



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:19 PM UTC

PDB ID : 1NGX / pdb_00001ngx
Title : Chimeric Germline Fab 7g12 with jeffamine fragment bound
Authors : Yin, J.; Andryski, S.E.; Beuscher, A.B.; Stevens, R.C.; Schultz, P.G.
Deposited on : 2002-12-18
Resolution : 1.80 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

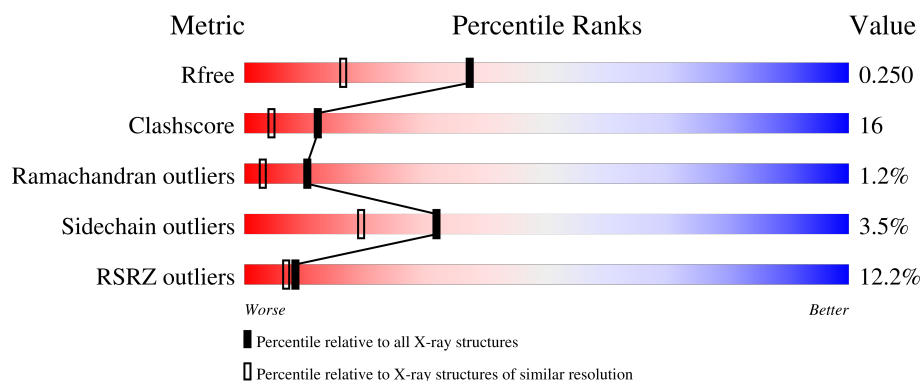
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	213	10% 74% 23% .
1	L	213	5% 74% 22% .
2	B	216	20% 69% 28% .
2	H	216	14% 72% 25% .

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	JEF	B	700	X	-	-	-
3	JEF	H	701	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7256 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.

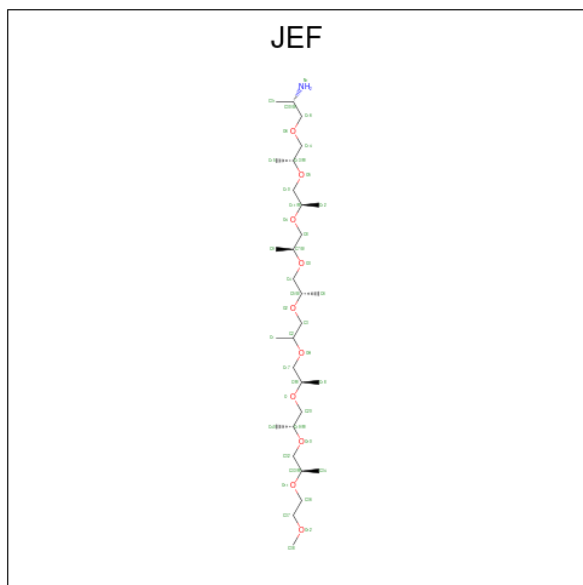
- Molecule 1 is a protein called Germline Metal Chelatase Catalytic Antibody, Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1643	1026	274	336	7			
1	L	213	Total	C	N	O	S	0	0	0
			1643	1026	274	336	7			

- Molecule 2 is a protein called Germline Metal Chelatase Catalytic Antibody, Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total	C	N	O	S	0	0	0
			1621	1023	271	321	6			
2	H	216	Total	C	N	O	S	0	0	0
			1621	1023	271	321	6			

- Molecule 3 is O-(O-(2-AMINOPROPYL)-O'-(2-METHOXYETHYL)POLYPROPYLENE GLYCOL 500) (CCD ID: JEF) (formula: C₃₀H₆₃NO₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			28	21	7		
3	H	1	Total	C	O	0	0
			28	21	7		

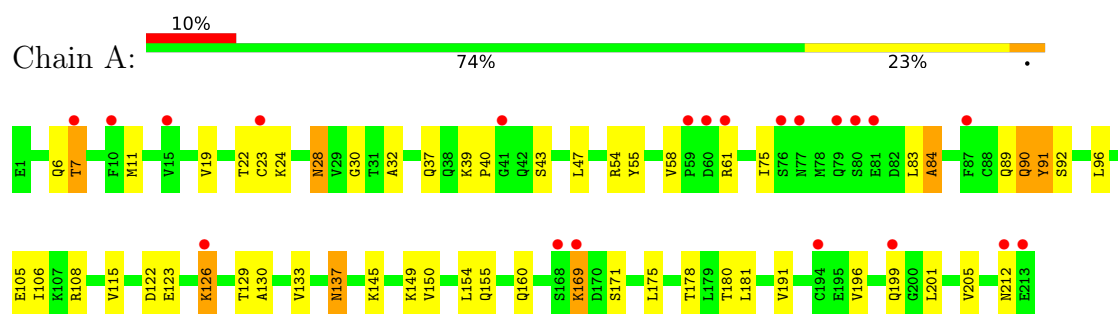
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	148	Total	O	0	0
			148	148		
4	B	143	Total	O	0	0
			143	143		
4	L	207	Total	O	0	0
			207	207		
4	H	174	Total	O	0	0
			174	174		

