Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:11 PM GMT

PDB ID	:	1EGJ
Title	:	DOMAIN 4 OF THE BETA COMMON CHAIN IN COMPLEX WITH AN ANTIBODY
Authors	:	Rossjohn, J.; McKinstry, W.J.; Woodcock, J.M.; McClure, B.J.; Hercus, T.R.; Parker, M.W.; Lopez, A.F.; Bagley, C.J.
Deposited on	:	2000-02-15
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 (i) symbol.

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

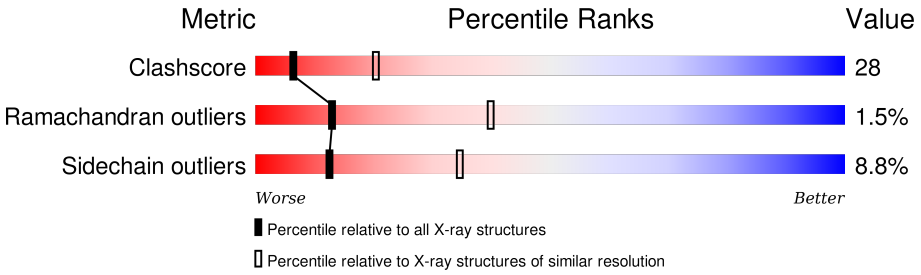
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	101	50% 42% 8%
2	L	215	49% 47% .
3	H	220	59% 35% 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4304 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 CYTOKINE RECEPTOR COMMON BETA CHAIN PRECURSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	101	Total	C	N	O	S	0	0	0
			844	526	151	163	4			

- Molecule 2 is a protein called ANTIBODY (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	215	Total	C	N	O	S	0	0	0
			1660	1033	281	340	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	80	THR	ALA	CONFLICT	EMBL 7024437
L	109	GLY	ALA	CONFLICT	EMBL 7024437
L	144	ALA	ILE	CONFLICT	EMBL 7024437
L	147	ALA	LYS	CONFLICT	EMBL 7024437

- Molecule 3 is a protein called ANTIBODY (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	220	Total	C	N	O	S	0	0	0
			1642	1034	270	330	8			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	39	HIS	GLN	CONFLICT	UNP P01865
H	105	GLN	HIS	CONFLICT	UNP P01865
H	108	THR	LEU	CONFLICT	UNP P01865
H	113	SER	ALA	CONFLICT	UNP P01865
H	118	ALA	PRO	CONFLICT	UNP P01865

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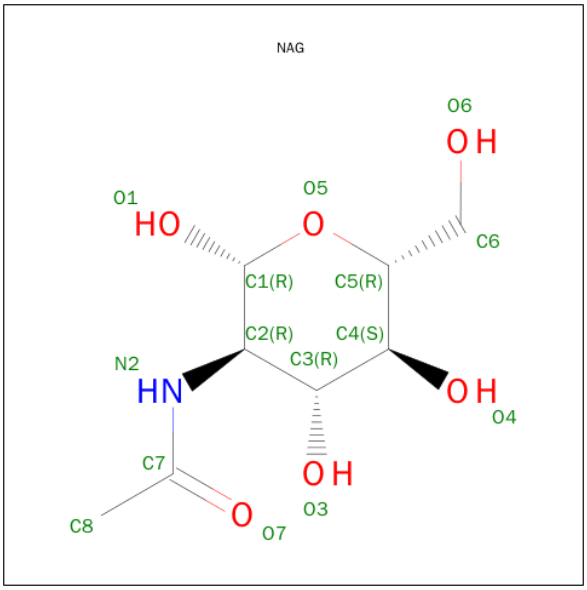
Chain	Residue	Modelled	Actual	Comment	Reference
H	127	VAL	GLY	CONFLICT	UNP P01865
H	128	CYS	SER	CONFLICT	UNP P01865
H	129	GLY	ALA	CONFLICT	UNP P01865
H	130	ASP	ALA	CONFLICT	UNP P01865
H	131	THR	GLN	CONFLICT	UNP P01865
H	133	GLY	ASN	CONFLICT	UNP P01865
H	135	SER	MET	CONFLICT	UNP P01865
H	152	LEU	VAL	CONFLICT	UNP P01865
H	192	THR	PRO	CONFLICT	UNP P01865
H	201	GLN	GLU	CONFLICT	UNP P01865
H	202	SER	THR	CONFLICT	UNP P01865
H	203	ILE	VAL	CONFLICT	UNP P01865
H	224	GLN	ARG	CONFLICT	UNP P01865
H	225	VAL	ASP	CONFLICT	UNP P01865

