



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:04 PM GMT

PDB ID : 3W11
Title : Insulin receptor ectodomain construct comprising domains L1-CR in complex with human insulin, Alpha-CT peptide(704-719) and FAB 83-7
Authors : Lawrence, M.C.; Smith, B.J.
Deposited on : 2012-11-06
Resolution : 3.90 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

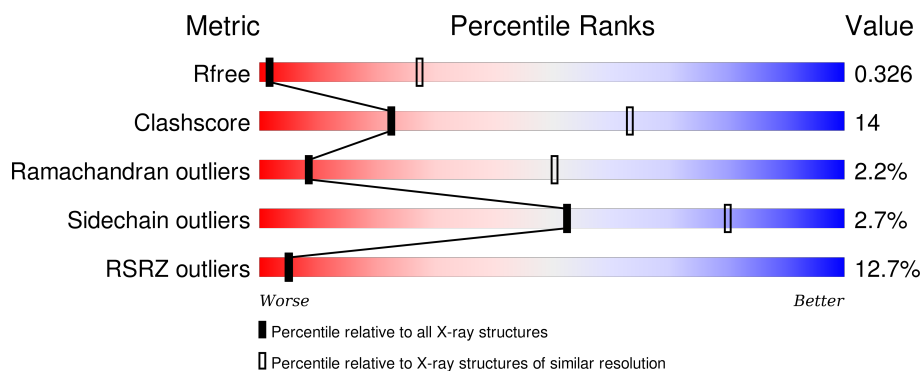
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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	1014 (4.28-3.52)
Clashscore	102246	1031 (4.24-3.56)
Ramachandran outliers	100387	1012 (4.26-3.54)
Sidechain outliers	100360	1004 (4.26-3.54)
RSRZ outliers	91569	1018 (4.28-3.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	21	<div> <div>14%</div> <div>67%</div> <div>24%</div> <div>10%</div> </div>
2	B	30	<div> <div>17%</div> <div>33%</div> <div>50%</div> </div>
3	C	118	<div> <div>19%</div> <div>80%</div> <div>19%</div> <div>•</div> </div>
4	D	114	<div> <div>18%</div> <div>77%</div> <div>21%</div> <div>•</div> </div>
5	E	310	<div> <div>8%</div> <div>73%</div> <div>19%</div> <div>•</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain	
				
6	F	16		

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 4597 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 Insulin A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			

- Molecule 2 is a protein called Insulin B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	15	Total	C	N	O	S	0	0	0
			109	69	17	21	2			

- Molecule 3 is a protein called monoclonal antibody fab 83-7 fragment - heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	118	Total	C	N	O	S	0	0	0
			904	568	153	178	5			

- Molecule 4 is a protein called monoclonal antibody fab 83-7 fragment - light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	114	Total	C	N	O	S	0	0	0
			891	565	149	173	4			

- Molecule 5 is a protein called Insulin receptor domains L1-CR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	288	Total	C	N	O	S	0	0	0
			2301	1449	397	423	32			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	144	HIS	TYR	SEE REMARK 999	UNP P06213

- Molecule 6 is a protein called Insulin receptor alpha-CT peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	F	11	Total	C	N	O	0	0	0
			98	67	14	17			

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	E	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	E	4	Total	C	N	O	0	0
			50	28	2	20		

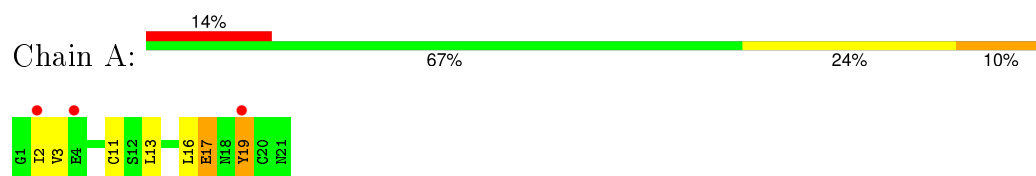
- Molecule 9 is a polymer of unknown type called SUGAR (3-MER).

