Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:19 PM GMT

PDB ID	:	1F45
Title	:	HUMAN INTERLEUKIN-12
Authors	:	Yoon, C.; Johnston, S.C.; Tang, J.; Tobin, J.F.; Somers, W.S.
Deposited on	:	2000-06-07
Resolution	:	2.80 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:

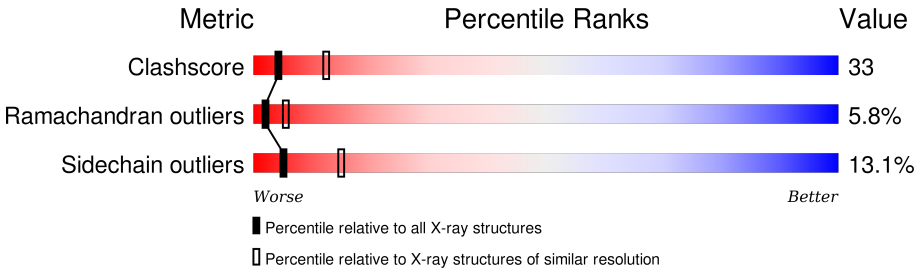
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.80 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	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	306	42% 39% 9% • 8%
2	B	197	40% 21% 5% • 32%

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
3	MAN	A	503	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3348 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 INTERLEUKIN-12 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	0	0
			2226	1411	357	446	12			

- Molecule 2 is a protein called INTERLEUKIN-12 ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	0	0
			1062	679	176	193	14			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	191	MET	THR	ENGINEERED	UNP P29459

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total	O	0	0
			14	14		
4	B	7	Total	O	0	0
			7	7		

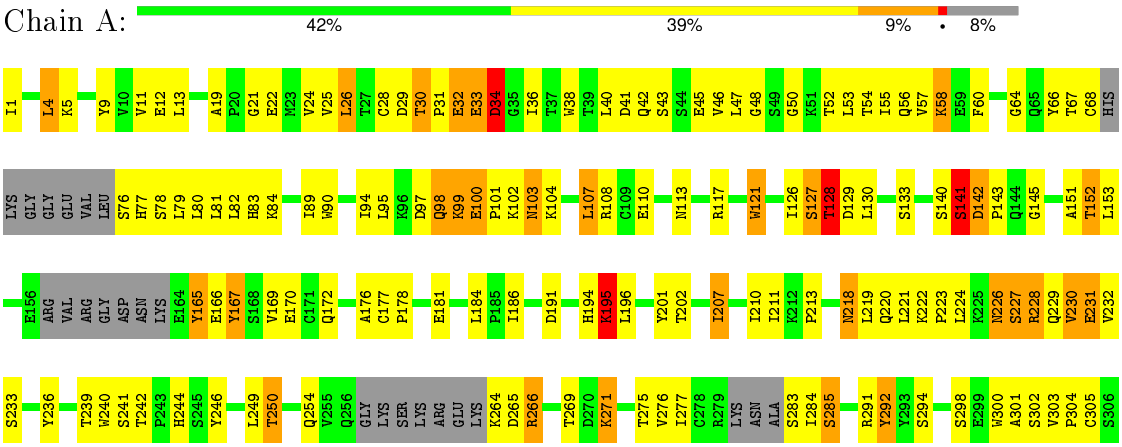
3 Residue-property plots (i)

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.

Note EDS was not executed.