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	31	Total	O	0	0
			31	31		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	67	Total O 67 67	0	0
5	L	46	Total O 46 46	0	0

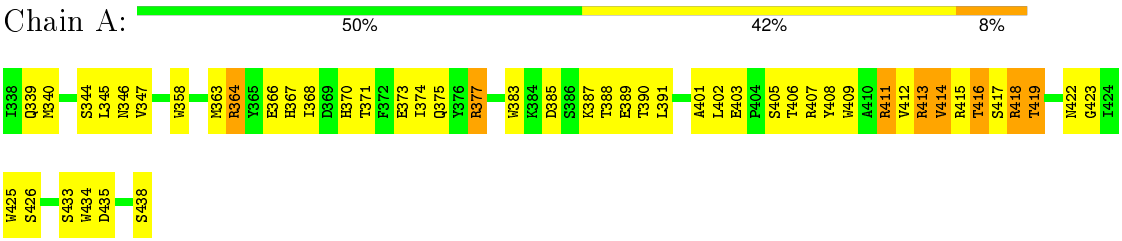
3 Residue-property plots (i)

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.

Note EDS was not executed.

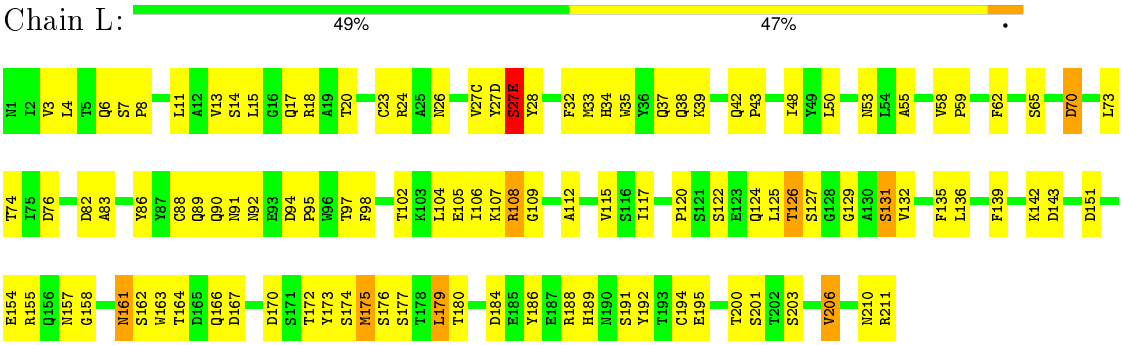
- Molecule 1: CYTOKINE RECEPTOR COMMON BETA CHAIN PRECURSOR

Chain A:



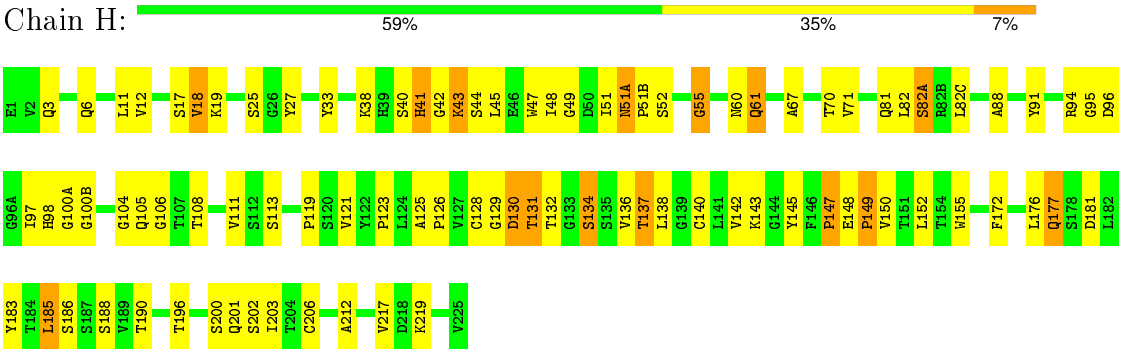
- Molecule 2: ANTIBODY (LIGHT CHAIN)