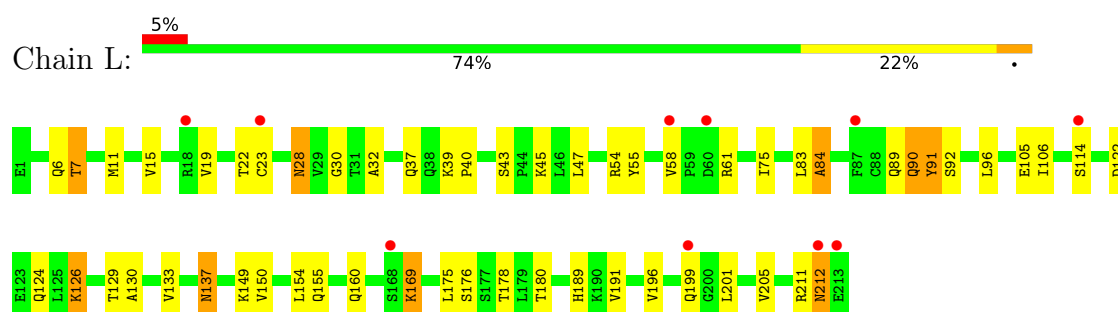
3 Residue-property plots [i](#)

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

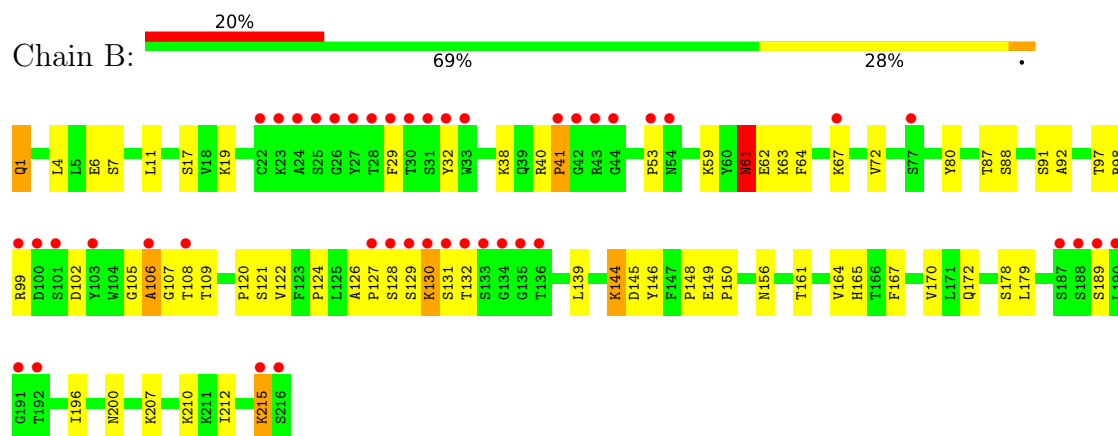
- Molecule 1: Germline Metal Chelatase Catalytic Antibody, Light chain



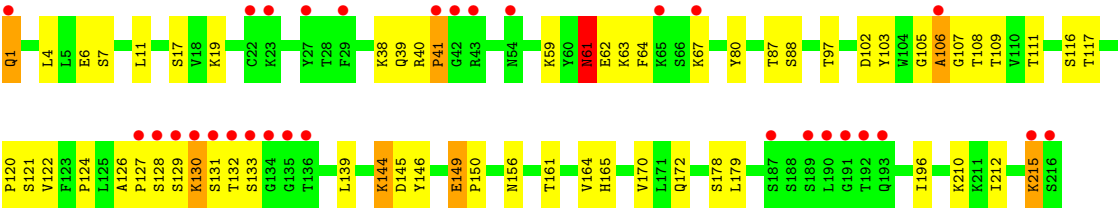
- Molecule 1: Germline Metal Chelatase Catalytic Antibody, Light chain



- Molecule 2: Germline Metal Chelatase Catalytic Antibody, Heavy chain



- Molecule 2: Germline Metal Chelatase Catalytic Antibody, Heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.67Å 64.72Å 93.38Å 90.00° 92.58° 90.00°	Depositor
Resolution (Å)	19.87 – 1.80 19.87 – 1.80	Depositor EDS
% Data completeness (in resolution range)	93.7 (19.87-1.80) 93.6 (19.87-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.84 (at 1.70Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.250 0.224 , 0.250	Depositor DCC
R_{free} test set	3696 reflections (4.22%)	wwPDB-VP
Wilson B-factor (Å ²)	18.6	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.055 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7256	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: JEF

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	0.34	0/1677	0.83	5/2274 (0.2%)
1	L	0.34	0/1677	0.83	5/2274 (0.2%)
2	B	0.32	0/1661	0.88	9/2260 (0.4%)
2	H	0.33	0/1661	0.89	10/2260 (0.4%)
All	All	0.33	0/6676	0.86	29/9068 (0.3%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	90	GLN	N-CA-C	8.78	125.07	113.30
1	A	90	GLN	N-CA-C	8.62	124.86	113.30
2	B	61	ASN	N-CA-C	-6.78	98.98	109.76
2	H	61	ASN	N-CA-C	-6.69	99.12	109.76
2	H	144	LYS	N-CA-C	6.36	120.07	109.95
2	B	145	ASP	N-CA-C	6.32	118.31	110.91
1	L	91	TYR	N-CA-C	6.29	124.20	110.80
2	B	144	LYS	N-CA-C	6.25	119.89	109.95
1	A	91	TYR	N-CA-C	6.17	123.93	110.80
2	B	126	ALA	N-CA-C	6.16	117.57	109.93
2	H	145	ASP	N-CA-C	6.13	118.08	110.91
2	H	126	ALA	N-CA-C	5.98	117.35	109.93
2	H	109	THR	N-CA-C	5.87	118.80	109.24
2	B	109	THR	N-CA-C	5.84	118.76	109.24
2	B	149	GLU	N-CA-C	-5.50	102.29	110.20
2	H	121	SER	N-CA-C	-5.48	100.76	109.59
1	A	137	ASN	N-CA-C	5.39	118.27	109.59
2	H	149	GLU	N-CA-C	-5.31	102.43	110.39
1	L	137	ASN	N-CA-C	5.28	118.09	109.59
1	A	191	VAL	N-CA-C	5.28	116.31	108.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	VAL	N-CA-C	5.20	116.46	108.71
2	H	126	ALA	CA-C-N	5.16	125.09	119.78
2	H	126	ALA	C-N-CA	5.16	125.09	119.78
2	H	107	GLY	N-CA-C	-5.13	101.02	113.18
1	L	114	SER	N-CA-C	-5.12	100.39	108.73
2	B	107	GLY	N-CA-C	-5.09	101.11	113.18
2	B	167	PHE	N-CA-C	5.09	117.67	110.24
1	L	191	VAL	N-CA-C	5.07	115.99	108.23
2	B	121	SER	N-CA-C	-5.02	100.99	109.07

