wwPDB X-ray Structure Validation Summary Report (i)

Sep 24, 2023 – 02:31 AM EDT

PDB ID	:	5TH9
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 (i)) were used in the production of this report:

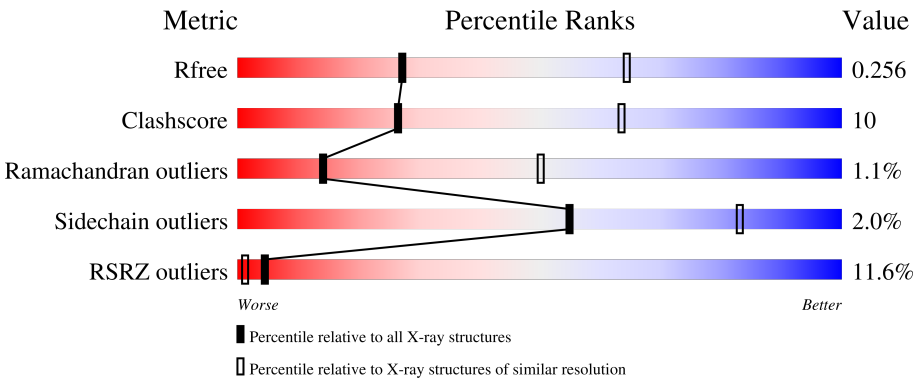
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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	92% 8%
1	N	214	30% 29% 17% • 50%
2	H	230	75% 16% 10%
2	I	230	77% 13% • 10%

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Mol	Chain	Length	Quality of chain
2	J	230	30% 21% 19% 5% 54%
3	A	231	81% 15%
3	B	231	84% 12%
3	C	231	28% 63% 28% 6%

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
			Total	C	N	O	S			
1	L	214	1656	1032	281	337	6	0	1	0
1	M	214	1646	1026	278	336	6	0	0	0
1	N	106	810	507	136	164	3	0	0	0

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

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

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

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

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

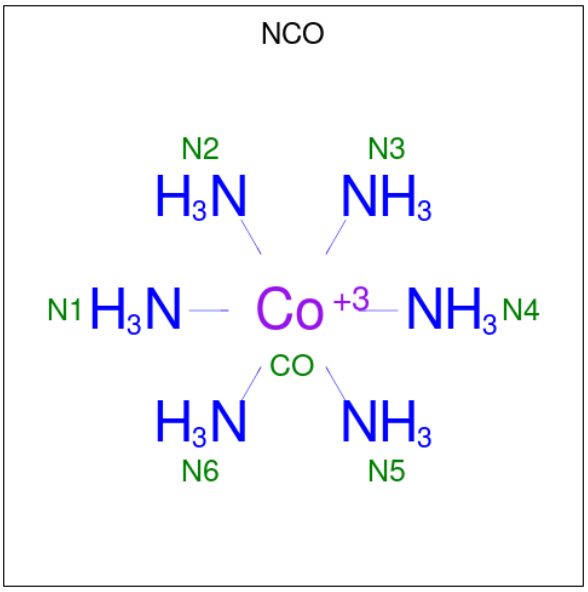
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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 (three-letter code: 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) (three-letter code: NCO) (formula: $CoH_{18}N_6$).



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

- Molecule 7 is water.

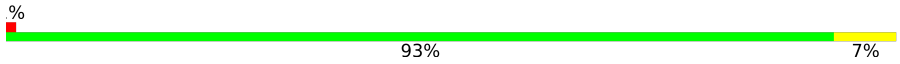
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	L	23	23	23	0	0
7	H	26	26	26	0	0
7	A	19	19	19	0	0
7	M	27	27	27	0	0
7	I	15	15	15	0	0
7	B	30	30	30	0	0

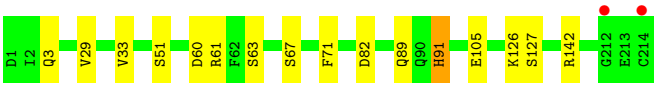
3 Residue-property plots (i)