Chain L:



- Molecule 3: ANTIBODY (HEAVY CHAIN)

Chain H:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	77.61Å 77.61Å 296.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.80)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.288	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4304	wwPDB-VP
Average B, all atoms (Å^2)	67.0	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

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	0.50	0/868	0.70	0/1177
2	L	0.47	0/1700	0.70	0/2314
3	H	0.54	0/1683	0.78	2/2294 (0.1%)
All	All	0.51	0/4251	0.73	2/5785 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	60	ASN	N-CA-C	-6.32	93.94	111.00
3	H	134	SER	N-CA-C	-5.54	96.06	111.00

There are no chirality outliers.

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	844	0	796	51	0
2	L	1660	0	1572	105	0
3	H	1642	0	1608	77	0
4	L	14	0	13	1	0
5	A	31	0	0	1	0
5	H	67	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	46	0	0	3	0
All	All	4304	0	3989	225	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 28.

All (225) 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:L:112:ALA:HB2	2:L:200:THR:HG21	1.34	1.05
3:H:12:VAL:HG11	3:H:18:VAL:HG13	1.48	0.93
3:H:96:ASP:OD1	3:H:97:ILE:HD13	1.70	0.90
2:L:124:GLN:HE22	2:L:131:SER:HB2	1.39	0.88
2:L:161:ASN:HB3	2:L:177:SER:HA	1.56	0.87
1:A:418:ARG:HD3	1:A:419:THR:HG23	1.57	0.87
1:A:377:ARG:HH11	1:A:377:ARG:HG2	1.43	0.82
3:H:51:ILE:HG13	3:H:55:GLY:O	1.83	0.78
3:H:47:TRP:CZ2	3:H:49:GLY:HA2	2.21	0.75
2:L:4:LEU:HD21	2:L:90:GLN:HB3	1.69	0.75
2:L:112:ALA:CB	2:L:200:THR:HG21	2.15	0.74
2:L:120:PRO:HD3	2:L:132:VAL:HG22	1.70	0.73
3:H:155:TRP:CZ3	3:H:206:CYS:HB2	2.24	0.73
2:L:33:MET:HE1	2:L:88:CYS:HB2	1.71	0.73
1:A:403:GLU:O	1:A:406:THR:HG22	1.89	0.73
3:H:121:VAL:HG21	3:H:217:VAL:CG2	2.20	0.72
2:L:195:GLU:HB3	2:L:206:VAL:HG12	1.70	0.72
1:A:339:GLN:NE2	1:A:426:SER:HA	2.04	0.71
2:L:155:ARG:NH2	2:L:157:ASN:HD22	1.87	0.71
2:L:82:ASP:O	2:L:104:LEU:HD21	1.91	0.71
3:H:12:VAL:HG11	3:H:18:VAL:CG1	2.20	0.69
3:H:51(A):ASN:HD22	3:H:52:SER:H	1.38	0.69
2:L:108:ARG:HD3	2:L:109:GLY:O	1.92	0.69
2:L:14:SER:HA	2:L:107:LYS:HB3	1.75	0.69
2:L:161:ASN:ND2	2:L:161:ASN:H	1.91	0.68
