Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2016 – 10:39 AM EDT

PDB ID	:	5DQ9
Title	:	Structure of S55-3 Fab in complex with Lipid A
Authors	:	Haji-Ghassemi, O.; Evans, S.V.
Deposited on	:	2015-09-14
Resolution	:	1.95 Å(reported)

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

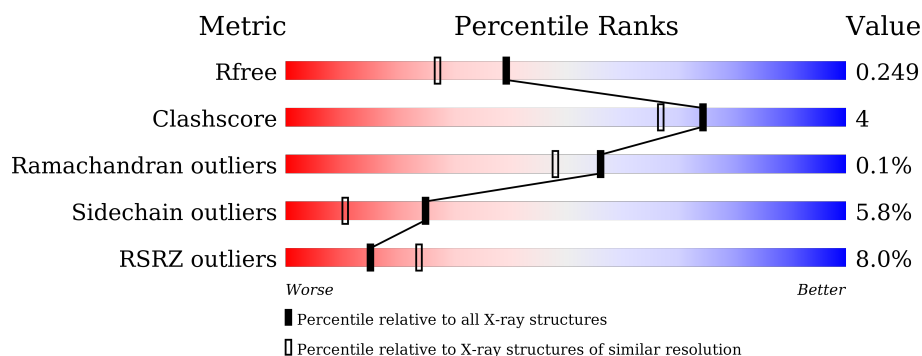|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0122
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

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 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	222	
1	C	222	
1	H	222	
2	B	218	
2	D	218	
2	L	218	

2 Entity composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10397 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.
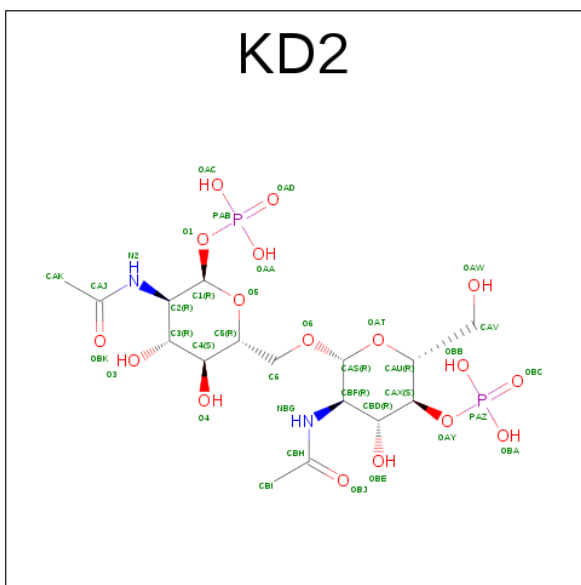
- Molecule 1 is a protein called S55-3 Fab (IgG2b) heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1615	1011	267	328	9			
1	C	217	Total	C	N	O	S	0	0	0
			1609	1008	266	326	9			
1	H	222	Total	C	N	O	S	0	0	0
			1639	1025	271	334	9			

- Molecule 2 is a protein called MAb 44B1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1648	1026	283	333	6			
2	D	211	Total	C	N	O	S	0	0	0
			1641	1022	282	331	6			
2	L	212	Total	C	N	O	S	0	0	0
			1649	1026	284	333	6			

- Molecule 3 is 2-(acetylamino)-6-O-[2-(acetylamino)-2-deoxy-4-O-phosphono-beta-D-glucopyranosyl]-2-deoxy-1-O-phosphono-alpha-D-glucopyranose (three-letter code: KD2) (formula: $C_{16}H_{30}N_2O_{17}P_2$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			37	16	2	17	2		
3	C	1	Total	C	N	O	P	0	0
			37	16	2	17	2		
3	H	1	Total	C	N	O	P	0	0
			37	16	2	17	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

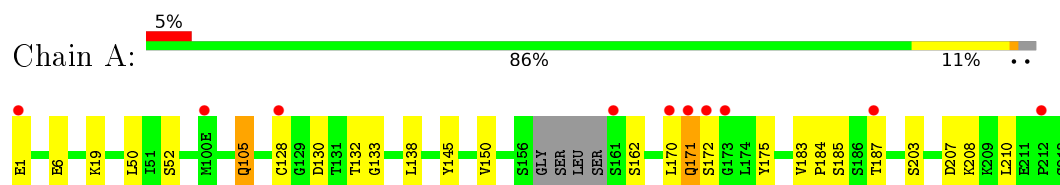| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	89	Total	O	0	0
			89	89		
5	B	60	Total	O	0	0
			60	60		
5	C	89	Total	O	0	0
			89	89		
5	D	66	Total	O	0	0
			66	66		