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

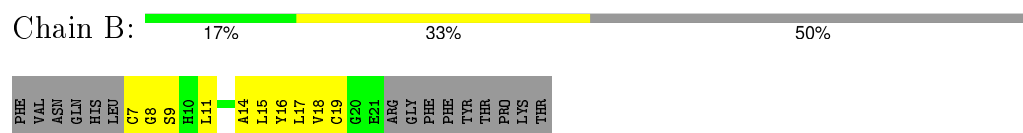
3 Residue-property plots [i](#)

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.

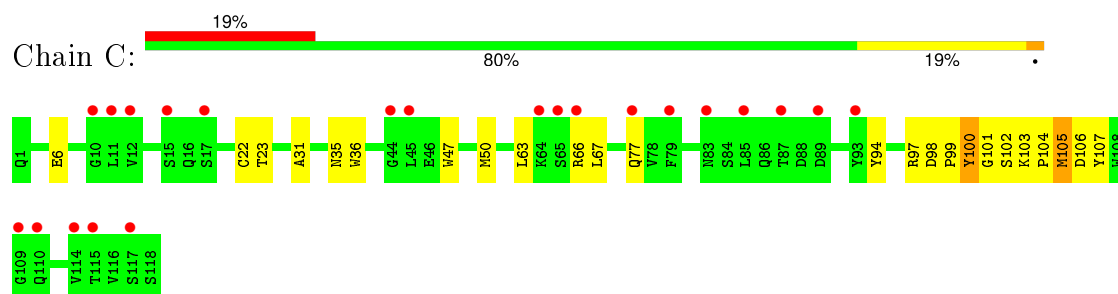
- Molecule 1: Insulin A chain



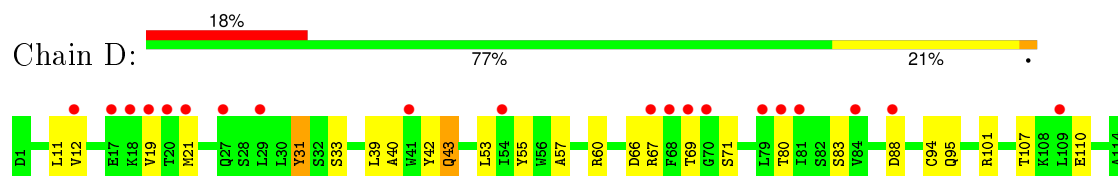
- Molecule 2: Insulin B chain



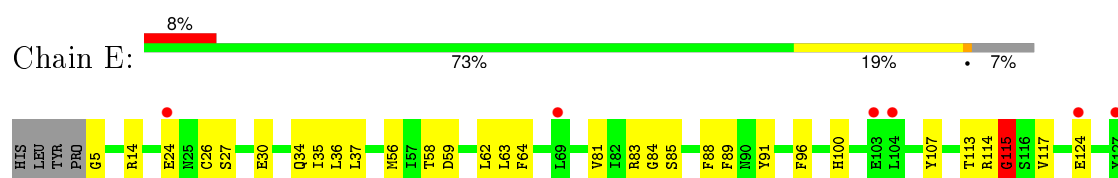
- Molecule 3: monoclonal antibody fab 83-7 fragment - heavy chain