3:H:121:VAL:HG21	3:H:217:VAL:HG21	1.75	0.68
1:A:415:ARG:NE	1:A:422:ASN:HB3	2.09	0.67
3:H:202:SER:O	3:H:203:ILE:HD13	1.95	0.67
2:L:161:ASN:HB3	2:L:177:SER:CA	2.25	0.67
1:A:417:SER:HB3	1:A:422:ASN:HD22	1.60	0.67
2:L:34:HIS:CD2	2:L:50:LEU:H	2.13	0.67
1:A:407:ARG:HD2	1:A:435:ASP:OD2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:23:CYS:SG	2:L:33:MET:HE1	2.36	0.66
3:H:51(A):ASN:ND2	3:H:52:SER:H	1.93	0.66
1:A:364:ARG:HG2	5:A:18:HOH:O	1.95	0.66
3:H:51:ILE:HD13	3:H:71:VAL:HG23	1.77	0.66
2:L:142:LYS:HB3	2:L:173:TYR:CD2	2.31	0.66
2:L:4:LEU:HD11	2:L:90:GLN:H	1.61	0.65
3:H:123:PRO:HD3	3:H:219:LYS:HE2	1.78	0.65
3:H:27:TYR:CE2	3:H:94:ARG:HD2	2.32	0.65
3:H:176:LEU:HD21	3:H:181:ASP:HA	1.79	0.65
2:L:86:TYR:HE1	2:L:104:LEU:HD22	1.60	0.65
2:L:20:THR:HG22	2:L:74:THR:HG22	1.79	0.65
4:L:501:NAG:O7	4:L:501:NAG:O3	2.13	0.65
2:L:34:HIS:HD2	2:L:50:LEU:H	1.44	0.64
2:L:27(C):VAL:HG13	2:L:92:ASN:HB2	1.79	0.64
2:L:139:PHE:CE1	2:L:174:SER:HA	2.33	0.64
3:H:51:ILE:O	3:H:51(B):PRO:HD3	1.97	0.63
3:H:42:GLY:C	3:H:43:LYS:HG2	2.18	0.63
1:A:366:GLU:HB2	3:H:33:TYR:CD2	2.34	0.63
2:L:112:ALA:HB2	2:L:200:THR:CG2	2.22	0.63
2:L:135:PHE:CE2	3:H:188:SER:HB3	2.34	0.63
3:H:51(A):ASN:HD22	3:H:51(A):ASN:C	2.01	0.63
2:L:38:GLN:HG3	2:L:42:GLN:O	1.99	0.63
3:H:148:GLU:OE2	3:H:149:PRO:HA	1.98	0.62
2:L:89:GLN:HB2	2:L:98:PHE:CD2	2.35	0.62
2:L:24:ARG:HD2	5:L:504:HOH:O	1.98	0.62
3:H:196:THR:C	3:H:200:SER:HB3	2.19	0.62
3:H:17:SER:HB3	3:H:82(A):SER:HA	1.82	0.61
2:L:27(E):SER:HG	2:L:28:TYR:HD1	1.47	0.61
2:L:11:LEU:HD13	2:L:13:VAL:HG23	1.82	0.61
2:L:151:ASP:OD2	2:L:189:HIS:HB3	2.01	0.61
1:A:383:TRP:CZ2	1:A:411:ARG:HG2	2.35	0.60
2:L:195:GLU:HB3	2:L:206:VAL:CG1	2.31	0.60
3:H:130:ASP:HB3	5:H:267:HOH:O	2.01	0.60
1:A:412:VAL:HG12	1:A:413:ARG:N	2.17	0.60
2:L:127:SER:HB2	5:L:534:HOH:O	2.01	0.60
3:H:3:GLN:HB2	3:H:25:SER:OG	2.02	0.60
1:A:377:ARG:NH1	1:A:377:ARG:HG2	2.16	0.60
3:H:152:LEU:HD23	3:H:152:LEU:C	2.21	0.60
3:H:121:VAL:CG2	3:H:217:VAL:HG21	2.32	0.59
1:A:408:TYR:O	1:A:433:SER:HB2	2.03	0.59
2:L:142:LYS:HD3	2:L:173:TYR:CZ	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:131:THR:HG22	3:H:132:THR:N	2.16	0.59
2:L:131:SER:OG	2:L:180:THR:HG23	2.02	0.59
1:A:340:MET:CE	1:A:414:VAL:HB	2.33	0.59