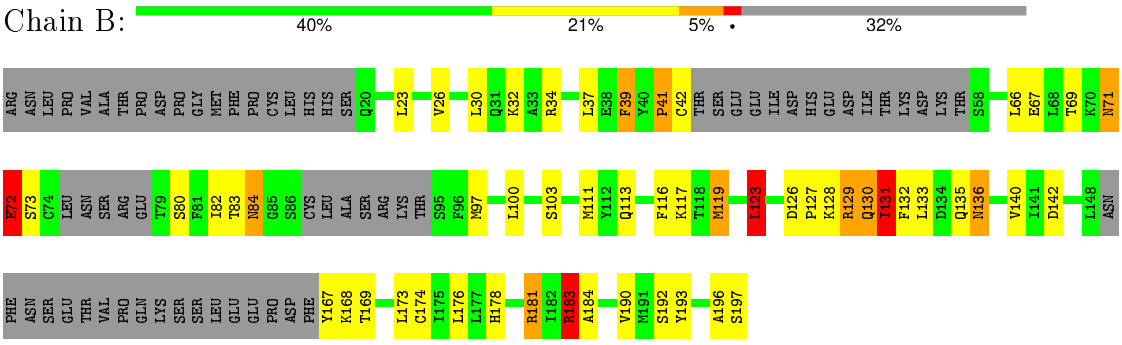
- Molecule 1: INTERLEUKIN-12 BETA CHAIN

Chain A:



- Molecule 2: INTERLEUKIN-12 ALPHA CHAIN

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	112.90Å 154.20Å 101.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (12.00-2.80)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3348	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.81	0/2280	0.99	3/3104 (0.1%)
2	B	0.98	0/1072	1.08	4/1435 (0.3%)
All	All	0.87	0/3352	1.02	7/4539 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
3	A	1	0
All	All	1	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	183	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	145	GLY	N-CA-C	5.72	127.39	113.10
2	B	142	ASP	CB-CG-OD1	5.65	123.38	118.30
2	B	131	ILE	N-CA-C	-5.33	96.62	111.00
1	A	176	ALA	N-CA-C	5.19	125.01	111.00
1	A	292	TYR	N-CA-C	5.19	125.01	111.00
2	B	42	CYS	CA-CB-SG	5.05	123.10	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	503	MAN	C1

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	246	TYR	Sidechain

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	2226	0	2102	164	0
2	B	1062	0	1095	52	0
3	A	39	0	34	6	0
4	A	14	0	0	1	0
4	B	7	0	0	1	0
All	All	3348	0	3231	218	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 33.

