wwPDB X-ray Structure Validation Summary Report (i)

Aug 4, 2026 – 05:42 AM EDT

PDB ID	:	5TH9 / pdb_00005th9
Title	:	Structure determination of a potent, selective antibody inhibitor of human MMP9 (GS-5745 bound to MMP-9)
Authors	:	Appleby, T.C.; Greenstein, A.E.; Kwon, H.J.
Deposited on	:	2016-09-29
Resolution	:	3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

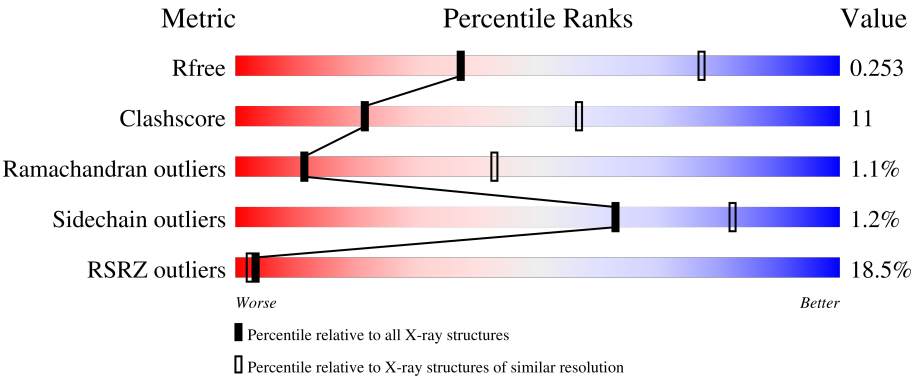
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 <=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	L	214	93% 7%
1	M	214	87% 12%
1	N	214	38% 29% 18% 50%
2	H	230	3% 75% 15% 10%
2	I	230	75% 15% 10%

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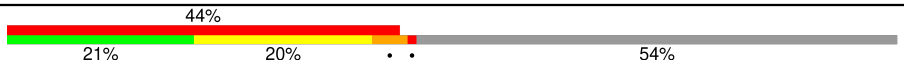
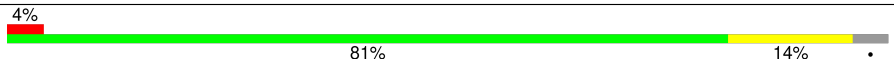
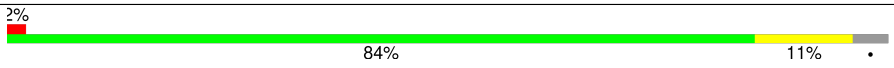
Mol	Chain	Length	Quality of chain
2	J	230	
3	A	231	
3	B	231	
3	C	231	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 13578 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 GS-5745 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	1	0
			1656	1032	281	337	6			
1	M	214	Total	C	N	O	S	0	0	0
			1646	1026	278	336	6			
1	N	106	Total	C	N	O	S	0	0	0
			810	507	136	164	3			

- Molecule 2 is a protein called GS-5745 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	208	Total	C	N	O	S	0	1	0
			1593	1017	258	311	7			
2	I	208	Total	C	N	O	S	0	1	0
			1593	1017	258	311	7			
2	J	106	Total	C	N	O	S	0	0	0
			839	539	135	160	5			

- Molecule 3 is a protein called Matrix metalloproteinase-9,Matrix metalloproteinase-9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	222	Total	C	N	O	S	0	0	0
			1767	1135	301	327	4			
3	B	222	Total	C	N	O	S	0	0	0
			1767	1135	301	327	4			
3	C	217	Total	C	N	O	S	0	0	0
			1734	1114	296	320	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	MET	-	initiating methionine	UNP P14780
A	39	ALA	-	expression tag	UNP P14780

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Chain	Residue	Modelled	Actual	Comment	Reference
B	38	MET	-	initiating methionine	UNP P14780
B	39	ALA	-	expression tag	UNP P14780
C	38	MET	-	initiating methionine	UNP P14780
C	39	ALA	-	expression tag	UNP P14780