3:H:18:VAL:HG22	3:H:82(C):LEU:HD11	1.86	0.58
2:L:164:THR:HG23	3:H:172:PHE:CD2	2.39	0.57
3:H:6:GLN:NE2	3:H:106:GLY:H	2.03	0.57
2:L:155:ARG:HH21	2:L:157:ASN:ND2	2.02	0.56
2:L:155:ARG:NH2	2:L:157:ASN:ND2	2.52	0.56
2:L:27(D):TYR:O	2:L:27(E):SER:HB3	2.04	0.56
1:A:416:THR:HG23	1:A:423:GLY:HA3	1.87	0.55
2:L:83:ALA:HB2	2:L:106:ILE:HG12	1.87	0.55
2:L:117:ILE:HD13	2:L:194:CYS:HB3	1.88	0.55
2:L:4:LEU:HD11	2:L:90:GLN:N	2.22	0.55
3:H:41:HIS:O	3:H:43:LYS:HG2	2.06	0.55
3:H:196:THR:O	3:H:200:SER:HB3	2.07	0.54
1:A:366:GLU:HB2	3:H:33:TYR:CE2	2.41	0.54
1:A:375:GLN:NE2	1:A:411:ARG:HH11	2.05	0.54
2:L:155:ARG:HH21	2:L:157:ASN:HD22	1.55	0.54
2:L:191:SER:OG	2:L:210:ASN:ND2	2.40	0.54
3:H:17:SER:HB2	3:H:82:LEU:O	2.08	0.54
2:L:86:TYR:CE1	2:L:104:LEU:HD22	2.41	0.54
1:A:339:GLN:HE21	1:A:426:SER:HA	1.72	0.53
2:L:122:SER:O	2:L:126:THR:HG23	2.08	0.53
1:A:418:ARG:HD2	2:L:28:TYR:HB3	1.90	0.53
3:H:17:SER:HA	3:H:82(C):LEU:CD1	2.38	0.53
3:H:152:LEU:HD23	3:H:152:LEU:O	2.08	0.53
2:L:11:LEU:HD12	2:L:11:LEU:O	2.10	0.52
1:A:418:ARG:HD3	1:A:419:THR:CG2	2.36	0.52
1:A:413:ARG:HD3	1:A:425:TRP:CE3	2.44	0.52
2:L:161:ASN:CB	2:L:177:SER:HA	2.33	0.52
2:L:161:ASN:HA	2:L:176:SER:O	2.10	0.52
1:A:403:GLU:O	1:A:406:THR:CG2	2.58	0.52
1:A:374:ILE:N	1:A:374:ILE:HD12	2.25	0.52
3:H:148:GLU:HG2	3:H:183:TYR:CE2	2.45	0.52
2:L:167:ASP:HB3	2:L:170:ASP:OD1	2.10	0.52
1:A:367:HIS:O	1:A:368:ILE:HG13	2.09	0.52
2:L:27(E):SER:OG	2:L:28:TYR:HD1	1.93	0.52
2:L:162:SER:O	2:L:175:MET:HA	2.10	0.52
3:H:97:ILE:N	3:H:97:ILE:HD12	2.24	0.51
3:H:67:ALA:HA	3:H:81:GLN:O	2.09	0.51
2:L:201:SER:C	2:L:203:SER:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:177:GLN:HB2	5:H:262:HOH:O	2.09	0.51
2:L:105:GLU:O	2:L:105:GLU:HG3	2.09	0.51
2:L:124:GLN:HG2	2:L:129:GLY:O	2.11	0.50
2:L:95:PRO:O	2:L:97:THR:HG23	2.11	0.50
3:H:140:CYS:HB2	3:H:155:TRP:CH2	2.47	0.50
3:H:142:VAL:HB	3:H:185:LEU:HD23	1.93	0.50
2:L:106:ILE:N	2:L:106:ILE:HD13	2.25	0.50
3:H:119:PRO:HB3	3:H:145:TYR:HB3	1.93	0.50
2:L:158:GLY:O	2:L:179:LEU:HA	2.11	0.50
3:H:137:THR:C	3:H:138:LEU:HD12	2.31	0.50
1:A:340:MET:HE3	1:A:414:VAL:HB	1.94	0.50
1:A:364:ARG:HB3	1:A:370:HIS:CE1	2.46	0.50
1:A:375:GLN:HB3	1:A:388:THR:HG22	1.94	0.50