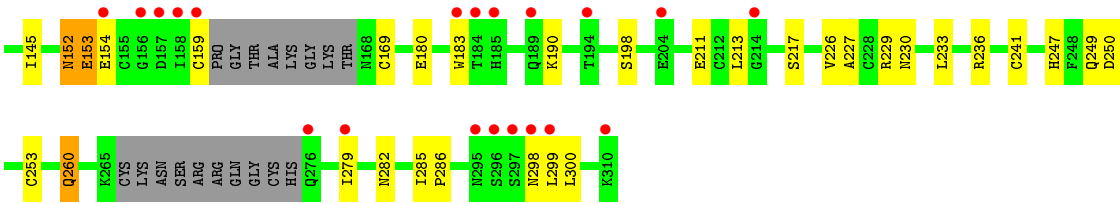


- Molecule 4: monoclonal antibody fab 83-7 fragment - light chain

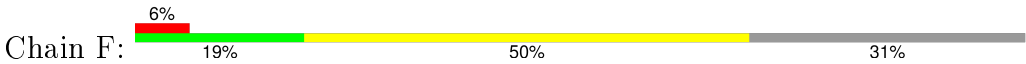


- Molecule 5: Insulin receptor domains L1-CR





• Molecule 6: Insulin receptor alpha-CT peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 3	Depositor
Cell constants a, b, c, α , β , γ	168.91Å 168.91Å 168.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.80 – 3.90 46.85 – 3.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (46.80-3.90) 98.4 (46.85-3.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 3.88Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.264 , 0.292 0.285 , 0.326	Depositor DCC
R_{free} test set	718 reflections (4.89%)	DCC
Wilson B-factor (Å ²)	187.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 296.6	EDS
Estimated twinning fraction	0.054 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 14691 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4597	wwPDB-VP
Average B, all atoms (Å ²)	228.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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: BMA, 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	0/164	0.94	0/220
2	B	0.47	0/110	0.95	0/148
3	C	0.53	0/926	0.77	0/1258
4	D	0.56	0/910	0.78	0/1228
5	E	0.57	0/2355	0.86	1/3192 (0.0%)
6	F	0.67	0/101	0.89	0/137
All	All	0.56	0/4566	0.83	1/6183 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	115	GLY	N-CA-C	5.18	126.06	113.10

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	163	0	149	21	0
2	B	109	0	102	13	0
3	C	904	0	879	34	0
4	D	891	0	882	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	2301	0	2201	54	0
6	F	98	0	87	15	0
7	E	42	0	39	3	0
8	E	50	0	43	0	0
9	E	39	0	34	0	0
All	All	4597	0	4416	123	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 14.