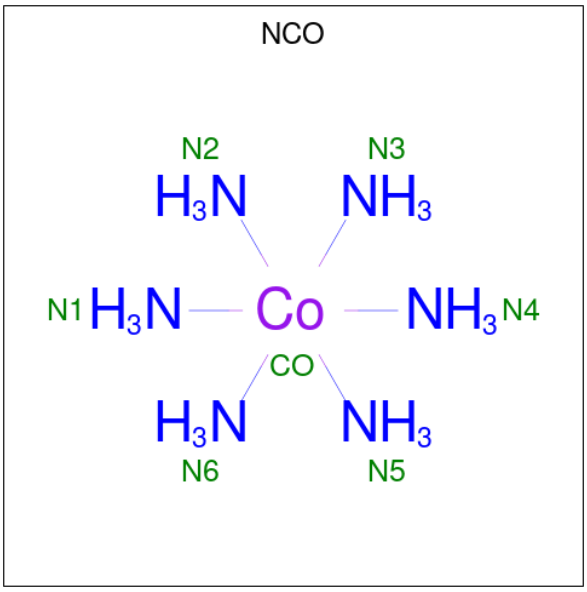
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Zn 2 2	0	0
4	B	2	Total Zn 2 2	0	0
4	C	2	Total Zn 2 2	0	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Ca 2 2	0	0
5	B	2	Total Ca 2 2	0	0
5	C	2	Total Ca 2 2	0	0

- Molecule 6 is COBALT HEXAMMINE(III) (CCD ID: NCO) (formula: $CoH_{18}N_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Co N 7 1 6	0	0
6	B	1	Total Co N 7 1 6	0	0
6	C	1	Total Co N 7 1 6	0	0

- Molecule 7 is water.

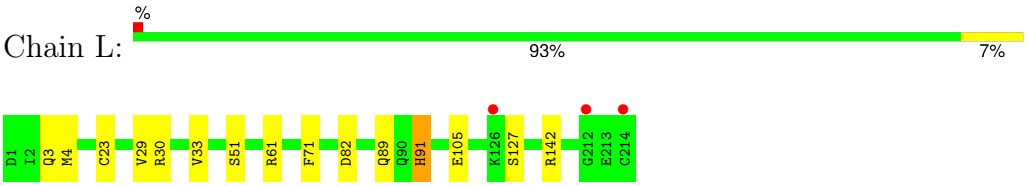
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	23	Total O 23 23	0	0
7	H	26	Total O 26 26	0	0
7	A	19	Total O 19 19	0	0
7	M	27	Total O 27 27	0	0
7	I	15	Total O 15 15	0	0
7	B	30	Total O 30 30	0	0

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.

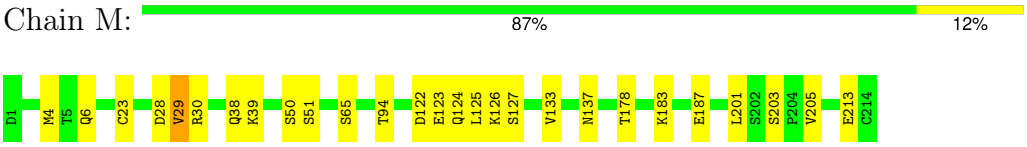
• Molecule 1: GS-5745 Fab light chain

Chain L:



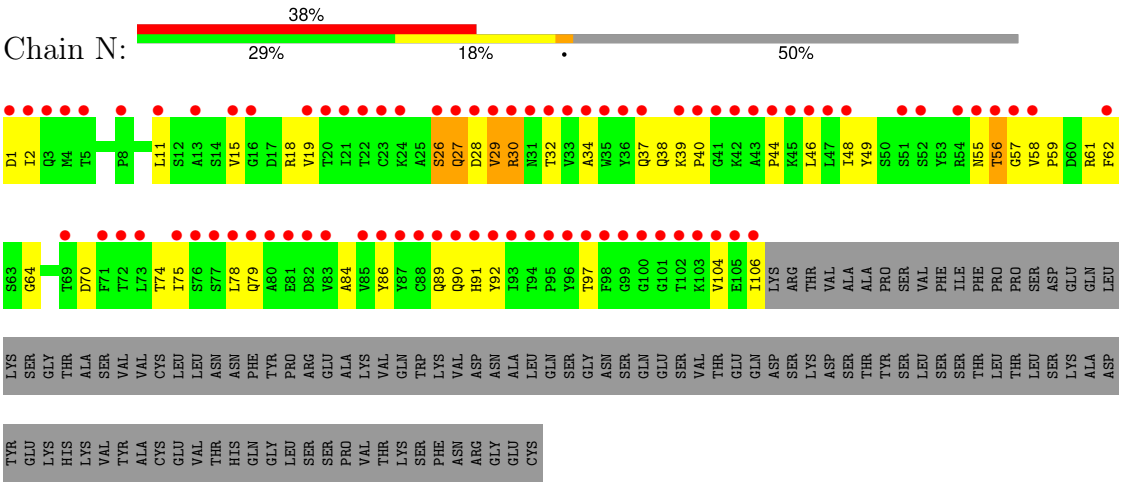
• Molecule 1: GS-5745 Fab light chain

Chain M:



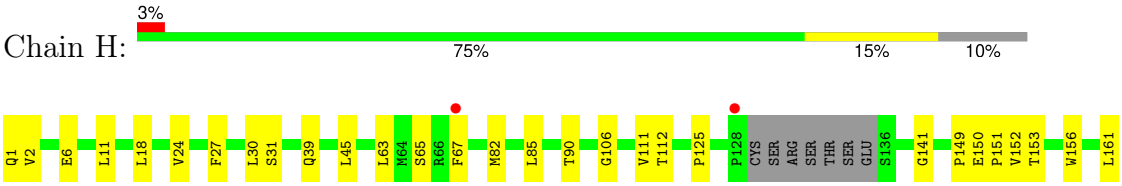
• Molecule 1: GS-5745 Fab light chain

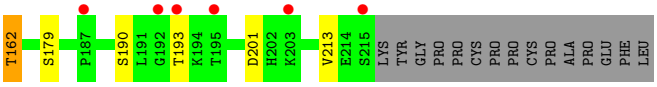
Chain N:



• Molecule 2: GS-5745 Fab heavy chain

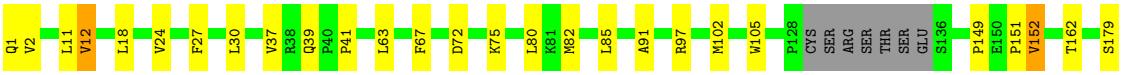
Chain H:

