89	GLU
1	A	92	GLN
1	A	101	THR
1	A	115	HIS
1	A	126	LEU
1	A	128	LYS
1	A	129	GLU
1	A	130	SER
1	A	135	LYS
1	A	136	LEU
1	A	140	GLN
1	A	160	LEU
1	A	181	LEU
1	A	192	GLN
1	A	193	ILE
1	A	196	ILE
1	A	224	GLU
1	A	230	LEU
1	A	241	LEU
1	A	244	GLU
1	A	255	VAL
1	A	262	ASN
1	A	271	ILE
1	A	303	ASN
1	A	306	ARG
1	A	324	PHE
1	A	331	LEU
1	A	333	ARG
1	A	342	TYR
1	A	343	GLN
1	A	347	GLN

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Mol	Chain	Res	Type
1	A	375	ASN
1	A	402	TRP
1	A	407	ASN
1	A	411	ILE
1	A	433	ILE
1	A	434	GLN
1	A	442	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	262	ASN

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 ⓘ

11 carbohydrates 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	NAG	A	484	1,2	14,14,15	0.72	1 (7%)	15,19,21	0.96	0
2	NAG	A	485	2	14,14,15	0.56	0	15,19,21	0.98	2 (13%)
2	MAN	A	486	2	11,11,12	0.60	0	14,15,17	0.79	0
2	FUC	A	487	2	10,10,11	0.59	0	14,14,16	0.70	0
3	NAG	A	488	1,3	14,14,15	0.43	0	15,19,21	1.18	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	489	3	14,14,15	0.55	0	15,19,21	0.73	0
4	NAG	A	490	1,4	14,14,15	0.43	0	15,19,21	1.05	1 (6%)
4	NAG	A	491	4	14,14,15	0.50	0	15,19,21	0.93	1 (6%)
4	FUC	A	492	4	10,10,11	0.60	0	14,14,16	1.15	2 (14%)
3	NAG	A	493	1,3	14,14,15	0.65	0	15,19,21	2.37	5 (33%)
3	NAG	A	494	3	14,14,15	0.60	0	15,19,21	1.37	3 (20%)

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	NAG	A	484	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	485	2	-	0/6/23/26	0/1/1/1
2	MAN	A	486	2	1/1/4/5	0/2/19/22	0/1/1/1
2	FUC	A	487	2	1/1/4/5	0/0/17/20	0/1/1/1
3	NAG	A	488	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	489	3	-	0/6/23/26	0/1/1/1
4	NAG	A	490	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	491	4	-	0/6/23/26	0/1/1/1
4	FUC	A	492	4	-	0/0/17/20	0/1/1/1
3	NAG	A	493	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	494	3	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	484	NAG	C1-C2	2.15	1.55	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	493	NAG	C3-C4-C5	-4.01	103.21	110.20
3	A	493	NAG	C4-C3-C2	-2.69	107.05	111.23
3	A	494	NAG	O7-C7-C8	-2.43	117.61	122.06
3	A	493	NAG	O4-C4-C3	2.14	115.15	110.34
2	A	485	NAG	C1-O5-C5	2.27	115.13	112.25
2	A	485	NAG	C4-C3-C2	2.35	114.89	111.23
3	A	493	NAG	O5-C5-C6	2.37	112.47	107.35
4	A	492	FUC	C1-O5-C5	2.46	116.17	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	492	FUC	O5-C5-C6	2.60	110.42	106.13
3	A	494	NAG	C1-O5-C5	2.64	115.59	112.25
3	A	494	NAG	C2-N2-C7	2.72	126.53	123.04
4	A	491	NAG	C1-O5-C5	2.85	115.87	112.25
3	A	488	NAG	C1-O5-C5	3.24	116.36	112.25
4	A	490	NAG	C1-O5-C5	3.50	116.69	112.25
3	A	493	NAG	C1-O5-C5	6.06	119.93	112.25

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	486	MAN	C1
2	A	487	FUC	C1
2	A	484	NAG	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	494	NAG	O7-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	484	NAG	1	0
3	A	489	NAG	1	0
4	A	490	NAG	3	0
4	A	491	NAG	2	0
3	A	493	NAG	2	0

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	479/483 (99%)	-0.09	26 (5%)	29 12	33, 80, 176, 190	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	425	VAL	5.3
1	A	340	GLU	4.6
1	A	482	ALA	4.4
1	A	459	ARG	4.2
1	A	399	LYS	4.1
1	A	394	ASN	4.0
1	A	480	THR	3.7
1	A	22	THR	3.5
1	A	200	GLN	3.1
1	A	461	SER	3.0
1	A	335	GLU	2.8
1	A	201	THR	2.7
1	A	452	THR	2.7
1	A	475	LYS	2.6
1	A	465	PHE	2.6
1	A	21	GLY	2.6
1	A	198	ASP	2.5
1	A	483	SER	2.4
1	A	393	ILE	2.4
1	A	19	PRO	2.4
1	A	144	ASN	2.3
1	A	20	SER	2.2
1	A	481	GLU	2.2
1	A	444	ALA	2.2
1	A	442	LEU	2.1
1	A	388	PHE	2.1

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](#)

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	A	488	14/15	0.92	0.23	1.32	102,104,105,107	0
2	NAG	A	484	14/15	0.92	0.17	-0.38	99,103,108,108	0
3	NAG	A	493	14/15	0.84	0.17	-0.48	89,91,93,95	0
2	FUC	A	487	10/11	0.90	0.17	-	96,97,97,98	10
3	NAG	A	489	14/15	0.88	0.26	-	108,109,111,111	0
2	MAN	A	486	11/12	0.89	0.13	-	116,117,117,117	0
2	NAG	A	485	14/15	0.93	0.19	-	110,112,115,115	0
4	FUC	A	492	10/11	0.96	0.30	-	102,104,104,104	0
4	NAG	A	490	14/15	0.93	0.15	-	85,90,100,100	0
4	NAG	A	491	14/15	0.84	0.25	-	104,107,108,108	0
3	NAG	A	494	14/15	0.87	0.26	-	97,99,102,103	0

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.