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

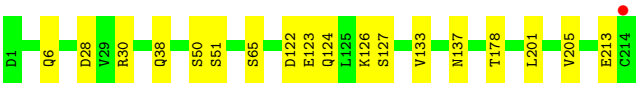
Chain L:





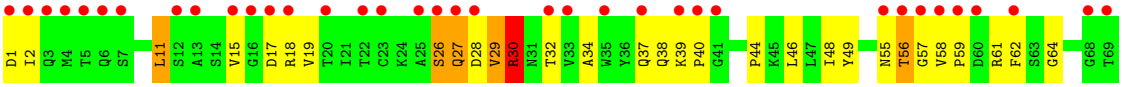
• Molecule 1: GS-5745 Fab light chain

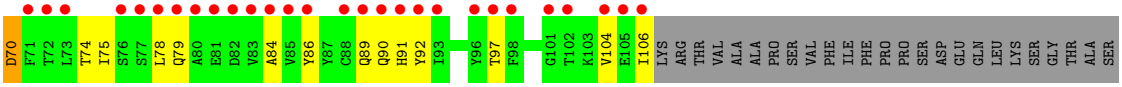
Chain M:

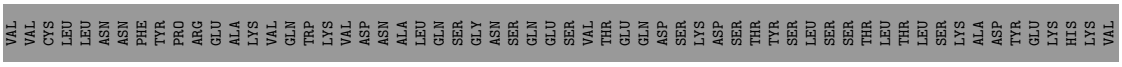


• Molecule 1: GS-5745 Fab light chain

Chain N:

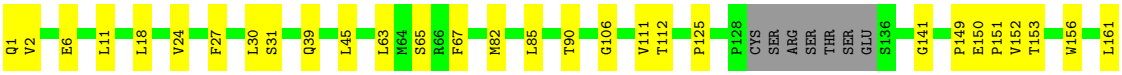


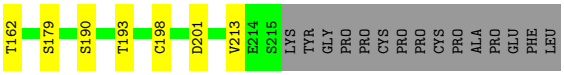




• Molecule 2: GS-5745 Fab heavy chain

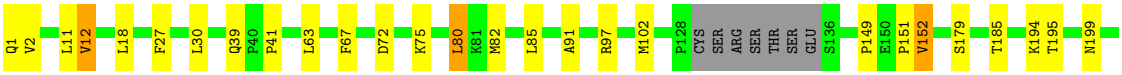
Chain H:





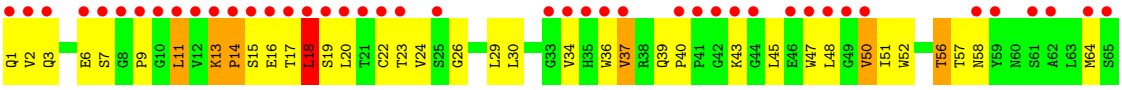
- Molecule 2: GS-5745 Fab heavy chain

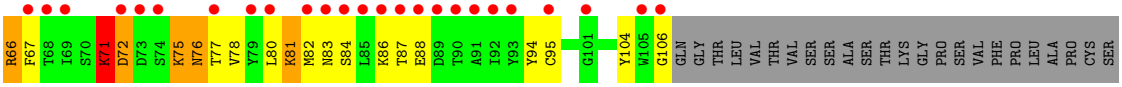
Chain I:



- Molecule 2: GS-5745 Fab heavy chain

Chain J:





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

Chain A:

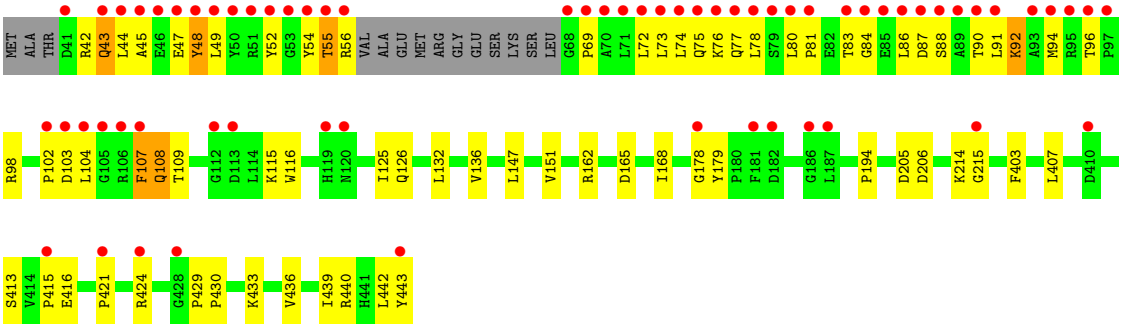
- Molecule 3: Matrix metalloproteinase-9,Matrix metalloproteinase-9

Chain B:

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

Chain C:

28%
63%
28%
6%


MET ALA THR D41 R42 Q43 L44 A45 E46 E47 Y48 L49 Y50 R51 Y52 G53 Y54 T55 R56 VAL ALA GLU MET ARG GLY GLU SER LYS SER LEU G68 P69 A70 L71 L72 L73 L74 Q75 K76 Q77 L78 S79 L80 P81 E82 T83 G84 E85 L86 D87 S88 A89 T90 L91 K92 A93 M94 R95 T96 P97
R98 P102 D103 L104 G105 R106 F107 Q108 T109 G112 D113 L114 K115 W116 H119 N120 I125 Q126 L132 V136 L147 V151 R162 D165 I168 G178 Y179 P180 F181 D182 G186 L187 P194 D205 D206 K214 G215 F403 L407 D410
S413 V414 P415 E416 P421 R424 G428 P429 P430 K433 V436 I439 R440 H441 L442 Y443

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) 94.5 (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 , 0.256	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 , 27.2	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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA, NCO

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	0.67	0/1691	0.57	0/2295
1	M	0.69	0/1680	0.63	0/2280
1	N	0.47	0/827	0.75	1/1124 (0.1%)
2	H	0.71	0/1635	0.62	0/2233
2	I	0.74	1/1635 (0.1%)	0.63	1/2233 (0.0%)
2	J	0.78	7/862 (0.8%)	0.89	3/1172 (0.3%)
3	A	0.72	0/1822	0.61	0/2478
3	B	0.63	0/1822	0.59	1/2478 (0.0%)
3	C	0.33	0/1789	0.60	1/2432 (0.0%)
All	All	0.65	8/13763 (0.1%)	0.64	7/18725 (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	71	LYS	CE-NZ	6.96	1.66	1.49
2	J	66	ARG	NE-CZ	-6.67	1.24	1.33
2	J	66	ARG	CZ-NH1	-6.59	1.24	1.33
2	J	66	ARG	CZ-NH2	-6.39	1.24	1.33
2	J	71	LYS	CD-CE	-5.88	1.36	1.51

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	18	LEU	CB-CG-CD1	8.66	125.73	111.00
2	J	71	LYS	CD-CE-NZ	-7.75	93.86	111.70
3	C	86	LEU	CA-CB-CG	7.42	132.38	115.30
2	I	80	LEU	CB-CG-CD1	-6.78	99.48	111.00
2	J	11	LEU	CA-CB-CG	6.61	130.51	115.30

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	6	0
1	M	1646	0	1599	12	0
1	N	810	0	787	34	0
2	H	1593	0	1563	20	0
2	I	1593	0	1563	21	0
2	J	839	0	813	73	0
3	A	1767	0	1672	31	0
3	B	1767	0	1672	20	0
3	C	1734	0	1635	75	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	270	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 10.