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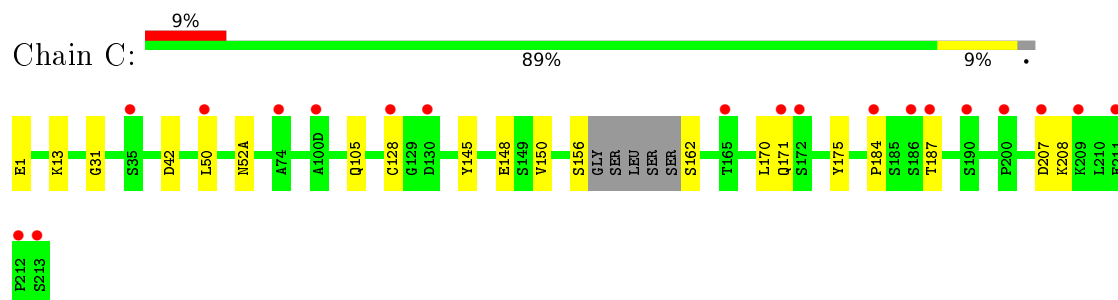| Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	96	Total　O 96　　96	0	0
5	L	83	Total　O 83　　83	0	0

3   Residue-property plots ⓘ

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.
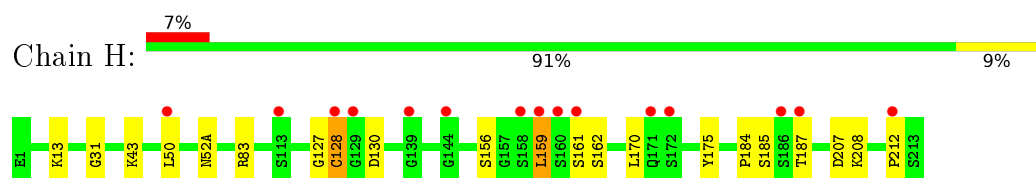
- Molecule 1: S55-3 Fab (IgG2b) heavy chain
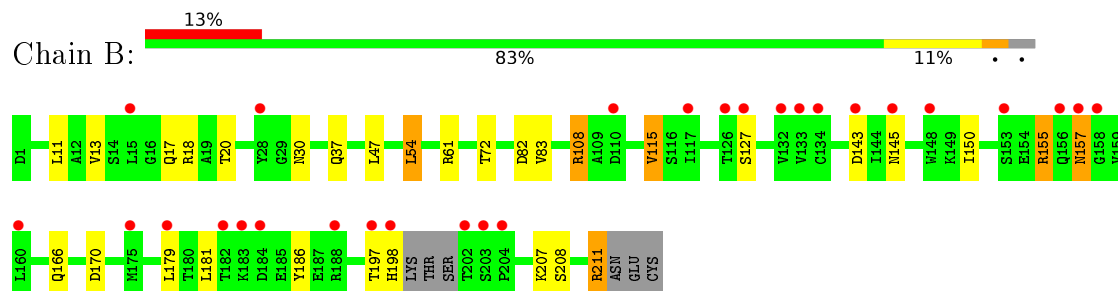

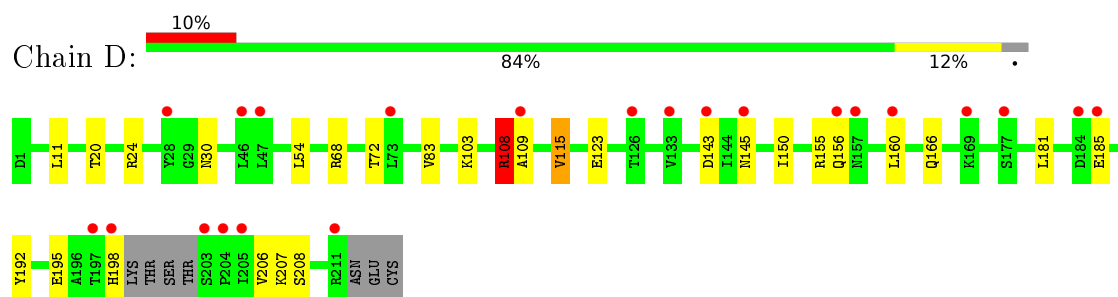- Molecule 1: S55-3 Fab (IgG2b) heavy chain
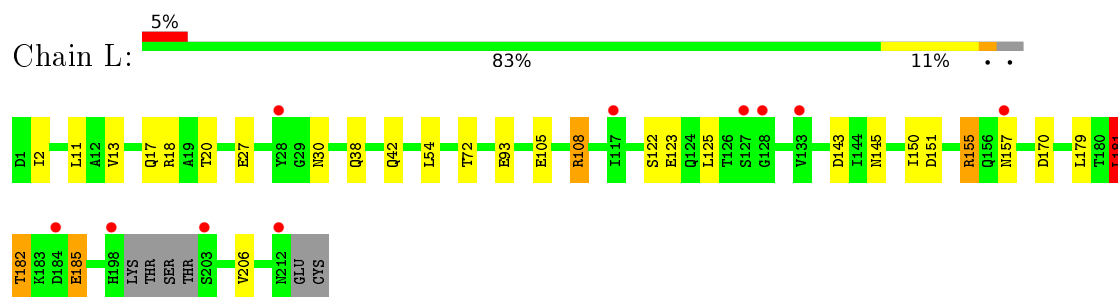