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	1643	0	1592	51	0
1	L	1643	0	1592	55	0
2	B	1621	0	1608	57	0
2	H	1621	0	1608	51	0
3	B	28	0	37	2	0
3	H	28	0	37	2	0
4	A	148	0	0	8	0
4	B	143	0	0	10	0
4	H	174	0	0	9	0
4	L	207	0	0	16	0
All	All	7256	0	6474	203	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 16.

All (203) 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:7:SER:H	2:B:108:THR:HG22	1.16	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:7:SER:H	2:H:108:THR:HG22	1.16	1.05
2:H:117:THR:HB	4:H:717:HOH:O	1.66	0.93
1:A:55:TYR:CE2	2:B:102:ASP:HB3	2.07	0.90
2:H:1:GLN:HE22	2:H:17:SER:H	1.26	0.83
2:B:1:GLN:HE22	2:B:17:SER:H	1.26	0.81
2:H:7:SER:N	2:H:108:THR:HG22	1.97	0.79
2:H:161:THR:O	2:H:164:VAL:HG12	1.81	0.79
2:B:161:THR:O	2:B:164:VAL:HG12	1.82	0.79
2:B:7:SER:N	2:B:108:THR:HG22	1.96	0.79
2:H:149:GLU:HG3	4:H:737:HOH:O	1.82	0.78
1:L:45:LYS:HE3	2:H:102:ASP:OD2	1.84	0.76
2:H:129:SER:HB3	4:H:764:HOH:O	1.87	0.75
1:A:169:LYS:HA	1:A:169:LYS:HZ3	1.54	0.73
1:A:150:VAL:HG22	1:A:155:GLN:NE2	2.04	0.73
1:L:150:VAL:HG22	1:L:155:GLN:NE2	2.03	0.73
1:A:54:ARG:HB3	1:A:58:VAL:CG2	2.19	0.72
1:L:55:TYR:O	1:L:58:VAL:HG22	1.89	0.72
1:A:90:GLN:O	1:A:92:SER:N	2.22	0.72
2:H:127:PRO:HG3	2:H:139:LEU:HB3	1.72	0.72
2:B:127:PRO:HG3	2:B:139:LEU:HB3	1.72	0.72
1:L:169:LYS:HA	1:L:169:LYS:NZ	2.05	0.72
2:H:116:SER:HB3	4:H:819:HOH:O	1.88	0.72
1:A:169:LYS:HA	1:A:169:LYS:NZ	2.05	0.71
1:A:55:TYR:O	1:A:58:VAL:HG22	1.90	0.71
1:L:54:ARG:HB3	1:L:58:VAL:CG2	2.20	0.71
1:A:137:ASN:HD21	2:B:165:HIS:CD2	2.07	0.71
2:B:29:PHE:HB2	4:B:823:HOH:O	1.90	0.70
1:L:7:THR:HB	4:L:379:HOH:O	1.92	0.70
1:A:89:GLN:HE22	3:B:700:JEF:H11	1.55	0.70
1:L:90:GLN:O	1:L:92:SER:N	2.24	0.69
1:L:176:SER:HB3	4:L:388:HOH:O	1.92	0.69
2:H:215:LYS:HB2	2:H:215:LYS:NZ	2.06	0.69
2:B:99:ARG:HG3	4:B:795:HOH:O	1.93	0.69
2:B:215:LYS:NZ	2:B:215:LYS:HB2	2.07	0.69
1:L:106:ILE:HG23	4:L:311:HOH:O	1.93	0.68
2:B:189:SER:HB2	4:B:778:HOH:O	1.94	0.67
2:B:1:GLN:NE2	2:B:17:SER:H	1.92	0.67
1:L:137:ASN:HD21	2:H:165:HIS:CD2	2.14	0.66
2:B:32:TYR:HB2	4:B:823:HOH:O	1.95	0.65
2:H:1:GLN:HE22	2:H:17:SER:N	1.95	0.65
2:H:1:GLN:NE2	2:H:17:SER:H	1.93	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:ASN:HD22	2:B:61:ASN:C	2.06	0.64
2:B:1:GLN:HE22	2:B:17:SER:N	1.95	0.63
1:L:199:GLN:H	1:L:199:GLN:CD	2.07	0.62
1:A:19:VAL:HB	1:A:75:ILE:HB	1.81	0.62
2:B:99:ARG:N	4:B:750:HOH:O	2.31	0.62
1:A:199:GLN:H	1:A:199:GLN:CD	2.07	0.62
2:H:120:PRO:HB3	2:H:146:TYR:HB3	1.81	0.62
1:L:169:LYS:HA	1:L:169:LYS:HZ3	1.63	0.62
2:H:61:ASN:C	2:H:61:ASN:HD22	2.06	0.62
2:H:133:SER:HA	4:H:856:HOH:O	1.99	0.62
2:B:97:THR:HG21	3:B:700:JEF:H102	1.82	0.61
2:H:105:GLY:O	2:H:106:ALA:O	2.18	0.61
1:L:19:VAL:HB	1:L:75:ILE:HB	1.81	0.61
2:B:61:ASN:HD22	2:B:62:GLU:N	1.99	0.61
2:B:105:GLY:O	2:B:106:ALA:O	2.18	0.61
2:B:120:PRO:HB3	2:B:146:TYR:HB3	1.83	0.61
2:H:61:ASN:HD22	2:H:62:GLU:N	1.99	0.60
1:A:108:ARG:HD2	1:A:171:SER:HB2	1.82	0.60
1:L:180:THR:HG23	4:L:218:HOH:O	2.01	0.59
2:H:215:LYS:HB2	2:H:215:LYS:HZ2	1.65	0.59
1:L:106:ILE:HD12	4:L:311:HOH:O	2.02	0.59