All (218) 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)
2:B:111:MET:CE	2:B:111:MET:SD	2.03	1.46
2:B:80:SER:HA	2:B:97:MET:HE2	1.26	1.15
2:B:130:GLN:HA	2:B:130:GLN:OE1	1.53	1.06
1:A:36:ILE:HB	1:A:50:GLY:O	1.67	0.92
2:B:130:GLN:NE2	2:B:131:ILE:HG12	1.85	0.91
1:A:108:ARG:HD2	1:A:121:TRP:CZ2	2.12	0.85
1:A:40:LEU:O	1:A:43:SER:HB3	1.78	0.83
1:A:227:SER:OG	1:A:229:GLN:HB3	1.79	0.82
1:A:46:VAL:O	1:A:46:VAL:HG12	1.79	0.82
3:A:502:NAG:O3	3:A:502:NAG:H83	1.80	0.81
1:A:133:SER:HB3	1:A:191:ASP:HB2	1.64	0.80
1:A:221:LEU:HD13	1:A:303:VAL:HG11	1.63	0.79
2:B:71:ASN:HD22	2:B:71:ASN:C	1.86	0.79
1:A:219:LEU:O	1:A:220:GLN:HG2	1.83	0.78
2:B:123:LEU:HD21	2:B:173:LEU:HD22	1.64	0.78
2:B:80:SER:HA	2:B:97:MET:CE	2.12	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ASP:O	1:A:76:SER:HB2	1.86	0.75
1:A:236:TYR:CE2	1:A:249:LEU:HD12	2.22	0.74
1:A:128:THR:OG1	1:A:129:ASP:N	2.19	0.74
1:A:22:GLU:O	1:A:57:VAL:HG22	1.88	0.74
1:A:22:GLU:H	1:A:57:VAL:HG23	1.54	0.73
1:A:79:LEU:O	1:A:80:LEU:HD23	1.90	0.70
1:A:33:GLU:O	1:A:34:ASP:O	2.09	0.70
1:A:219:LEU:C	1:A:220:GLN:HG2	2.12	0.69
2:B:39:PHE:H	2:B:39:PHE:HD1	1.40	0.69
1:A:141:SER:O	1:A:142:ASP:HB3	1.91	0.69
2:B:126:ASP:OD1	2:B:128:LYS:HD3	1.92	0.69
1:A:250:THR:HG22	1:A:291:ARG:HA	1.75	0.69
1:A:81:LEU:HD22	1:A:196:LEU:HA	1.74	0.68
2:B:39:PHE:N	2:B:39:PHE:CD1	2.60	0.68
2:B:127:PRO:C	2:B:129:ARG:H	1.94	0.68
1:A:140:SER:O	1:A:143:PRO:HD3	1.93	0.68
2:B:130:GLN:HE22	2:B:131:ILE:HG12	1.59	0.67
1:A:303:VAL:HG13	1:A:304:PRO:HD2	1.76	0.67
1:A:152:THR:O	1:A:167:TYR:HA	1.96	0.66
1:A:34:ASP:O	1:A:36:ILE:HG13	1.95	0.66
1:A:40:LEU:HD13	1:A:66:TYR:CE2	2.31	0.66
2:B:71:ASN:HD22	2:B:72:GLU:N	1.93	0.66
1:A:25:VAL:HG13	1:A:52:THR:HG23	1.78	0.65
1:A:221:LEU:N	1:A:221:LEU:HD12	2.10	0.65
1:A:117:ARG:HB2	1:A:172:GLN:NE2	2.12	0.65
1:A:222:LYS:HE2	1:A:231:GLU:OE1	1.97	0.65
1:A:97:ASP:C	1:A:99:LYS:H	1.99	0.65
1:A:226:ASN:O	1:A:227:SER:HB2	1.96	0.64
1:A:227:SER:HG	1:A:229:GLN:HB3	1.62	0.64
1:A:103:ASN:O	1:A:104:LYS:HB2	1.97	0.64
1:A:54:THR:O	1:A:55:ILE:HG23	1.98	0.64
1:A:221:LEU:CD1	1:A:303:VAL:HG11	2.28	0.64
1:A:108:ARG:HD2	1:A:121:TRP:CH2	2.32	0.64
1:A:213:PRO:O	1:A:298:SER:HB2	1.97	0.63
1:A:101:PRO:HD3	1:A:108:ARG:NH2	2.13	0.63
1:A:11:VAL:HG13	1:A:22:GLU:OE1	1.99	0.62
1:A:40:LEU:HD13	1:A:66:TYR:HE2	1.65	0.62
1:A:223:PRO:O	1:A:224:LEU:HD23	2.01	0.61
2:B:130:GLN:HE22	2:B:131:ILE:CG1	2.14	0.60
1:A:12:GLU:HG2	1:A:90:TRP:CH2	2.36	0.60
1:A:79:LEU:HD12	1:A:80:LEU:H	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:502:NAG:H4	3:A:503:MAN:O2	2.02	0.60
1:A:167:TYR:N	1:A:167:TYR:CD1	2.68	0.60
1:A:30:THR:O	1:A:32:GLU:N	2.35	0.59
1:A:228:ARG:HG3	1:A:228:ARG:HH11	1.66	0.59
1:A:285:SER:HB2	1:A:300:TRP:CE3	2.37	0.59
1:A:81:LEU:CD2	1:A:196:LEU:HA	2.32	0.59
1:A:9:TYR:HB2	1:A:80:LEU:CD2	2.32	0.59
2:B:67:GLU:CD	2:B:67:GLU:H	2.05	0.59
1:A:1:ILE:O	1:A:1:ILE:HG23	2.00	0.59
1:A:264:LYS:HG3	1:A:265:ASP:H	1.68	0.58
1:A:100:GLU:CB	1:A:101:PRO:HD3	2.34	0.58
1:A:55:ILE:CD1	1:A:66:TYR:HE1	2.17	0.58
2:B:136:ASN:O	2:B:140:VAL:HG23	2.04	0.58
1:A:264:LYS:CG	1:A:265:ASP:H	2.17	0.57
1:A:19:ALA:O	1:A:58:LYS:NZ	2.35	0.57
1:A:52:THR:HG22	1:A:52:THR:O	2.03	0.57