All (123) 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)
3:C:35:ASN:OD1	3:C:50:MET:HB3	1.39	1.17
3:C:35:ASN:OD1	3:C:50:MET:CB	2.08	1.01
4:D:60:ARG:HH11	4:D:66:ASP:HA	1.30	0.95
3:C:99:PRO:HG2	3:C:103:LYS:HB2	1.51	0.92
1:A:2:ILE:HG12	2:B:11:LEU:HD21	1.51	0.90
5:E:81:VAL:HG21	5:E:213:LEU:HD23	1.55	0.89
1:A:16:LEU:HB3	2:B:18:VAL:HG21	1.63	0.81
1:A:2:ILE:CG1	2:B:11:LEU:HD21	2.12	0.79
1:A:2:ILE:HG12	2:B:11:LEU:CD2	2.13	0.78
1:A:2:ILE:HD11	2:B:11:LEU:HD11	1.64	0.78
1:A:3:VAL:CG2	6:F:710:HIS:HB2	2.13	0.77
5:E:14:ARG:HG2	5:E:36:LEU:HD11	1.67	0.76
3:C:99:PRO:HD2	3:C:103:LYS:O	1.88	0.74
5:E:241:CYS:H	5:E:247:HIS:CE1	2.05	0.74
1:A:2:ILE:CD1	2:B:11:LEU:HD21	2.19	0.73
5:E:241:CYS:H	5:E:247:HIS:HE1	1.40	0.70
3:C:63:LEU:HD23	3:C:66:ARG:HB2	1.74	0.69
3:C:100:TYR:HE2	5:E:233:LEU:HD21	1.57	0.69
5:E:14:ARG:HG2	5:E:36:LEU:CD1	2.23	0.68
3:C:63:LEU:HD22	3:C:67:LEU:HB2	1.75	0.68
5:E:213:LEU:HB3	5:E:227:ALA:CB	2.23	0.68
3:C:104:PRO:HG2	4:D:55:TYR:HB3	1.76	0.67
4:D:12:VAL:HG12	4:D:110:GLU:HB2	1.75	0.67
5:E:198:SER:O	5:E:213:LEU:O	2.15	0.64
3:C:100:TYR:HE2	5:E:233:LEU:CD2	2.10	0.64
5:E:96:PHE:CE2	6:F:709:LEU:CD2	2.80	0.64
5:E:211:GLU:OE2	5:E:230:ASN:ND2	2.32	0.63
3:C:99:PRO:HG2	3:C:103:LYS:CB	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:43:GLN:HB2	4:D:53:LEU:HD11	1.83	0.60
3:C:104:PRO:HA	4:D:101:ARG:HH12	1.67	0.60
4:D:60:ARG:NH1	4:D:66:ASP:HA	2.09	0.60
3:C:106:ASP:O	3:C:107:TYR:HB2	2.03	0.59
5:E:213:LEU:HB3	5:E:227:ALA:HB1	1.83	0.59
4:D:67:ARG:NH2	4:D:88:ASP:OD1	2.34	0.59
3:C:31:ALA:O	5:E:236:ARG:NH1	2.37	0.57
1:A:16:LEU:CB	2:B:18:VAL:HG21	2.34	0.57
3:C:98:ASP:OD1	4:D:101:ARG:NH2	2.37	0.57
5:E:96:PHE:CE2	6:F:709:LEU:HD22	2.40	0.57
5:E:190:LYS:HD3	7:E:507:NAG:H81	1.88	0.55
3:C:97:ARG:O	3:C:105:MET:HA	2.06	0.55
5:E:213:LEU:HB3	5:E:227:ALA:HB3	1.87	0.55
6:F:708:TYR:O	6:F:712:VAL:HG12	2.06	0.55
1:A:3:VAL:HG23	6:F:710:HIS:HB2	1.88	0.55
4:D:39:LEU:HD22	4:D:95:GLN:O	2.07	0.54
5:E:58:THR:HG22	5:E:85:SER:OG	2.08	0.54
5:E:233:LEU:HD12	5:E:253:CYS:HB2	1.90	0.54
4:D:39:LEU:HD13	4:D:40:ALA:N	2.23	0.53
5:E:298:ASN:ND2	5:E:300:LEU:HD12	2.23	0.53
3:C:101:GLY:H	5:E:236:ARG:NH2	2.07	0.53
5:E:152:ASN:O	5:E:154:GLU:N	2.37	0.52
5:E:226:VAL:HG12	5:E:226:VAL:O	2.09	0.52
1:A:16:LEU:HD23	2:B:18:VAL:HG21	1.91	0.52
5:E:30:GLU:CG	5:E:249:GLN:HG2	2.39	0.52
5:E:30:GLU:HG3	5:E:249:GLN:HG2	1.91	0.52
3:C:35:ASN:HD21	4:D:101:ARG:HD2	1.74	0.52
5:E:36:LEU:HD13	5:E:37:LEU:HG	1.92	0.52
5:E:5:GLY:HA3	5:E:27:SER:OG	2.09	0.52
4:D:31:TYR:HE1	5:E:282:ASN:OD1	1.92	0.52
4:D:21:MET:HB2	4:D:107:THR:HG21	1.92	0.51
1:A:17:GLU:C	1:A:17:GLU:CD	2.69	0.51
3:C:47:TRP:CD2	4:D:101:ARG:O	2.63	0.51
5:E:64:PHE:HA	5:E:96:PHE:O	2.10	0.51
6:F:715:VAL:HG12	6:F:715:VAL:O	2.11	0.51
1:A:13:LEU:O	1:A:13:LEU:HD12	2.10	0.51
3:C:35:ASN:HD22	3:C:105:MET:CE	2.24	0.50