1:L:180:THR:HG22	4:L:266:HOH:O	2.03	0.58
1:L:83:LEU:O	1:L:84:ALA:HB2	2.03	0.58
1:L:61:ARG:NH1	4:L:296:HOH:O	2.37	0.57
2:H:97:THR:HG21	3:H:701:JEF:H102	1.85	0.57
1:A:83:LEU:O	1:A:84:ALA:HB2	2.04	0.57
1:A:150:VAL:O	1:A:150:VAL:HG23	2.03	0.57
2:B:156:ASN:ND2	2:B:196:ILE:H	2.03	0.57
1:L:150:VAL:HG23	1:L:150:VAL:O	2.04	0.57
2:B:38:LYS:HE2	2:B:40:ARG:HD2	1.87	0.56
1:A:181:LEU:HD23	4:A:300:HOH:O	2.03	0.56
2:H:156:ASN:ND2	2:H:196:ILE:H	2.03	0.56
2:B:87:THR:HG22	2:B:88:SER:N	2.22	0.55
2:H:38:LYS:HE2	2:H:40:ARG:HD2	1.87	0.55
1:A:149:LYS:HE3	1:A:154:LEU:HD11	1.89	0.55
2:H:87:THR:HG22	2:H:88:SER:N	2.22	0.55
2:B:98:ARG:HB3	4:B:750:HOH:O	2.06	0.55
2:H:130:LYS:NZ	2:H:130:LYS:HB2	2.22	0.54
1:L:89:GLN:HE22	3:H:701:JEF:H11	1.71	0.54
1:A:105:GLU:HB2	4:A:355:HOH:O	2.07	0.54
2:B:130:LYS:HB2	2:B:130:LYS:NZ	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.90	0.54
1:A:43:SER:OG	2:B:106:ALA:O	2.22	0.54
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.90	0.53
1:A:61:ARG:HD3	4:A:275:HOH:O	2.07	0.53
1:A:196:VAL:HB	1:A:205:VAL:HG13	1.91	0.53
1:L:201:LEU:HD13	1:L:205:VAL:HG12	1.90	0.53
2:H:64:PHE:CD2	2:H:67:LYS:HE2	2.44	0.53
1:A:199:GLN:CD	1:A:199:GLN:N	2.67	0.53
1:A:201:LEU:HD13	1:A:205:VAL:HG12	1.91	0.53
2:B:19:LYS:HE3	2:B:80:TYR:CD1	2.44	0.53
1:L:28:ASN:ND2	1:L:30:GLY:H	2.06	0.53
2:B:178:SER:HB3	4:B:799:HOH:O	2.08	0.52
1:A:122:ASP:O	1:A:126:LYS:HG3	2.10	0.52
2:B:215:LYS:HB2	2:B:215:LYS:HZ3	1.72	0.52
1:L:45:LYS:HD2	2:H:103:TYR:CZ	2.44	0.52
1:L:180:THR:CG2	4:L:266:HOH:O	2.57	0.52
1:L:149:LYS:HE3	1:L:154:LEU:HD11	1.91	0.52
1:L:122:ASP:O	1:L:126:LYS:HG3	2.11	0.51
1:L:54:ARG:HB3	1:L:58:VAL:HG23	1.93	0.51
1:L:199:GLN:CD	1:L:199:GLN:N	2.67	0.51
2:B:129:SER:C	2:B:131:SER:H	2.19	0.51
1:L:196:VAL:HB	1:L:205:VAL:HG13	1.92	0.51
1:A:54:ARG:HB3	1:A:58:VAL:HG23	1.93	0.51
1:A:28:ASN:ND2	1:A:30:GLY:H	2.08	0.50
1:A:133:VAL:HG22	1:A:178:THR:HG22	1.93	0.50
2:B:64:PHE:CD2	2:B:67:LYS:HE2	2.45	0.50
2:H:129:SER:C	2:H:131:SER:H	2.19	0.50
1:L:133:VAL:HG22	1:L:178:THR:HG22	1.92	0.49
1:L:189:HIS:HD2	4:L:384:HOH:O	1.95	0.49
2:B:122:VAL:O	2:B:210:LYS:HE3	2.12	0.49
1:A:39:LYS:HB3	1:A:40:PRO:HD2	1.94	0.49
1:A:105:GLU:HG2	1:A:106:ILE:N	2.27	0.49
1:L:32:ALA:O	1:L:90:GLN:O	2.31	0.49
1:A:180:THR:HG22	4:A:257:HOH:O	2.12	0.48
2:B:19:LYS:HE2	4:B:739:HOH:O	2.12	0.48
2:H:19:LYS:HE3	2:H:80:TYR:CD1	2.48	0.48
1:A:11:MET:SD	1:A:19:VAL:HG13	2.53	0.48
2:B:19:LYS:HE3	2:B:80:TYR:CG	2.48	0.48
2:H:178:SER:HB3	4:H:833:HOH:O	2.12	0.48
1:A:32:ALA:O	1:A:90:GLN:O	2.31	0.48
2:H:122:VAL:O	2:H:210:LYS:HE3	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:TYR:HE1	4:B:795:HOH:O	1.96	0.48
4:L:300:HOH:O	2:H:130:LYS:HE2	2.13	0.48
2:H:111:THR:HG21	4:H:722:HOH:O	2.15	0.47
2:H:128:SER:O	2:H:132:THR:HB	2.14	0.47
1:L:15:VAL:HG22	4:L:245:HOH:O	2.13	0.47
2:H:11:LEU:HA	2:H:111:THR:OG1	2.14	0.47
2:B:128:SER:O	2:B:132:THR:HB	2.14	0.47
1:L:7:THR:HG23	1:L:22:THR:HG1	1.78	0.47
1:A:6:GLN:HG3	1:A:23:CYS:SG	2.55	0.47
1:A:24:LYS:HE3	4:A:245:HOH:O	2.14	0.47
2:B:6:GLU:HA	2:B:108:THR:HG21	1.95	0.47
1:L:39:LYS:HB3	1:L:40:PRO:HD2	1.95	0.47