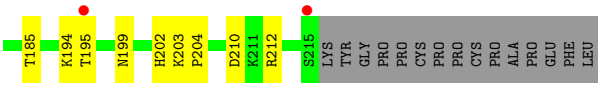




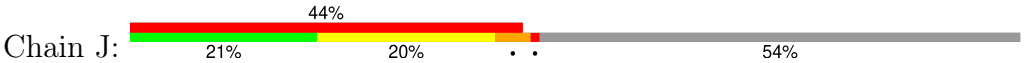
• Molecule 2: GS-5745 Fab heavy chain



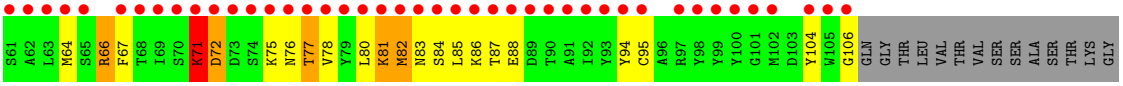


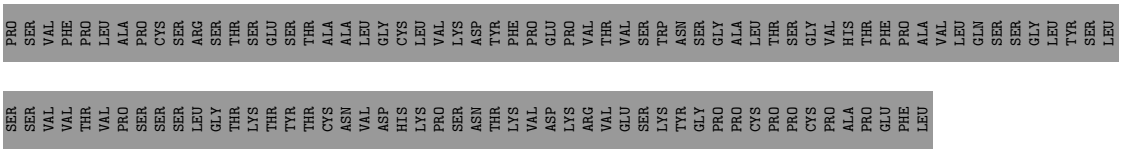


• Molecule 2: GS-5745 Fab heavy chain

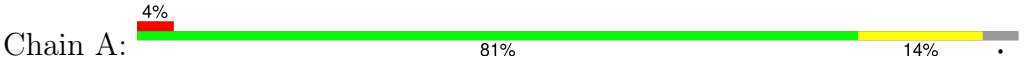


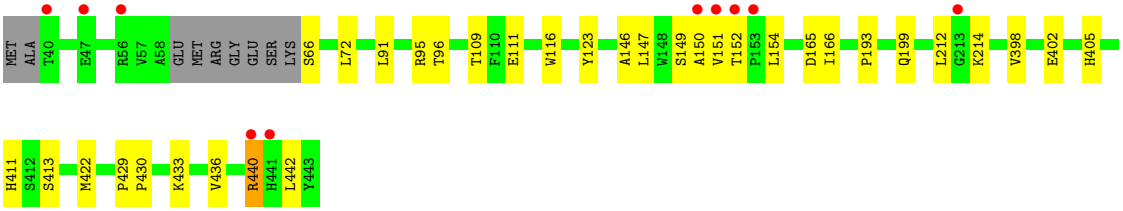




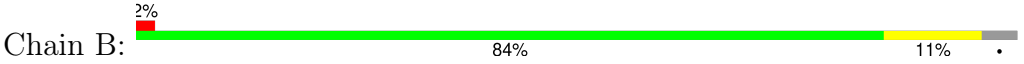


• Molecule 3: Matrix metalloproteinase-9,Matrix metalloproteinase-9

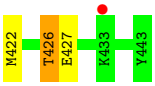




• Molecule 3: Matrix metalloproteinase-9,Matrix metalloproteinase-9



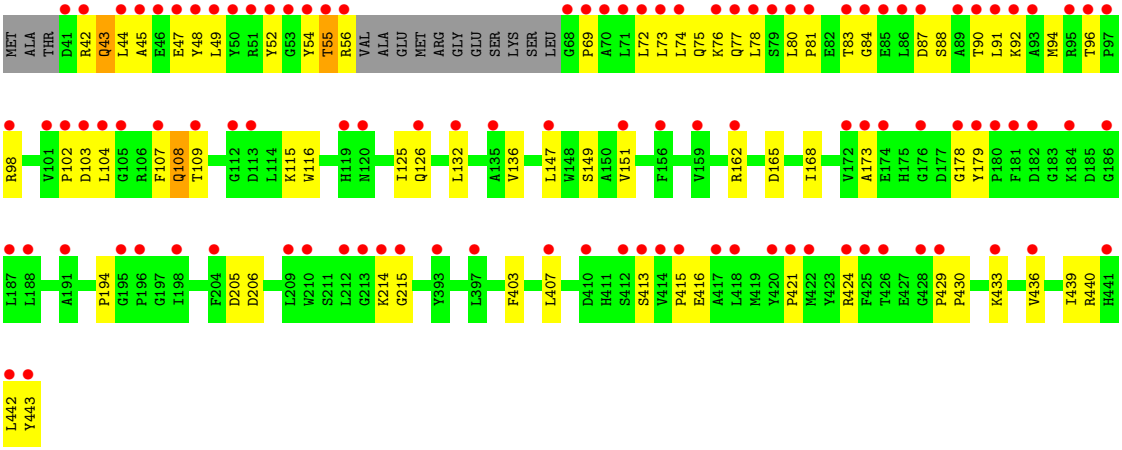




• Molecule 3: Matrix metalloproteinase-9,Matrix metalloproteinase-9

Chain C:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	168.17Å 168.17Å 234.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.64 – 3.00 46.64 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.64-3.00) 94.4 (46.64-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.74 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.218 , 0.257 0.219 , 0.253	Depositor DCC
R_{free} test set	2000 reflections (2.95%)	wwPDB-VP
Wilson B-factor (Å^2)	36.2	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 27.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	13578	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: NCO, ZN, CA