5:E:56:MET:HG3	5:E:81:VAL:HB	1.93	0.50
3:C:23:THR:HG22	3:C:77:GLN:HG2	1.92	0.50
6:F:712:VAL:HG13	6:F:713:VAL:HG23	1.94	0.50
1:A:3:VAL:HG21	6:F:707:ASP:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:169:CYS:HB2	5:E:180:GLU:HG2	1.93	0.49
3:C:47:TRP:CE3	4:D:101:ARG:O	2.65	0.49
5:E:24:GLU:HG2	7:E:502:NAG:H82	1.93	0.49
3:C:35:ASN:OD1	3:C:50:MET:HB2	2.06	0.49
5:E:88:PHE:CZ	6:F:712:VAL:HG11	2.48	0.49
1:A:2:ILE:HD13	2:B:11:LEU:HD21	1.94	0.49
5:E:81:VAL:CG2	5:E:213:LEU:HD23	2.36	0.49
1:A:2:ILE:HB	1:A:19:TYR:CE2	2.48	0.48
5:E:96:PHE:CD2	6:F:709:LEU:HD22	2.48	0.48
5:E:56:MET:SD	5:E:83:ARG:HD2	2.52	0.48
5:E:117:VAL:HG12	5:E:145:ILE:HD11	1.95	0.48
3:C:97:ARG:HG2	3:C:98:ASP:N	2.28	0.48
3:C:104:PRO:HG2	4:D:55:TYR:CB	2.41	0.48
5:E:260:GLN:HA	5:E:299:LEU:HD11	1.95	0.48
5:E:285:ILE:HG13	5:E:286:PRO:HD2	1.96	0.47
4:D:39:LEU:HD21	4:D:94:CYS:HB2	1.97	0.47
3:C:35:ASN:ND2	4:D:101:ARG:HD2	2.30	0.46
5:E:114:ARG:O	5:E:115:GLY:O	2.34	0.46
3:C:100:TYR:CE2	5:E:233:LEU:CD2	2.96	0.46
3:C:104:PRO:CG	4:D:55:TYR:HB3	2.45	0.45
5:E:96:PHE:CD2	6:F:709:LEU:CD2	2.99	0.45
5:E:226:VAL:O	5:E:226:VAL:CG1	2.64	0.45
3:C:6:GLU:OE2	3:C:94:TYR:HA	2.16	0.45
5:E:217:SER:HA	7:E:507:NAG:H62	1.99	0.45
1:A:19:TYR:HE1	6:F:715:VAL:C	2.19	0.44
3:C:104:PRO:CG	4:D:55:TYR:CB	2.95	0.44
3:C:35:ASN:HD22	3:C:105:MET:HE3	1.81	0.44
2:B:14:ALA:O	2:B:18:VAL:HG23	2.18	0.44
3:C:6:GLU:OE1	3:C:6:GLU:N	2.49	0.44
5:E:279:ILE:HB	5:E:300:LEU:HD23	2.00	0.44
4:D:31:TYR:HE1	5:E:282:ASN:CG	2.21	0.44
1:A:17:GLU:O	1:A:17:GLU:CD	2.56	0.44
5:E:159:CYS:HB3	5:E:169:CYS:SG	2.58	0.44
6:F:713:VAL:HG12	6:F:713:VAL:O	2.18	0.43
1:A:2:ILE:HD12	1:A:19:TYR:CE2	2.54	0.43
4:D:43:GLN:CB	4:D:53:LEU:HD11	2.48	0.43
3:C:105:MET:HB2	4:D:42:TYR:OH	2.19	0.43
5:E:83:ARG:HA	5:E:113:THR:HB	2.00	0.42
5:E:89:PHE:O	5:E:91:TYR:CD2	2.73	0.42
1:A:3:VAL:HG11	6:F:707:ASP:HB3	2.02	0.42
1:A:16:LEU:HB3	2:B:18:VAL:HG11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:59:ASP:O	5:E:84:GLY:HA2	2.20	0.41
5:E:153:GLU:HG2	5:E:153:GLU:O	2.20	0.41
1:A:2:ILE:HB	1:A:19:TYR:CZ	2.55	0.41
3:C:22:CYS:HB2	3:C:36:TRP:CH2	2.56	0.41
5:E:34:GLN:HG2	5:E:62:LEU:HD23	2.02	0.41
4:D:19:VAL:O	4:D:80:THR:HA	2.21	0.41
4:D:11:LEU:CD2	4:D:19:VAL:HG13	2.51	0.41
2:B:16:TYR:O	2:B:17:LEU:C	2.60	0.41
2:B:15:LEU:CD2	6:F:714:PHE:CE1	3.04	0.40
3:C:47:TRP:CE2	4:D:101:ARG:HB2	2.56	0.40
5:E:285:ILE:CG1	5:E:286:PRO:HD2	2.51	0.40
5:E:35:ILE:HB	5:E:63:LEU:CD1	2.52	0.40
5:E:107:TYR:HA	5:E:183:TRP:CD1	2.57	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	19/21 (90%)	18 (95%)	1 (5%)	0	100	100
2	B	13/30 (43%)	9 (69%)	1 (8%)	3 (23%)	0	1
3	C	116/118 (98%)	108 (93%)	6 (5%)	2 (2%)	11	55
4	D	112/114 (98%)	103 (92%)	6 (5%)	3 (3%)	6	46
5	E	282/310 (91%)	258 (92%)	20 (7%)	4 (1%)	14	58
6	F	9/16 (56%)	7 (78%)	2 (22%)	0	100	100
All	All	551/609 (90%)	503 (91%)	36 (6%)	12 (2%)	8	50