1:A:55:TYR:CZ	2:B:102:ASP:HB3	2.50	0.47
2:B:11:LEU:HB2	2:B:148:PRO:HG3	1.97	0.47
2:H:6:GLU:HA	2:H:108:THR:HG21	1.96	0.47
1:L:11:MET:SD	1:L:19:VAL:HG13	2.55	0.46
1:L:6:GLN:HG3	1:L:23:CYS:SG	2.55	0.46
1:L:160:GLN:HB3	2:H:170:VAL:HG11	1.97	0.46
2:B:215:LYS:HD3	2:B:215:LYS:C	2.41	0.46
1:L:105:GLU:HG2	1:L:106:ILE:N	2.30	0.46
1:L:124:GLN:NE2	4:L:230:HOH:O	2.49	0.46
2:B:19:LYS:CE	4:B:739:HOH:O	2.62	0.46
2:H:156:ASN:HD21	2:H:196:ILE:H	1.64	0.46
2:B:179:LEU:C	2:B:179:LEU:HD23	2.41	0.46
2:H:61:ASN:ND2	2:H:63:LYS:H	2.14	0.46
2:H:105:GLY:O	2:H:106:ALA:C	2.59	0.46
2:H:179:LEU:HD23	2:H:179:LEU:C	2.42	0.45
2:B:130:LYS:HB2	2:B:130:LYS:HZ2	1.82	0.45
1:L:40:PRO:HG3	4:L:355:HOH:O	2.16	0.45
1:L:58:VAL:HG23	1:L:58:VAL:O	2.17	0.45
1:A:54:ARG:HD2	4:A:318:HOH:O	2.16	0.45
2:H:39:GLN:HG3	4:H:730:HOH:O	2.17	0.45
1:A:7:THR:HG23	1:A:22:THR:HG1	1.82	0.45
2:B:105:GLY:O	2:B:106:ALA:C	2.60	0.44
2:B:144:LYS:HE3	2:B:172:GLN:HE22	1.82	0.44
2:H:19:LYS:HE3	2:H:80:TYR:CG	2.52	0.44
1:L:7:THR:HG23	1:L:22:THR:OG1	2.16	0.44
2:H:215:LYS:C	2:H:215:LYS:HD3	2.41	0.44
2:B:61:ASN:C	2:B:61:ASN:ND2	2.75	0.44
1:A:175:LEU:C	1:A:175:LEU:HD23	2.43	0.44
2:H:144:LYS:HE3	2:H:172:GLN:HE22	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:ASN:ND2	2:B:63:LYS:H	2.15	0.44
1:A:150:VAL:CG2	1:A:155:GLN:NE2	2.79	0.43
1:L:199:GLN:HG2	4:L:343:HOH:O	2.18	0.43
1:A:126:LYS:NZ	1:A:126:LYS:HB2	2.33	0.43
2:H:61:ASN:C	2:H:61:ASN:ND2	2.76	0.43
1:L:175:LEU:C	1:L:175:LEU:HD23	2.44	0.43
2:B:156:ASN:HD21	2:B:196:ILE:H	1.64	0.43
1:A:129:THR:HG21	2:B:144:LYS:HZ1	1.84	0.43
1:L:126:LYS:NZ	1:L:126:LYS:HB2	2.34	0.43
1:A:58:VAL:HG23	1:A:58:VAL:O	2.17	0.43
2:B:129:SER:O	2:B:130:LYS:HB2	2.19	0.42
2:B:6:GLU:HA	2:B:108:THR:CG2	2.49	0.42
1:A:7:THR:HG23	1:A:22:THR:OG1	2.19	0.42
1:A:123:GLU:HA	1:A:126:LYS:HE3	2.02	0.42
2:H:129:SER:O	2:H:130:LYS:HB2	2.20	0.42
1:A:83:LEU:C	1:A:83:LEU:HD12	2.45	0.42
1:A:196:VAL:HB	1:A:205:VAL:CG1	2.49	0.42
2:H:87:THR:HG23	4:H:815:HOH:O	2.19	0.42
1:L:83:LEU:O	1:L:84:ALA:CB	2.68	0.41
1:A:180:THR:CG2	4:A:257:HOH:O	2.68	0.41
2:B:200:ASN:OD1	2:B:207:LYS:HG2	2.19	0.41
1:A:145:LYS:HG3	4:A:350:HOH:O	2.21	0.41
1:L:196:VAL:HB	1:L:205:VAL:CG1	2.51	0.41
2:B:91:SER:O	2:B:92:ALA:HB2	2.21	0.41
1:L:129:THR:HG22	1:L:130:ALA:N	2.36	0.41
2:B:53:PRO:HA	2:B:72:VAL:HG21	2.03	0.41
2:B:124:PRO:CB	2:B:212:ILE:HD12	2.51	0.41
1:A:129:THR:HG22	1:A:130:ALA:N	2.36	0.41
1:L:43:SER:OG	2:H:106:ALA:O	2.30	0.41
1:L:199:GLN:CD	4:L:343:HOH:O	2.63	0.41
2:H:124:PRO:CB	2:H:212:ILE:HD12	2.51	0.41
1:A:83:LEU:O	1:A:84:ALA:CB	2.69	0.41
2:B:1:GLN:NE2	2:B:1:GLN:N	2.69	0.40
1:L:178:THR:CG2	4:L:346:HOH:O	2.68	0.40
1:L:211:ARG:O	1:L:212:ASN:HB3	2.21	0.40
1:A:160:GLN:HB3	2:B:170:VAL:HG11	2.01	0.40
2:H:6:GLU:HA	2:H:108:THR:CG2	2.51	0.40
1:L:83:LEU:C	1:L:83:LEU:HD12	2.46	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	211/213 (99%)	203 (96%)	5 (2%)	3 (1%)	9	2
1	L	211/213 (99%)	203 (96%)	5 (2%)	3 (1%)	9	2
2	B	214/216 (99%)	198 (92%)	14 (6%)	2 (1%)	14	5
2	H	214/216 (99%)	198 (92%)	14 (6%)	2 (1%)	14	5
All	All	850/858 (99%)	802 (94%)	38 (4%)	10 (1%)	10	3