1:A:377:ARG:HH11	1:A:377:ARG:CG	2.18	0.50
1:A:340:MET:HE1	1:A:414:VAL:HB	1.93	0.49
3:H:70:THR:HG22	3:H:71:VAL:H	1.78	0.49
3:H:11:LEU:HB2	3:H:147:PRO:HG3	1.94	0.49
2:L:37:GLN:OE1	2:L:39:LYS:HE3	2.12	0.49
2:L:24:ARG:CZ	2:L:70:ASP:OD2	2.60	0.48
2:L:124:GLN:NE2	2:L:131:SER:HB2	2.19	0.48
1:A:418:ARG:HD2	2:L:28:TYR:CB	2.43	0.48
1:A:415:ARG:HE	1:A:422:ASN:HB3	1.78	0.48
1:A:401:ALA:O	1:A:402:LEU:HD12	2.13	0.48
3:H:61:GLN:OE1	3:H:61:GLN:HA	2.13	0.48
2:L:65:SER:HB2	5:L:503:HOH:O	2.12	0.48
2:L:27(C):VAL:O	2:L:27(C):VAL:HG12	2.14	0.48
1:A:417:SER:HB3	1:A:422:ASN:ND2	2.25	0.48
2:L:135:PHE:CD2	3:H:188:SER:HB3	2.49	0.48
3:H:131:THR:HG22	3:H:132:THR:H	1.76	0.48
1:A:418:ARG:HG2	1:A:418:ARG:HH11	1.79	0.48
1:A:377:ARG:NH1	1:A:383:TRP:CD2	2.82	0.48
1:A:405:SER:OG	1:A:438:SER:HB2	2.14	0.48
3:H:6:GLN:NE2	3:H:106:GLY:N	2.61	0.47
2:L:154:GLU:HG2	2:L:155:ARG:H	1.80	0.47
3:H:125:ALA:HB1	3:H:126:PRO:HD2	1.97	0.47
3:H:95:GLY:HA2	3:H:100(B):GLY:O	2.14	0.47
2:L:8:PRO:O	2:L:102:THR:HG23	2.14	0.47
2:L:86:TYR:HE1	2:L:104:LEU:CD2	2.27	0.47
3:H:147:PRO:HD2	3:H:212:ALA:CB	2.45	0.47
1:A:390:THR:HG22	1:A:391:LEU:N	2.30	0.47
1:A:418:ARG:HE	2:L:32:PHE:HZ	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:33:MET:CE	2:L:88:CYS:HB2	2.44	0.47
2:L:37:GLN:HG3	2:L:86:TYR:CE2	2.50	0.47
2:L:3:VAL:HB	2:L:26:ASN:HB2	1.97	0.47
1:A:412:VAL:CG1	1:A:413:ARG:N	2.78	0.46
1:A:344:SER:O	1:A:358:TRP:HA	2.15	0.46
2:L:50:LEU:HD23	2:L:50:LEU:HA	1.73	0.46
2:L:166:GLN:HB2	2:L:173:TYR:CZ	2.51	0.46
2:L:89:GLN:NE2	2:L:91:ASN:HB2	2.32	0.45
1:A:413:ARG:HG2	1:A:414:VAL:N	2.28	0.45
2:L:162:SER:O	2:L:175:MET:HB2	2.16	0.45
2:L:115:VAL:HA	2:L:135:PHE:O	2.16	0.45
3:H:155:TRP:CH2	3:H:206:CYS:HB2	2.52	0.45
1:A:406:THR:HG23	1:A:408:TYR:CE1	2.50	0.45
3:H:150:VAL:HG13	3:H:150:VAL:O	2.16	0.45
3:H:142:VAL:HB	3:H:185:LEU:CD2	2.47	0.45
2:L:59:PRO:HD2	2:L:62:PHE:HD1	1.81	0.45
3:H:82:LEU:HB2	3:H:82(C):LEU:HD21	1.99	0.45
2:L:59:PRO:HD2	2:L:62:PHE:CD1	2.52	0.45
2:L:48:ILE:HG23	2:L:53:ASN:O	2.17	0.45
3:H:12:VAL:O	3:H:111:VAL:HA	2.16	0.45
1:A:406:THR:CG2	1:A:408:TYR:HE1	2.30	0.45
2:L:15:LEU:HG	2:L:106:ILE:HG22	1.99	0.45
2:L:135:PHE:O	2:L:136:LEU:HD12	2.16	0.45
3:H:136:VAL:O	3:H:190:THR:HG23	2.17	0.45