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	100	TYR
5	E	115	GLY
5	E	153	GLU
2	B	8	GLY
4	D	83	SER
5	E	100	HIS
3	C	105	MET
4	D	57	ALA
5	E	124	GLU
4	D	33	SER
2	B	9	SER
2	B	19	CYS

5.3.2 Protein sidechains ⓘ

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	20/20 (100%)	17 (85%)	3 (15%)	3	25
2	B	12/26 (46%)	11 (92%)	1 (8%)	14	51
3	C	101/101 (100%)	100 (99%)	1 (1%)	82	91
4	D	100/100 (100%)	96 (96%)	4 (4%)	38	73
5	E	268/286 (94%)	263 (98%)	5 (2%)	65	86
6	F	11/16 (69%)	11 (100%)	0	100	100
All	All	512/549 (93%)	498 (97%)	14 (3%)	52	80

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	CYS
1	A	17	GLU
1	A	19	TYR
2	B	7	CYS
3	C	102	SER
4	D	31	TYR
4	D	43	GLN

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Mol	Chain	Res	Type
4	D	69	THR
4	D	71	SER
5	E	26	CYS
5	E	152	ASN
5	E	229	ARG
5	E	250	ASP
5	E	260	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
3	C	16	GLN
3	C	35	ASN
4	D	43	GLN
4	D	95	GLN
5	E	32	HIS
5	E	247	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 ⓘ

7 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
8	NAG	E	503	8,5	14,14,15	0.29	0	15,19,21	1.13	1 (6%)
8	NAG	E	504	8	14,14,15	0.27	0	15,19,21	0.46	0
8	BMA	E	505	8	11,11,12	0.31	0	14,15,17	1.06	1 (7%)
8	MAN	E	506	8	11,11,12	0.44	0	14,15,17	0.94	1 (7%)
9	NAG	E	508	9,5	14,14,15	0.27	0	15,19,21	0.87	1 (6%)
9	NAG	E	509	9	14,14,15	0.41	0	15,19,21	1.52	4 (26%)
9	BMA	E	510	9	11,11,12	0.30	0	14,15,17	1.01	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
8	NAG	E	503	8,5	-	0/6/23/26	0/1/1/1
8	NAG	E	504	8	-	0/6/23/26	0/1/1/1
8	BMA	E	505	8	-	0/2/19/22	0/1/1/1
8	MAN	E	506	8	-	0/2/19/22	0/1/1/1
9	NAG	E	508	9,5	-	0/6/23/26	0/1/1/1
9	NAG	E	509	9	-	0/6/23/26	0/1/1/1
9	BMA	E	510	9	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	509	NAG	C2-N2-C7	2.10	125.73	123.04
9	E	509	NAG	O4-C4-C3	2.29	115.50	110.34
9	E	508	NAG	C1-O5-C5	2.59	115.53	112.25
8	E	506	MAN	C1-C2-C3	2.68	112.71	109.54
8	E	505	BMA	C1-O5-C5	2.78	115.78	112.25
9	E	509	NAG	O4-C4-C5	3.02	117.25	109.24
8	E	503	NAG	C1-O5-C5	3.22	116.34	112.25
9	E	510	BMA	C1-O5-C5	3.40	116.57	112.25
9	E	509	NAG	C1-O5-C5	3.84	117.12	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

3 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	$\# Z > 2$
7	NAG	E	501	5	14,14,15	0.32	0	15,19,21	1.09	1 (6%)
7	NAG	E	502	5	14,14,15	0.42	0	15,19,21	1.12	1 (6%)
7	NAG	E	507	5	14,14,15	0.35	0	15,19,21	0.81	0