2:B:130:GLN:HB3	2:B:135:GLN:OE1	2.04	0.57
1:A:167:TYR:N	1:A:167:TYR:HD1	2.00	0.57
2:B:196:ALA:O	2:B:197:SER:HB3	2.04	0.57
1:A:283:SER:HB3	1:A:303:VAL:O	2.05	0.57
1:A:117:ARG:HB2	1:A:172:GLN:HE22	1.68	0.57
1:A:46:VAL:HG13	1:A:48:GLY:O	2.04	0.57
1:A:128:THR:HG1	1:A:129:ASP:H	1.49	0.57
1:A:220:GLN:C	1:A:221:LEU:HD12	2.25	0.57
1:A:126:ILE:HD12	1:A:126:ILE:N	2.19	0.56
1:A:213:PRO:O	1:A:298:SER:CB	2.53	0.56
1:A:292:TYR:O	2:B:34:ARG:HD3	2.05	0.56
1:A:9:TYR:HB2	1:A:80:LEU:HD22	1.88	0.56
1:A:79:LEU:HD12	1:A:80:LEU:N	2.21	0.55
1:A:32:GLU:HG2	1:A:32:GLU:O	2.06	0.55
2:B:71:ASN:ND2	2:B:71:ASN:C	2.57	0.55
1:A:219:LEU:H	1:A:219:LEU:HD12	1.72	0.55
1:A:221:LEU:HD21	1:A:284:ILE:HD12	1.90	0.55
2:B:131:ILE:O	2:B:135:GLN:NE2	2.40	0.54
2:B:174:CYS:O	2:B:178:HIS:HD2	1.89	0.54
1:A:41:ASP:OD1	1:A:42:GLN:HG2	2.07	0.54
1:A:28:CYS:SG	1:A:30:THR:CG2	2.96	0.54
1:A:29:ASP:HB3	1:A:76:SER:OG	2.08	0.53
1:A:221:LEU:CD1	1:A:221:LEU:N	2.72	0.53
1:A:55:ILE:CD1	1:A:66:TYR:CE1	2.91	0.53
1:A:26:LEU:HD23	1:A:26:LEU:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:VAL:HG22	1:A:170:GLU:N	2.24	0.52
1:A:38:TRP:CZ3	1:A:68:CYS:HB3	2.45	0.52
2:B:130:GLN:HE22	2:B:131:ILE:CD1	2.23	0.52
2:B:126:ASP:OD1	2:B:126:ASP:C	2.47	0.52
1:A:83:HIS:HD2	3:A:501:NAG:O6	1.93	0.52
2:B:80:SER:CA	2:B:97:MET:HE2	2.18	0.52
1:A:25:VAL:CG1	1:A:52:THR:HG23	2.40	0.52
1:A:117:ARG:HE	1:A:172:GLN:HE21	1.56	0.52
1:A:141:SER:O	1:A:142:ASP:CB	2.59	0.51
1:A:38:TRP:HB2	1:A:48:GLY:O	2.11	0.51
1:A:113:ASN:ND2	1:A:239:THR:O	2.42	0.50
1:A:21:GLY:HA3	1:A:57:VAL:O	2.11	0.50
1:A:97:ASP:C	1:A:99:LYS:N	2.63	0.50
1:A:186:ILE:HD12	1:A:207:ILE:CD1	2.41	0.50
1:A:55:ILE:HD11	1:A:66:TYR:HE1	1.76	0.50
1:A:55:ILE:HD11	1:A:66:TYR:CE1	2.47	0.50
1:A:38:TRP:CE3	1:A:68:CYS:HB3	2.46	0.50
1:A:29:ASP:C	1:A:76:SER:HB2	2.32	0.50
1:A:117:ARG:HE	1:A:172:GLN:NE2	2.09	0.50
1:A:165:TYR:CD1	1:A:165:TYR:N	2.80	0.49
1:A:126:ILE:HG21	1:A:130:LEU:HG	1.95	0.49
1:A:181:GLU:OE1	2:B:183:ARG:NH1	2.46	0.49
2:B:126:ASP:O	2:B:129:ARG:N	2.45	0.49
1:A:38:TRP:CE2	1:A:53:LEU:HB2	2.47	0.49
1:A:236:TYR:CD2	1:A:249:LEU:HD12	2.47	0.49
1:A:140:SER:O	1:A:142:ASP:N	2.46	0.49
1:A:83:HIS:CD2	3:A:501:NAG:O6	2.66	0.49
1:A:98:GLN:O	1:A:100:GLU:N	2.45	0.48
1:A:11:VAL:HA	4:A:516:HOH:O	2.12	0.48
3:A:501:NAG:H83	3:A:501:NAG:O3	2.13	0.48
1:A:201:TYR:N	1:A:201:TYR:CD1	2.81	0.48
1:A:38:TRP:HB3	1:A:53:LEU:HD13	1.95	0.48
1:A:121:TRP:CD1	1:A:121:TRP:N	2.82	0.48
3:A:502:NAG:C4	3:A:503:MAN:O2	2.61	0.48
2:B:83:THR:HG22	2:B:84:ASN:H	1.77	0.48
1:A:64:GLY:HA2	1:A:196:LEU:HD21	1.96	0.47
1:A:55:ILE:HD13	1:A:66:TYR:CE1	2.50	0.47
1:A:55:ILE:HD13	1:A:66:TYR:OH	2.15	0.47
2:B:128:LYS:N	2:B:128:LYS:HD2	2.29	0.47
2:B:127:PRO:C	2:B:129:ARG:N	2.62	0.47
1:A:227:SER:OG	1:A:229:GLN:CB	2.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:VAL:HG22	2:B:140:VAL:CG1	2.45	0.47
2:B:126:ASP:OD1	2:B:128:LYS:HB2	2.14	0.46
1:A:186:ILE:HD12	1:A:207:ILE:HD12	1.97	0.46
2:B:82:ILE:HG13	2:B:193:TYR:HE2	1.80	0.46
2:B:83:THR:HG22	2:B:84:ASN:N	2.29	0.46
1:A:126:ILE:CG2	1:A:127:SER:N	2.78	0.46
1:A:4:LEU:HD23	1:A:5:LYS:HE3	1.98	0.46
1:A:223:PRO:HA	1:A:230:VAL:HG13	1.98	0.46