- Molecule 1: S55-3 Fab (IgG2b) heavy chain

- Molecule 2: MAb 44B1 light chain

- Molecule 2: MAb 44B1 light chain

Chain D:

• Molecule 2: MAb 44B1 light chain

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	338.12Å　52.87Å　75.39Å 90.00°　100.95°　90.00°	Depositor
Resolution (Å)	25.00　–　1.95 24.98　–　1.95	Depositor EDS
% Data completeness (in resolution range)	98.3 (25.00-1.95) 98.4 (24.98-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.20 (at 1.95Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.212　,　0.245 0.220　,　0.249	Depositor DCC
R_{free} test set	4730 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	30.0	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 38.5	EDS
Estimated twinning fraction	0.014 for -h-2*l,-k,l	Xtriage
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Outliers	1 of 94048 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10397	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.18 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.6189e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: KD2, CL

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	0.51	0/1653	0.69	0/2253
1	C	0.49	0/1647	0.71	2/2245 (0.1%)
1	H	0.51	0/1678	0.68	0/2288
2	B	0.47	0/1685	0.74	3/2289 (0.1%)
2	D	0.48	0/1678	0.82	2/2279 (0.1%)
2	L	0.50	0/1686	0.74	4/2290 (0.2%)
All	All	0.49	0/10027	0.73	11/13644 (0.1%)

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
1	A	0	1
2	B	0	1
All	All	0	2

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	108	ARG	NE-CZ-NH1	14.60	127.60	120.30
2	D	108	ARG	NE-CZ-NH2	-13.52	113.54	120.30
2	L	18	ARG	NE-CZ-NH1	5.98	123.29	120.30
2	B	108	ARG	NE-CZ-NH1	-5.72	117.44	120.30
2	B	155	ARG	CG-CD-NE	5.57	123.50	111.80
2	L	151	ASP	CB-CG-OD2	-5.57	113.29	118.30
2	L	108	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	C	42	ASP	N-CA-C	5.43	125.66	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	108	ARG	NE-CZ-NH2	5.25	122.92	120.30
2	L	181	LEU	CA-CB-CG	5.08	126.98	115.30
1	C	148	GLU	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	THR	Peptide
2	B	157	ASN	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	A	1615	0	1567	16	1
1	C	1609	0	1562	9	0
1	H	1639	0	1592	15	0
2	B	1648	0	1576	18	0
2	D	1641	0	1569	11	0
2	L	1649	0	1575	11	0
3	A	37	0	0	2	0
3	C	37	0	0	0	0
3	H	37	0	0	0	0
4	C	1	0	0	0	0
4	H	1	0	0	0	0
5	A	89	0	0	3	0
5	B	60	0	0	3	0
5	C	89	0	0	0	0
5	D	66	0	0	1	0
5	H	96	0	0	3	0
5	L	83	0	0	0	0
All	All	10397	0	9441	77	1

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 4.