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	TYR
2	B	106	ALA
1	L	91	TYR
2	H	106	ALA
2	B	41	PRO
2	H	41	PRO
1	A	84	ALA
1	A	212	ASN
1	L	84	ALA
1	L	212	ASN

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	188/188 (100%)	183 (97%)	5 (3%)	39	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	188/188 (100%)	183 (97%)	5 (3%)	39	27
2	B	185/185 (100%)	177 (96%)	8 (4%)	26	13
2	H	185/185 (100%)	177 (96%)	8 (4%)	26	13
All	All	746/746 (100%)	720 (96%)	26 (4%)	32	19

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	28	ASN
1	A	96	LEU
1	A	126	LYS
1	A	169	LYS
2	B	1	GLN
2	B	4	LEU
2	B	41	PRO
2	B	59	LYS
2	B	61	ASN
2	B	130	LYS
2	B	150	PRO
2	B	215	LYS
1	L	7	THR
1	L	28	ASN
1	L	96	LEU
1	L	126	LYS
1	L	169	LYS
2	H	1	GLN
2	H	4	LEU
2	H	41	PRO
2	H	59	LYS
2	H	61	ASN
2	H	130	LYS
2	H	150	PRO
2	H	215	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	42	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	89	GLN
1	A	124	GLN
1	A	137	ASN
1	A	160	GLN
1	A	189	HIS
2	B	1	GLN
2	B	54	ASN
2	B	61	ASN
2	B	156	ASN
2	B	172	GLN
2	B	205	ASN
1	L	28	ASN
1	L	37	GLN
1	L	42	GLN
1	L	89	GLN
1	L	124	GLN
1	L	137	ASN
1	L	160	GLN
1	L	189	HIS
2	H	1	GLN
2	H	54	ASN
2	H	61	ASN
2	H	82	GLN
2	H	156	ASN
2	H	165	HIS
2	H	172	GLN
2	H	205	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	JEF	H	701	-	27,27,40	1.20	2 (7%)	31,32,48	2.04	4 (12%)
3	JEF	B	700	-	27,27,40	1.21	1 (3%)	31,32,48	2.15	5 (16%)

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	JEF	H	701	-	1/1/6/9	10/31/31/46	-
3	JEF	B	700	-	1/1/6/9	11/31/31/46	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	700	JEF	C3-C2	2.13	1.55	1.50
3	H	701	JEF	O-C	2.05	1.47	1.44
3	H	701	JEF	C3-C2	2.04	1.55	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	701	JEF	OH-C2-C1	8.35	140.47	110.22
3	B	700	JEF	OH-C2-C1	8.26	140.15	110.22
3	B	700	JEF	C3-O2-C5	-3.75	109.52	115.05
3	B	700	JEF	O-C-C18	3.58	123.20	110.22
3	B	700	JEF	C17-OH-C2	-3.51	109.87	115.05
3	H	701	JEF	O-C-C18	3.48	122.82	110.22
3	H	701	JEF	C17-OH-C2	-3.46	109.94	115.05
3	H	701	JEF	C3-O2-C5	-2.89	110.78	115.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	700	JEF	C4-O3-C7	2.68	119.00	115.05