1:A:242:THR:HG22	1:A:244:HIS:CE1	2.50	0.46
1:A:28:CYS:SG	1:A:30:THR:HG22	2.55	0.45
1:A:229:GLN:HG2	1:A:275:THR:CG2	2.45	0.45
1:A:207:ILE:O	1:A:211:ILE:HG13	2.17	0.45
1:A:97:ASP:O	1:A:99:LYS:N	2.49	0.45
1:A:26:LEU:HD11	1:A:66:TYR:CD1	2.51	0.45
2:B:82:ILE:HG13	2:B:193:TYR:CE2	2.52	0.45
2:B:131:ILE:O	2:B:132:PHE:CG	2.70	0.45
1:A:126:ILE:N	1:A:126:ILE:CD1	2.80	0.45
1:A:194:HIS:O	1:A:195:LYS:HB2	2.17	0.44
1:A:40:LEU:O	1:A:41:ASP:OD1	2.35	0.44
2:B:100:LEU:HD23	2:B:100:LEU:HA	1.73	0.44
2:B:119:MET:CA	2:B:119:MET:HE3	2.47	0.44
1:A:94:ILE:O	1:A:94:ILE:HG22	2.17	0.44
1:A:169:VAL:CG2	1:A:170:GLU:N	2.80	0.44
1:A:219:LEU:HD12	1:A:219:LEU:N	2.32	0.44
1:A:219:LEU:HB2	1:A:303:VAL:HG21	1.99	0.44
1:A:64:GLY:HA2	1:A:196:LEU:CD2	2.48	0.44
1:A:165:TYR:HD1	1:A:165:TYR:N	2.15	0.44
1:A:45:GLU:O	1:A:47:LEU:N	2.51	0.44
2:B:126:ASP:O	2:B:128:LYS:N	2.51	0.44
2:B:32:LYS:HE2	2:B:32:LYS:HB2	1.71	0.43
1:A:4:LEU:CD2	1:A:5:LYS:HE3	2.47	0.43
1:A:240:TRP:CG	1:A:241:SER:N	2.87	0.43
1:A:38:TRP:CG	1:A:53:LEU:HD13	2.53	0.43
1:A:195:LYS:HB3	1:A:196:LEU:H	1.42	0.43
1:A:229:GLN:HA	1:A:276:VAL:O	2.18	0.43
1:A:223:PRO:CA	1:A:230:VAL:HG13	2.49	0.43
2:B:131:ILE:C	2:B:132:PHE:CD1	2.92	0.43
1:A:26:LEU:CD1	1:A:66:TYR:CD1	3.02	0.43
1:A:26:LEU:CD1	1:A:66:TYR:HD1	2.32	0.43
1:A:38:TRP:CB	1:A:53:LEU:HD13	2.49	0.43
2:B:196:ALA:O	2:B:197:SER:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:GLU:C	1:A:210:ILE:HD12	2.40	0.42
1:A:219:LEU:HD22	1:A:303:VAL:HG23	2.01	0.42
1:A:152:THR:HG23	1:A:153:LEU:N	2.35	0.42
1:A:166:GLU:C	1:A:167:TYR:CD1	2.93	0.42
1:A:84:LYS:O	1:A:90:TRP:HE3	2.03	0.42
2:B:126:ASP:OD1	2:B:128:LYS:CD	2.64	0.42
2:B:30:LEU:HD21	2:B:184:ALA:HB3	2.00	0.42
2:B:167:TYR:O	2:B:168:LYS:C	2.58	0.42
2:B:37:LEU:HA	2:B:37:LEU:HD23	1.89	0.42
1:A:211:ILE:O	1:A:294:SER:OG	2.29	0.41
1:A:107:LEU:CD1	1:A:107:LEU:N	2.83	0.41
1:A:194:HIS:O	1:A:195:LYS:CB	2.68	0.41
1:A:285:SER:HA	1:A:301:ALA:O	2.20	0.41
1:A:126:ILE:HG22	1:A:127:SER:N	2.34	0.41
1:A:95:LEU:HD12	1:A:201:TYR:CE1	2.55	0.41
2:B:66:LEU:O	2:B:69:THR:HB	2.19	0.41
1:A:24:VAL:HG23	1:A:57:VAL:HG22	2.02	0.41
1:A:254:GLN:OE1	1:A:266:ARG:NH1	2.54	0.41
1:A:97:ASP:CG	1:A:104:LYS:H	2.23	0.41
1:A:28:CYS:SG	1:A:30:THR:HG21	2.60	0.41
1:A:32:GLU:O	1:A:34:ASP:N	2.54	0.41
2:B:113:GLN:O	2:B:117:LYS:HG3	2.20	0.41
2:B:130:GLN:HE22	2:B:131:ILE:HD11	1.85	0.41
1:A:104:LYS:HA	1:A:104:LYS:HD3	1.86	0.41
1:A:60:PHE:CD1	1:A:82:LEU:HD12	2.56	0.41
1:A:302:SER:O	1:A:303:VAL:HG23	2.21	0.40
1:A:25:VAL:HG13	1:A:52:THR:CG2	2.50	0.40
1:A:177:CYS:HA	1:A:178:PRO:HD3	1.94	0.40
1:A:184:LEU:HD23	1:A:184:LEU:HA	1.91	0.40
1:A:269:THR:OG1	1:A:271:LYS:HG3	2.21	0.40
2:B:181:ARG:HB3	4:B:202:HOH:O	2.22	0.40
1:A:218:ASN:CG	1:A:218:ASN:O	2.60	0.40
1:A:40:LEU:HD11	1:A:64:GLY:HA3	2.03	0.40
1:A:79:LEU:C	1:A:80:LEU:HD23	2.42	0.40
1:A:277:ILE:HG22	1:A:277:ILE:O	2.21	0.40
1:A:219:LEU:HA	1:A:233:SER:O	2.21	0.40
2:B:123:LEU:HA	2:B:123:LEU:HD12	1.81	0.40
2:B:116:PHE:CE2	2:B:176:LEU:HD23	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	272/306 (89%)	224 (82%)	31 (11%)	17 (6%)	2	4
2	B	123/197 (62%)	107 (87%)	10 (8%)	6 (5%)	3	8
All	All	395/503 (78%)	331 (84%)	41 (10%)	23 (6%)	2	5