All (77) 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:61:ARG:HH12	2:B:82:ASP:CG	1.58	1.05
2:B:61:ARG:NH1	2:B:82:ASP:OD2	2.00	0.94
1:A:52:SER:HA	3:A:301:KD2:OAW	1.69	0.92
1:H:127:GLY:O	1:H:130:ASP:HB2	1.77	0.84
2:B:61:ARG:NH1	2:B:82:ASP:OD1	2.10	0.83
2:B:61:ARG:NH1	2:B:82:ASP:CG	2.33	0.81
2:L:182:THR:HG22	2:L:185:GLU:HG3	1.64	0.80
1:H:159:LEU:HD11	5:H:407:HOH:O	1.81	0.80
1:H:159:LEU:HD13	1:H:187:THR:HG21	1.71	0.72
1:H:128:CYS:HB2	1:H:212:PRO:CB	2.20	0.71
1:H:159:LEU:HD13	1:H:187:THR:CG2	2.21	0.70
1:A:1:GLU:HG2	5:A:426:HOH:O	1.94	0.68
2:L:150:ILE:HD11	2:L:179:LEU:HD21	1.78	0.65
2:B:150:ILE:HD11	2:B:179:LEU:HD21	1.78	0.63
2:D:195:GLU:HG2	2:D:206:VAL:HG22	1.80	0.63
1:H:128:CYS:HB2	1:H:212:PRO:HB3	1.80	0.62
1:A:6:GLU:H	1:A:105:GLN:HE22	1.47	0.62
1:C:1:GLU:O	1:C:1:GLU:HG2	1.99	0.62
1:A:138:LEU:HB3	1:A:210:LEU:HD23	1.82	0.61
2:D:150:ILE:HD12	2:D:192:TYR:CD2	2.37	0.60
1:H:184:PRO:O	1:H:187:THR:HG22	2.01	0.60
1:C:184:PRO:O	1:C:187:THR:HG22	2.02	0.59
1:H:208:LYS:NZ	2:L:123:GLU:OE1	2.32	0.59
2:B:83:VAL:HG21	2:B:166:GLN:HB3	1.86	0.57
2:D:108:ARG:HD3	2:D:109:ALA:O	2.04	0.57
1:A:184:PRO:HB2	1:A:187:THR:HG23	1.86	0.56
2:D:83:VAL:HG21	2:D:166:GLN:HB3	1.87	0.56
2:L:38:GLN:OE1	2:L:42:GLN:O	2.24	0.56
1:H:156:SER:O	1:H:159:LEU:HG	2.06	0.56
1:A:19:LYS:NZ	5:A:402:HOH:O	2.35	0.54
1:C:31:GLY:H	1:C:52(A):ASN:ND2	2.06	0.53
1:C:50:LEU:HD12	1:C:50:LEU:C	2.29	0.53
2:B:83:VAL:CG2	5:B:337:HOH:O	2.56	0.53
1:A:50:LEU:HD12	1:A:50:LEU:C	2.30	0.52
1:H:50:LEU:C	1:H:50:LEU:HD12	2.30	0.52
1:H:31:GLY:H	1:H:52(A):ASN:ND2	2.08	0.52
2:B:83:VAL:HG23	5:B:337:HOH:O	2.09	0.51
1:A:145:TYR:CE2	1:A:150:VAL:CG1	2.94	0.51
2:B:197:THR:O	2:B:198:HIS:HB2	2.10	0.50
1:A:1:GLU:HB3	5:A:461:HOH:O	2.13	0.49
2:D:150:ILE:HD12	2:D:192:TYR:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:TYR:CE2	1:C:150:VAL:CG1	2.96	0.49
2:L:181:LEU:N	2:L:181:LEU:HD23	2.28	0.48
1:H:128:CYS:HB3	5:H:492:HOH:O	2.13	0.48
2:L:179:LEU:HG	2:L:181:LEU:HD22	1.97	0.47
2:B:186:TYR:CE2	2:B:211:ARG:HD2	2.50	0.47
1:A:133:GLY:HA2	1:A:185:SER:OG	2.16	0.45
2:B:115:VAL:HG22	2:B:207:LYS:CG	2.47	0.45
2:D:115:VAL:HG22	2:D:207:LYS:HG3	1.99	0.45
1:A:171:GLN:O	1:A:172:SER:HB3	2.17	0.45
2:D:115:VAL:HG22	2:D:207:LYS:CG	2.47	0.44
2:B:54:LEU:HD13	5:B:310:HOH:O	2.17	0.44
2:L:20:THR:HG23	2:L:72:THR:CG2	2.48	0.43
1:A:52:SER:CA	3:A:301:KD2:OAW	2.55	0.43
1:C:105:GLN:HG3	1:C:105:GLN:O	2.17	0.43
2:B:13:VAL:HG13	2:B:17:GLN:HB2	2.01	0.42
2:B:20:THR:HG23	2:B:72:THR:CG2	2.49	0.42
2:D:20:THR:HG23	2:D:72:THR:CG2	2.49	0.42
1:H:128:CYS:HB2	1:H:212:PRO:HB2	1.98	0.42
1:H:208:LYS:NZ	5:H:406:HOH:O	2.53	0.42
1:C:171:GLN:HB2	2:D:160:LEU:HD21	2.01	0.42
2:L:2:ILE:CD1	2:L:93:GLU:HG2	2.50	0.42
1:C:170:LEU:HD13	1:C:175:TYR:CZ	2.55	0.41
1:A:105:GLN:HE21	1:A:105:GLN:H	1.68	0.41
1:H:170:LEU:HD13	1:H:175:TYR:CZ	2.54	0.41
2:B:37:GLN:HB2	2:B:47:LEU:HD11	2.03	0.41
2:L:13:VAL:HG13	2:L:17:GLN:HB2	2.03	0.41
2:D:24:ARG:HD3	5:D:316:HOH:O	2.21	0.41
1:A:170:LEU:HD13	1:A:175:TYR:CZ	2.56	0.41
2:B:115:VAL:HG22	2:B:207:LYS:HG3	2.01	0.41
2:L:108:ARG:HD2	2:L:170:ASP:O	2.21	0.41
1:C:208:LYS:NZ	2:D:123:GLU:OE1	2.40	0.41
1:A:138:LEU:HB3	1:A:210:LEU:CD2	2.49	0.41
1:A:171:GLN:O	1:A:171:GLN:HG3	2.21	0.40
2:B:186:TYR:CZ	2:B:211:ARG:HD2	2.56	0.40
2:L:150:ILE:HD12	2:L:155:ARG:HG3	2.04	0.40
2:B:108:ARG:HD2	2:B:170:ASP:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ASP:OD1	1:A:130:ASP:OD1[2_555]	1.65	0.55