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	L	0.58	0/1691	0.52	1/2295 (0.0%)
1	M	0.62	0/1680	0.61	1/2280 (0.0%)
1	N	0.46	1/827 (0.1%)	0.72	0/1124
2	H	0.62	0/1635	0.54	0/2233
2	I	0.64	0/1635	0.58	0/2233
2	J	0.79	6/862 (0.7%)	0.91	5/1172 (0.4%)
3	A	0.63	1/1822 (0.1%)	0.55	0/2478
3	B	0.55	0/1822	0.55	0/2478
3	C	0.26	0/1789	0.56	1/2432 (0.0%)
All	All	0.58	8/13763 (0.1%)	0.60	8/18725 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	J	0	3
3	C	0	1
All	All	0	4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	66	ARG	NE-CZ	-7.89	1.24	1.33
2	J	66	ARG	CD-NE	-6.89	1.36	1.46
2	J	66	ARG	CZ-NH2	-6.70	1.24	1.33
2	J	66	ARG	CZ-NH1	-5.91	1.24	1.32
3	A	440	ARG	NE-CZ	-5.78	1.26	1.33

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	29	VAL	N-CA-C	-6.11	107.34	113.20
2	J	82	MET	N-CA-C	5.91	118.68	109.52
2	J	71	LYS	CD-CE-NZ	-5.64	93.86	111.90
2	J	14	PRO	N-CA-C	5.60	124.00	112.47
2	J	77	THR	CB-CA-C	-5.48	104.25	111.82

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	43	GLN	Peptide
2	J	47	TRP	Peptide
2	J	72	ASP	Peptide
2	J	81	LYS	Peptide

5.2 Too-close contacts (i)

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	L	1656	0	1605	7	0
1	M	1646	0	1599	15	0
1	N	810	0	787	35	0
2	H	1593	0	1563	20	0
2	I	1593	0	1563	23	0
2	J	839	0	813	78	0
3	A	1767	0	1672	33	0
3	B	1767	0	1672	20	0
3	C	1734	0	1635	79	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
6	A	7	0	0	0	0
6	B	7	0	0	0	0
6	C	7	0	0	1	0
7	A	19	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	30	0	0	2	0
7	H	26	0	0	0	0
7	I	15	0	0	0	0
7	L	23	0	0	0	0
7	M	27	0	0	0	0
All	All	13578	0	12909	287	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 11.

The worst 5 of 287 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:J:14:PRO:C	2:J:16:GLU:OE1	1.79	1.25
3:C:49:LEU:HD21	3:C:55:THR:HG23	1.18	1.10
3:A:440:ARG:HD3	3:C:440:ARG:HH12	1.26	1.00
2:J:29:LEU:HG	2:J:71:LYS:HE2	1.43	0.99
3:C:75:GLN:HE22	3:C:83:THR:HG22	1.28	0.98

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	L	213/214 (100%)	200 (94%)	12 (6%)	1 (0%)	24 60
1	M	212/214 (99%)	200 (94%)	12 (6%)	0	100 100
1	N	104/214 (49%)	89 (86%)	9 (9%)	6 (6%)	1 8
2	H	205/230 (89%)	196 (96%)	9 (4%)	0	100 100
2	I	205/230 (89%)	199 (97%)	6 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	J	104/230 (45%)	81 (78%)	17 (16%)	6 (6%)	1 8
3	A	218/231 (94%)	205 (94%)	11 (5%)	2 (1%)	14 48
3	B	218/231 (94%)	209 (96%)	8 (4%)	1 (0%)	24 60
3	C	213/231 (92%)	186 (87%)	25 (12%)	2 (1%)	14 48
All	All	1692/2025 (84%)	1565 (92%)	109 (6%)	18 (1%)	11 43