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
7	NAG	E	501	5	-	0/6/23/26	0/1/1/1
7	NAG	E	502	5	-	0/6/23/26	0/1/1/1
7	NAG	E	507	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	502	NAG	C1-O5-C5	3.83	117.11	112.25
7	E	501	NAG	C1-O5-C5	3.94	117.25	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	502	NAG	1	0
7	E	507	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	21/21 (100%)	0.75	3 (14%) 4 3	225, 255, 288, 296	0
2	B	15/30 (50%)	0.22	0 100 100	200, 230, 271, 301	0
3	C	118/118 (100%)	1.04	22 (18%) 2 2	173, 266, 318, 322	0
4	D	114/114 (100%)	0.88	20 (17%) 2 2	186, 216, 286, 356	0
5	E	288/310 (92%)	0.49	26 (9%) 12 8	166, 211, 275, 342	0
6	F	11/16 (68%)	0.38	1 (9%) 11 8	179, 189, 214, 215	0
All	All	567/609 (93%)	0.68	72 (12%) 5 5	166, 220, 299, 356	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	154	GLU	7.5
4	D	20	THR	6.7
3	C	115	THR	5.6
5	E	158	ILE	5.5
4	D	68	PHE	5.0
3	C	77	GLN	4.9
3	C	83	ASN	4.8
3	C	11	LEU	4.4
4	D	21	MET	4.0
3	C	109	GLY	4.0
3	C	17	SER	4.0
3	C	114	VAL	3.8
3	C	12	VAL	3.8
4	D	17	GLU	3.8
5	E	299	LEU	3.7
4	D	19	VAL	3.6
1	A	2	ILE	3.5
5	E	156	GLY	3.3
4	D	54	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
4	D	18	LYS	3.3
5	E	185	HIS	3.2
3	C	10	GLY	3.2
3	C	66	ARG	3.1
4	D	27	GLN	3.1
3	C	45	LEU	3.1
3	C	93	TYR	3.0
5	E	184	THR	3.0
5	E	183	TRP	3.0
3	C	79	PHE	3.0
5	E	204	GLU	3.0
4	D	80	THR	2.9
5	E	157	ASP	2.9
4	D	29	LEU	2.9
4	D	84	VAL	2.9
1	A	19	TYR	2.9
5	E	159	CYS	2.8
4	D	69	THR	2.8
4	D	79	LEU	2.8
5	E	310	LYS	2.8
5	E	214	GLY	2.8
5	E	295	ASN	2.8
5	E	189	GLN	2.6
5	E	104	LEU	2.6
5	E	103	GLU	2.6
3	C	44	GLY	2.5
4	D	109	LEU	2.5
3	C	110	GLN	2.5
1	A	4	GLU	2.5
3	C	85	LEU	2.5
4	D	81	ILE	2.5
5	E	298	ASN	2.4
5	E	124	GLU	2.4
4	D	41	TRP	2.4
4	D	88	ASP	2.3
5	E	24	GLU	2.3
5	E	194	THR	2.2
3	C	117	SER	2.2
4	D	67	ARG	2.2
6	F	714	PHE	2.2
3	C	89	ASP	2.2
5	E	69	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
4	D	12	VAL	2.2
5	E	296	SER	2.2
5	E	297	SER	2.1
4	D	70	GLY	2.1
3	C	65	SER	2.1
3	C	15	SER	2.1
5	E	127	TYR	2.1
5	E	279	ILE	2.1
5	E	276	GLN	2.1
3	C	64	LYS	2.1
3	C	87	THR	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](#)

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(Å ²)	Q<0.9
8	NAG	E	503	14/15	0.90	0.26	-0.80	208,210,215,216	0
8	MAN	E	506	11/12	0.78	0.37	-	266,275,281,284	0
8	NAG	E	504	14/15	0.94	0.21	-	213,217,222,227	0
9	NAG	E	509	14/15	0.57	0.44	-	266,293,324,348	0
8	BMA	E	505	11/12	0.88	0.22	-	236,241,247,256	0
9	BMA	E	510	11/12	0.42	0.41	-	370,378,383,384	0
9	NAG	E	508	14/15	0.84	0.26	-	241,250,263,274	0

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, 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
7	NAG	E	507	14/15	0.79	0.36	0.53	244,252,259,259	0
7	NAG	E	502	14/15	0.62	0.65	-	250,269,284,292	0
7	NAG	E	501	14/15	0.67	0.41	-	305,329,354,355	0

6.5 Other polymers [i](#)

There are no such residues in this entry.