2:L:55:ALA:O	2:L:58:VAL:HG23	2.17	0.44
3:H:196:THR:HA	3:H:200:SER:HB3	1.99	0.44
2:L:24:ARG:NH1	2:L:70:ASP:OD2	2.50	0.44
2:L:166:GLN:HB2	2:L:173:TYR:CE1	2.52	0.44
2:L:135:PHE:C	2:L:136:LEU:HD12	2.37	0.44
3:H:98:HIS:C	3:H:98:HIS:CD2	2.91	0.44
2:L:27(C):VAL:CG1	2:L:92:ASN:HB2	2.47	0.44
2:L:201:SER:C	2:L:203:SER:N	2.71	0.43
2:L:161:ASN:HB3	2:L:177:SER:CB	2.47	0.43
3:H:51(A):ASN:ND2	3:H:51(A):ASN:C	2.71	0.43
2:L:184:ASP:O	2:L:188:ARG:HG3	2.19	0.43
2:L:18:ARG:HG3	2:L:76:ASP:HB2	2.01	0.43
3:H:82:LEU:CB	3:H:82(C):LEU:HD21	2.48	0.43
3:H:121:VAL:HG21	3:H:217:VAL:HG22	1.99	0.43
3:H:6:GLN:HE21	3:H:104:GLY:HA3	1.83	0.43
3:H:17:SER:CB	3:H:82:LEU:O	2.67	0.42
2:L:14:SER:O	2:L:17:GLN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:VAL:HG21	1:A:434:TRP:CE3	2.54	0.42
3:H:38:LYS:HB2	3:H:48:ILE:HD11	2.01	0.42
2:L:211:ARG:HH11	2:L:211:ARG:HB3	1.84	0.42
2:L:35:TRP:CE2	2:L:73:LEU:HB2	2.55	0.42
1:A:371:THR:HB	1:A:415:ARG:HG3	2.01	0.42
2:L:7:SER:HA	2:L:8:PRO:HA	1.89	0.42
3:H:105:GLN:HG3	5:H:264:HOH:O	2.19	0.42
2:L:90:GLN:C	2:L:90:GLN:OE1	2.58	0.42
3:H:17:SER:HA	3:H:82(C):LEU:HD11	2.02	0.41
1:A:418:ARG:HH11	1:A:419:THR:HG22	1.85	0.41
3:H:185:LEU:HG	3:H:186:SER:N	2.34	0.41
2:L:179:LEU:O	2:L:179:LEU:HD23	2.20	0.41
2:L:186:TYR:HA	2:L:192:TYR:OH	2.21	0.41
3:H:3:GLN:OE1	3:H:3:GLN:HA	2.20	0.41
2:L:170:ASP:O	2:L:172:THR:HG23	2.20	0.41
3:H:11:LEU:HD12	5:H:266:HOH:O	2.19	0.41
1:A:406:THR:HG23	1:A:408:TYR:HE1	1.85	0.41
2:L:163:TRP:CZ2	2:L:175:MET:HE2	2.56	0.41
1:A:387:LYS:HE2	1:A:389:GLU:CG	2.51	0.41
3:H:143:LYS:HB2	3:H:143:LYS:HE3	1.83	0.41
2:L:43:PRO:HB3	3:H:91:TYR:CE2	2.56	0.41
1:A:409:TRP:CE3	1:A:433:SER:HB3	2.57	0.40
2:L:6:GLN:HG2	2:L:88:CYS:SG	2.61	0.40
2:L:83:ALA:HB2	2:L:106:ILE:CG1	2.50	0.40
1:A:377:ARG:NH1	1:A:377:ARG:CG	2.78	0.40
2:L:125:LEU:C	2:L:127:SER:H	2.25	0.40
3:H:40:SER:HA	3:H:88:ALA:HB1	2.03	0.40
1:A:418:ARG:CD	1:A:419:THR:HG23	2.40	0.40
3:H:125:ALA:HB1	3:H:126:PRO:CD	2.51	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	99/101 (98%)	92 (93%)	7 (7%)	0	100 100
2	L	213/215 (99%)	198 (93%)	13 (6%)	2 (1%)	21 55
3	H	218/220 (99%)	187 (86%)	25 (12%)	6 (3%)	6 21
All	All	530/536 (99%)	477 (90%)	45 (8%)	8 (2%)	13 40