The worst 5 of 270 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	1.20
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%)	29 68
1	M	212/214 (99%)	200 (94%)	12 (6%)	0	100 100
1	N	104/214 (49%)	89 (86%)	9 (9%)	6 (6%)	1 10
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	10
3	A	218/231 (94%)	205 (94%)	11 (5%)	2 (1%)	17	55
3	B	218/231 (94%)	209 (96%)	8 (4%)	1 (0%)	29	68
3	C	213/231 (92%)	186 (87%)	25 (12%)	2 (1%)	17	55
All	All	1692/2025 (84%)	1565 (92%)	109 (6%)	18 (1%)	14	50

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%)	181 (96%)	8 (4%)	30	66
1	M	188/188 (100%)	187 (100%)	1 (0%)	88	96
1	N	91/188 (48%)	87 (96%)	4 (4%)	28	65
2	H	182/201 (90%)	179 (98%)	3 (2%)	62	86
2	I	182/201 (90%)	180 (99%)	2 (1%)	73	90
2	J	92/201 (46%)	87 (95%)	5 (5%)	22	57
3	A	181/188 (96%)	178 (98%)	3 (2%)	60	85
3	B	181/188 (96%)	180 (99%)	1 (1%)	86	95
3	C	177/188 (94%)	174 (98%)	3 (2%)	60	85
All	All	1463/1731 (84%)	1433 (98%)	30 (2%)	55	82

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	65	SER
3	C	48	TYR
3	B	426	THR
3	C	107	PHE
2	J	64	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	89	GLN
3	C	126	GLN
3	B	199	GLN
3	C	401	HIS
3	C	75	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 monosaccharides 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	4.48	6 (100%)	-		
6	NCO	B	505	-	6,6,6	4.87	6 (100%)	-		
6	NCO	A	505	-	6,6,6	5.57	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	-5.80	1.76	1.96
6	A	505	NCO	CO-N4	-5.66	1.77	1.96
6	A	505	NCO	CO-N3	-5.52	1.77	1.96
6	A	505	NCO	CO-N5	-5.50	1.77	1.96
6	A	505	NCO	CO-N1	-5.48	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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.29	2 (0%)	84	63	6, 23, 44, 96	0
1	M	214/214 (100%)	-0.42	1 (0%)	91	75	3, 18, 43, 87	0
1	N	106/214 (49%)	2.47	64 (60%)	0	0	85, 106, 128, 140	0
2	H	208/230 (90%)	-0.32	0	100	100	5, 17, 66, 86	0
2	I	208/230 (90%)	-0.27	0	100	100	4, 16, 50, 72	0
2	J	106/230 (46%)	3.04	68 (64%)	0	0	96, 123, 141, 151	0
3	A	222/231 (96%)	-0.35	0	100	100	5, 18, 56, 77	0
3	B	222/231 (96%)	-0.37	0	100	100	5, 20, 46, 72	0
3	C	217/231 (93%)	1.47	65 (29%)	0	0	61, 92, 126, 142	0
All	All	1717/2025 (84%)	0.27	200 (11%)	4	1	3, 25, 122, 151	0

The worst 5 of 200 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	10	GLY	9.9
2	J	49	GLY	9.1
1	N	80	ALA	9.0
1	N	83	VAL	8.6
2	J	11	LEU	8.5

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 monosaccharides 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	0.85	0.19	92,112,119,149	0
5	CA	C	504	1/1	0.92	0.17	101,101,101,101	0
5	CA	B	503	1/1	0.92	0.09	24,24,24,24	0
4	ZN	C	501	1/1	0.93	0.06	81,81,81,81	0
5	CA	C	503	1/1	0.93	0.10	75,75,75,75	0
4	ZN	C	502	1/1	0.97	0.07	78,78,78,78	0
5	CA	A	504	1/1	0.98	0.08	13,13,13,13	0
5	CA	B	504	1/1	0.99	0.06	12,12,12,12	0
5	CA	A	503	1/1	0.99	0.10	26,26,26,26	0
4	ZN	A	502	1/1	0.99	0.09	5,5,5,5	0
6	NCO	A	505	7/7	0.99	0.13	10,13,17,22	0
6	NCO	B	505	7/7	0.99	0.15	27,31,50,70	0
4	ZN	B	501	1/1	0.99	0.12	13,13,13,13	0
4	ZN	B	502	1/1	1.00	0.08	2,2,2,2	0
4	ZN	A	501	1/1	1.00	0.09	15,15,15,15	0

6.5 Other polymers (i)

There are no such residues in this entry.