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	PRO
1	A	33	GLU
1	A	34	ASP
1	A	100	GLU
1	A	142	ASP
2	B	41	PRO
1	A	58	LYS
1	A	78	SER
1	A	99	LYS
1	A	102	LYS
1	A	103	ASN
1	A	151	ALA
1	A	227	SER
2	B	123	LEU
2	B	131	ILE
1	A	98	GLN
1	A	128	THR
1	A	195	LYS
2	B	84	ASN
2	B	72	GLU
1	A	4	LEU
1	A	141	SER
2	B	73	SER

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	252/277 (91%)	221 (88%)	31 (12%)	6 18
2	B	121/183 (66%)	103 (85%)	18 (15%)	4 11
All	All	373/460 (81%)	324 (87%)	49 (13%)	5 15

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	26	LEU
1	A	30	THR
1	A	32	GLU
1	A	34	ASP
1	A	56	GLN
1	A	67	THR
1	A	77	HIS
1	A	89	ILE
1	A	107	LEU
1	A	121	TRP
1	A	127	SER
1	A	128	THR
1	A	141	SER
1	A	152	THR
1	A	165	TYR
1	A	167	TYR
1	A	195	LYS
1	A	202	THR
1	A	207	ILE
1	A	218	ASN
1	A	226	ASN
1	A	228	ARG
1	A	230	VAL
1	A	231	GLU
1	A	232	VAL
1	A	250	THR