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	700	JEF	C2
3	H	701	JEF	C2

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	700	JEF	C18-C-O-C20
3	B	700	JEF	C1-C2-C3-O2
3	B	700	JEF	O3-C4-C5-O2
3	B	700	JEF	C9-C7-C8-O4
3	B	700	JEF	O5-C13-C14-O6
3	H	701	JEF	C18-C-O-C20
3	H	701	JEF	C9-C7-C8-O4
3	H	701	JEF	O5-C13-C14-O6
3	H	701	JEF	C1-C2-OH-C17
3	B	700	JEF	O3-C4-C5-C6
3	B	700	JEF	C15-C13-C14-O6
3	H	701	JEF	C1-C2-C3-O2
3	H	701	JEF	C15-C13-C14-O6
3	B	700	JEF	O-C-C17-OH
3	B	700	JEF	O5-C10-C11-O4
3	H	701	JEF	O-C-C17-OH
3	H	701	JEF	C13-C14-O6-C16
3	B	700	JEF	C13-C14-O6-C16
3	B	700	JEF	C9-C7-O3-C4
3	H	701	JEF	C9-C7-O3-C4
3	H	701	JEF	C7-C8-O4-C11

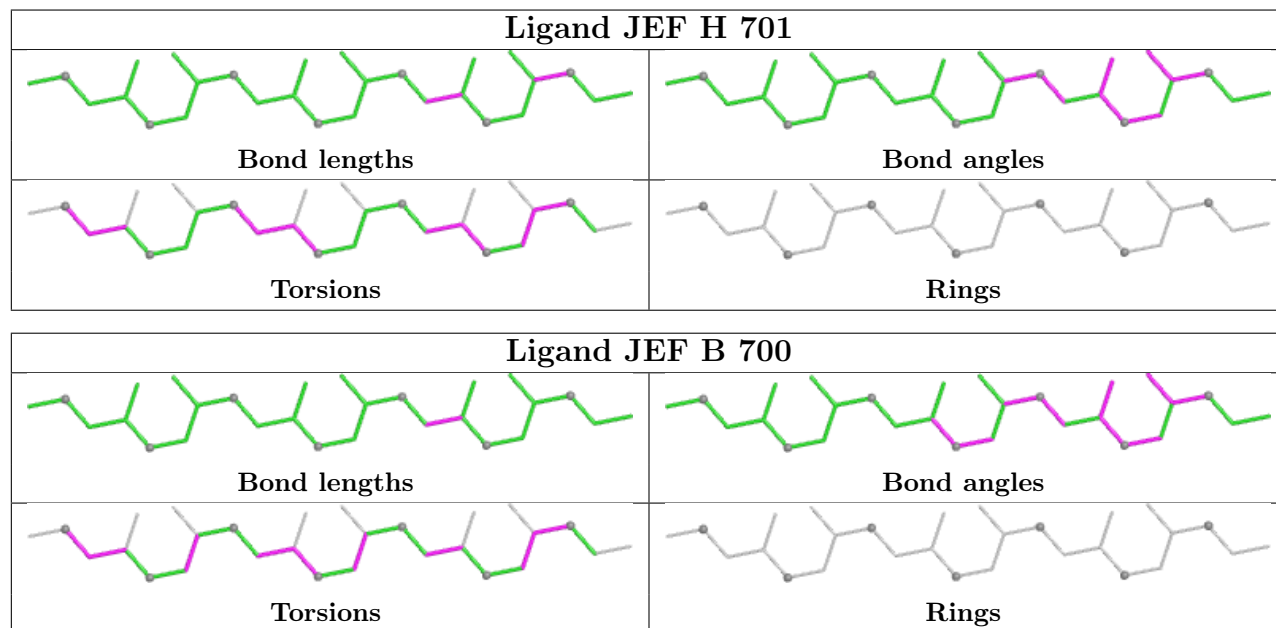
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	701	JEF	2	0
3	B	700	JEF	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	213/213 (100%)	0.48	21 (9%)	13 11	10, 18, 32, 71	0
1	L	213/213 (100%)	0.24	10 (4%)	36 35	9, 16, 29, 71	0
2	B	216/216 (100%)	0.93	44 (20%)	3 2	11, 20, 50, 67	0
2	H	216/216 (100%)	0.73	30 (13%)	6 5	9, 18, 48, 66	0
All	All	858/858 (100%)	0.60	105 (12%)	8 7	9, 18, 42, 71	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	134	GLY	7.7
2	B	32	TYR	7.4
1	L	87	PHE	7.0
2	H	129	SER	6.3
2	H	106	ALA	6.1
2	B	129	SER	6.0
2	B	133	SER	5.6
2	B	25	SER	5.4
2	B	27	TYR	5.4
2	H	131	SER	5.3
2	H	133	SER	5.2
2	B	132	THR	5.1
2	B	128	SER	4.8
2	H	132	THR	4.8
2	H	130	LYS	4.8
2	B	191	GLY	4.7
1	A	168	SER	4.6
2	B	26	GLY	4.6
1	L	213	GLU	4.5
2	B	190	LEU	4.4
2	B	192	THR	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	27	TYR	4.3
1	A	87	PHE	4.2
2	B	24	ALA	4.2
2	B	33	TRP	4.2
1	L	212	ASN	4.1
1	A	213	GLU	4.1
2	B	106	ALA	4.0
2	B	42	GLY	4.0
1	A	212	ASN	4.0
2	B	22	CYS	3.9
2	B	100	ASP	3.9
1	L	199	GLN	3.9
2	H	1	GLN	3.7
2	H	135	GLY	3.7
1	A	10	PHE	3.6
2	B	28	THR	3.6
2	B	30	THR	3.6
2	B	134	GLY	3.6
2	B	41	PRO	3.6
2	B	131	SER	3.6
2	H	128	SER	3.5
2	H	215	LYS	3.5
1	A	81	GLU	3.5
2	B	54	ASN	3.5
2	B	29	PHE	3.5
2	B	215	LYS	3.5
2	H	191	GLY	3.4
2	B	31	SER	3.4
2	B	130	LYS	3.4
2	B	189	SER	3.3
2	B	23	LYS	3.2
2	B	135	GLY	3.1
1	L	60	ASP	3.0
1	L	168	SER	3.0
2	H	23	LYS	3.0
1	L	114	SER	3.0
2	B	53	PRO	3.0
1	A	76	SER	3.0
1	A	169	LYS	3.0
1	L	58	VAL	2.9
2	B	101	SER	2.9
2	H	65	LYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	67	LYS	2.9
2	H	136	THR	2.8
2	B	99	ARG	2.8
2	B	187	SER	2.7
2	H	127	PRO	2.7
2	B	77	SER	2.6
1	A	199	GLN	2.6
1	L	18	ARG	2.6
2	H	43	ARG	2.6
2	H	192	THR	2.5
1	A	60	ASP	2.5
2	H	216	SER	2.5
1	A	61	ARG	2.4
1	A	77	ASN	2.4
2	B	108	THR	2.4
1	A	23	CYS	2.4
2	H	22	CYS	2.4
2	H	187	SER	2.4
2	H	189	SER	2.4
2	H	190	LEU	2.4
1	A	41	GLY	2.4
1	A	7	THR	2.4
2	H	41	PRO	2.4
2	H	193	GLN	2.4
2	B	44	GLY	2.4
2	H	42	GLY	2.4
2	B	216	SER	2.4
2	H	29	PHE	2.3
1	A	15	VAL	2.3
1	A	194	CYS	2.3
1	L	23	CYS	2.3
2	B	103	TYR	2.3
2	H	54	ASN	2.3
1	A	126	LYS	2.2
1	A	80	SER	2.2
2	B	127	PRO	2.2
2	B	188	SER	2.2
2	B	43	ARG	2.2
2	B	67	LYS	2.1
1	A	59	PRO	2.1
1	A	79	GLN	2.1
2	B	136	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](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