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	19	VAL
1	N	30	ARG
2	J	14	PRO
3	C	55	THR
1	L	127	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	L	189/188 (100%)	185 (98%)	4 (2%)	47 75
1	M	188/188 (100%)	183 (97%)	5 (3%)	39 71
1	N	91/188 (48%)	91 (100%)	0	100 100
2	H	182/201 (90%)	179 (98%)	3 (2%)	55 79
2	I	182/201 (90%)	177 (97%)	5 (3%)	39 71
2	J	92/201 (46%)	91 (99%)	1 (1%)	65 83
3	A	181/188 (96%)	181 (100%)	0	100 100
3	B	181/188 (96%)	180 (99%)	1 (1%)	78 88
3	C	177/188 (94%)	177 (100%)	0	100 100
All	All	1463/1731 (84%)	1444 (99%)	19 (1%)	63 81

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	152	VAL
3	B	426	THR
2	J	95	CYS
2	I	179	SER
1	M	39	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	91	HIS
2	J	76	ASN
2	J	58	ASN
3	C	75	GLN
3	A	199	GLN

5.3.3 RNA (i)

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)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 12 are monoatomic - leaving 3 for Mogul analysis.

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	$\#\|Z\|>2$
6	NCO	C	505	-	6,6,6	4.98	6 (100%)	-		
6	NCO	A	505	-	6,6,6	6.20	6 (100%)	-		
6	NCO	B	505	-	6,6,6	5.41	6 (100%)	-		

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	505	NCO	CO-N2	-6.45	1.76	1.96
6	A	505	NCO	CO-N4	-6.29	1.77	1.96
6	A	505	NCO	CO-N3	-6.14	1.77	1.96
6	A	505	NCO	CO-N5	-6.11	1.77	1.96
6	A	505	NCO	CO-N1	-6.10	1.77	1.96

There are no bond angle outliers.

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
6	C	505	NCO	1	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	L	214/214 (100%)	-0.26	3 (1%) 73 51	6, 23, 44, 96	1 (0%)
1	M	214/214 (100%)	-0.37	0 100 100	3, 18, 43, 87	0
1	N	106/214 (49%)	2.98	81 (76%) 0 0	85, 106, 128, 140	0
2	H	208/230 (90%)	-0.12	8 (3%) 44 24	5, 17, 66, 86	1 (0%)
2	I	208/230 (90%)	-0.28	2 (0%) 79 59	4, 16, 50, 72	1 (0%)
2	J	106/230 (46%)	3.79	101 (95%) 0 0	96, 123, 141, 151	0
3	A	222/231 (96%)	-0.18	10 (4%) 38 20	5, 18, 56, 77	0
3	B	222/231 (96%)	-0.24	4 (1%) 67 44	5, 20, 46, 72	0
3	C	217/231 (93%)	2.31	108 (49%) 0 0	61, 92, 126, 142	0
All	All	1717/2025 (84%)	0.53	317 (18%) 3 2	3, 25, 122, 151	3 (0%)

The worst 5 of 317 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	34	VAL	8.1
1	N	91	HIS	7.5
1	N	83	VAL	7.5
2	J	49	GLY	7.3
2	J	10	GLY	7.1

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

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

6.3 Carbohydrates

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(Å^2)	Q<0.9
6	NCO	C	505	7/7	0.81	0.10	92,112,119,149	0
5	CA	B	503	1/1	0.95	0.06	24,24,24,24	0
5	CA	C	504	1/1	0.97	0.14	101,101,101,101	0
6	NCO	B	505	7/7	0.97	0.11	27,31,50,70	0
5	CA	A	503	1/1	0.97	0.05	26,26,26,26	0
5	CA	A	504	1/1	0.98	0.03	13,13,13,13	0
4	ZN	C	501	1/1	0.98	0.08	81,81,81,81	0
5	CA	C	503	1/1	0.98	0.05	75,75,75,75	0
4	ZN	C	502	1/1	0.99	0.04	78,78,78,78	0
6	NCO	A	505	7/7	0.99	0.05	10,13,17,22	0
4	ZN	A	502	1/1	1.00	0.01	5,5,5,5	0
4	ZN	B	501	1/1	1.00	0.01	13,13,13,13	0
4	ZN	B	502	1/1	1.00	0.03	2,2,2,2	0
4	ZN	A	501	1/1	1.00	0.01	15,15,15,15	0
5	CA	B	504	1/1	1.00	0.02	12,12,12,12	0

6.5 Other polymers (i)

There are no such residues in this entry.