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Mol	Chain	Res	Type
1	A	266	ARG
1	A	271	LYS
1	A	285	SER
1	A	305	CYS
2	B	23	LEU
2	B	39	PHE
2	B	41	PRO
2	B	71	ASN
2	B	72	GLU
2	B	103	SER
2	B	119	MET
2	B	123	LEU
2	B	129	ARG
2	B	130	GLN
2	B	131	ILE
2	B	133	LEU
2	B	136	ASN
2	B	169	THR
2	B	181	ARG
2	B	183	ARG
2	B	190	VAL
2	B	192	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	HIS
1	A	98	GLN
1	A	144	GLN
1	A	172	GLN
1	A	226	ASN
1	A	229	GLN
2	B	20	GLN
2	B	71	ASN
2	B	130	GLN
2	B	135	GLN
2	B	178	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

3 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	$\#\|Z\| > 2$
3	NAG	A	501	1,3	14,14,15	0.76	0	15,19,21	1.13	1 (6%)
3	NAG	A	502	3	14,14,15	1.10	1 (7%)	15,19,21	1.13	1 (6%)
3	MAN	A	503	3	11,11,12	0.74	0	14,15,17	1.23	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	501	1,3	-	2/6/23/26	0/1/1/1
3	NAG	A	502	3	-	0/6/23/26	0/1/1/1
3	MAN	A	503	3	1/1/4/5	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	NAG	C1-C2	-2.40	1.49	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	NAG	C2-N2-C7	-3.67	118.32	123.04
3	A	501	NAG	C2-N2-C7	-2.46	119.88	123.04
3	A	503	MAN	C1-C2-C3	3.54	113.72	109.54

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	503	MAN	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	NAG	C8-C7-N2-C2
3	A	501	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	NAG	3	0
3	A	502	NAG	3	0
3	A	503	MAN	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 (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.