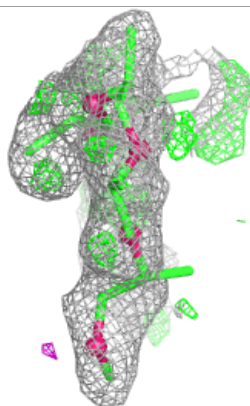
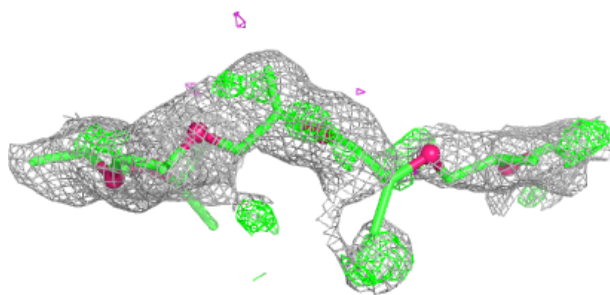
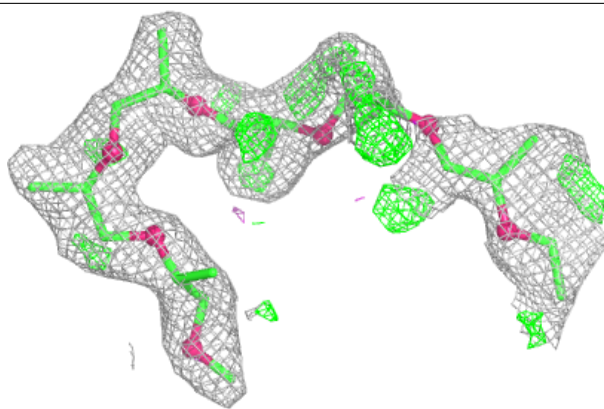
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	JEF	H	701	28/41	0.71	0.20	29,36,44,46	0
3	JEF	B	700	28/41	0.82	0.14	28,36,41,41	0

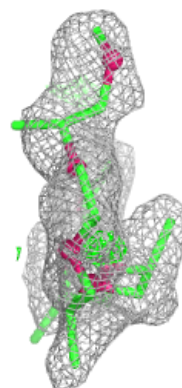
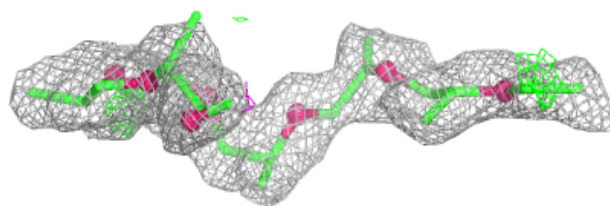
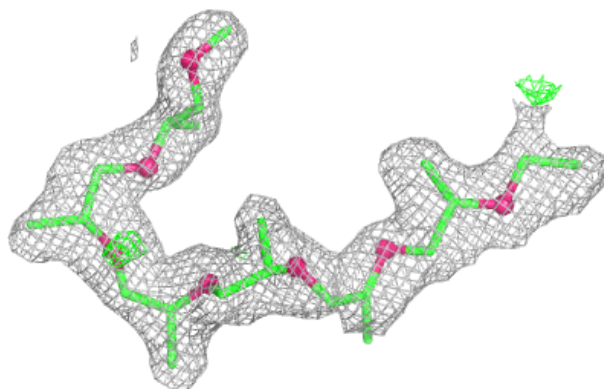
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around JEF H 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around JEF B 700:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.