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	131	THR
2	L	27(E)	SER
2	L	126	THR
3	H	100(A)	GLY
3	H	129	GLY
3	H	55	GLY
3	H	147	PRO
3	H	149	PRO

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	91/91 (100%)	78 (86%)	13 (14%)	4 12
2	L	186/186 (100%)	176 (95%)	10 (5%)	27 60
3	H	189/189 (100%)	171 (90%)	18 (10%)	11 30
All	All	466/466 (100%)	425 (91%)	41 (9%)	12 35

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	345	LEU
1	A	346	ASN
1	A	363	MET
1	A	364	ARG
1	A	373	GLU

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Mol	Chain	Res	Type
1	A	377	ARG
1	A	385	ASP
1	A	411	ARG
1	A	413	ARG
1	A	414	VAL
1	A	416	THR
1	A	418	ARG
1	A	419	THR
2	L	27(E)	SER
2	L	70	ASP
2	L	94	ASP
2	L	108	ARG
2	L	131	SER
2	L	143	ASP
2	L	161	ASN
2	L	175	MET
2	L	179	LEU
2	L	206	VAL
3	H	18	VAL
3	H	19	LYS
3	H	41	HIS
3	H	43	LYS
3	H	44	SER
3	H	45	LEU
3	H	51(A)	ASN
3	H	61	GLN
3	H	82(A)	SER
3	H	108	THR
3	H	113	SER
3	H	128	CYS
3	H	130	ASP
3	H	134	SER
3	H	137	THR
3	H	177	GLN
3	H	185	LEU
3	H	201	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	339	GLN
1	A	346	ASN

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Mol	Chain	Res	Type
1	A	375	GLN
1	A	392	GLN
1	A	422	ASN
2	L	34	HIS
2	L	91	ASN
2	L	124	GLN
2	L	156	GLN
2	L	157	ASN
2	L	161	ASN
2	L	210	ASN
3	H	6	GLN
3	H	51(A)	ASN
3	H	98	HIS
3	H	170	HIS

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

1 ligand is 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	$\#\|Z\|>2$
4	NAG	L	501	2	14,14,15	1.10	1 (7%)	15,19,21	2.34	4 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	L	501	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	501	NAG	O5-C5	-2.08	1.38	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	501	NAG	C2-N2-C7	-2.34	120.03	123.04
4	L	501	NAG	C1-O5-C5	2.28	115.14	112.25
4	L	501	NAG	C4-C3-C2	4.98	118.97	111.23
4	L	501	NAG	C6-C5-C4	6.02	127.85	113.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	501	NAG	1	0

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

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.