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	214/222 (96%)	210 (98%)	4 (2%)	0	100	100
1	C	213/222 (96%)	210 (99%)	3 (1%)	0	100	100
1	H	220/222 (99%)	217 (99%)	3 (1%)	0	100	100
2	B	208/218 (95%)	201 (97%)	7 (3%)	0	100	100
2	D	207/218 (95%)	200 (97%)	6 (3%)	1 (0%)	34	21
2	L	208/218 (95%)	202 (97%)	6 (3%)	0	100	100
All	All	1270/1320 (96%)	1240 (98%)	29 (2%)	1 (0%)	56	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	68	ARG

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	184/187 (98%)	176 (96%)	8 (4%)	35	20
1	C	183/187 (98%)	178 (97%)	5 (3%)	52	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	187/187 (100%)	178 (95%)	9 (5%)	31	15
2	B	186/192 (97%)	173 (93%)	13 (7%)	19	6
2	D	185/192 (96%)	171 (92%)	14 (8%)	16	5
2	L	186/192 (97%)	171 (92%)	15 (8%)	15	4
All	All	1111/1137 (98%)	1047 (94%)	64 (6%)	25	10

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	128	CYS
1	A	162	SER
1	A	171	GLN
1	A	183	VAL
1	A	203	SER
1	A	207	ASP
1	A	208	LYS
2	B	11	LEU
2	B	18	ARG
2	B	30	ASN
2	B	54	LEU
2	B	115	VAL
2	B	127	SER
2	B	143	ASP
2	B	145	ASN
2	B	155	ARG
2	B	157	ASN
2	B	181	LEU
2	B	208	SER
2	B	211	ARG
1	C	13	LYS
1	C	128	CYS
1	C	156	SER
1	C	162	SER
1	C	207	ASP
2	D	11	LEU
2	D	30	ASN
2	D	54	LEU
2	D	103	LYS
2	D	108	ARG
2	D	115	VAL

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Mol	Chain	Res	Type
2	D	143	ASP
2	D	145	ASN
2	D	155	ARG
2	D	156	GLN
2	D	181	LEU
2	D	185	GLU
2	D	198	HIS
2	D	208	SER
1	H	13	LYS
1	H	43	LYS
1	H	83	ARG
1	H	128	CYS
1	H	159	LEU
1	H	161	SER
1	H	162	SER
1	H	185	SER
1	H	207	ASP
2	L	11	LEU
2	L	27	GLU
2	L	30	ASN
2	L	54	LEU
2	L	105	GLU
2	L	122	SER
2	L	125	LEU
2	L	143	ASP
2	L	145	ASN
2	L	155	ARG
2	L	157	ASN
2	L	181	LEU
2	L	182	THR
2	L	185	GLU
2	L	206	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	171	GLN
2	B	76	ASN
1	C	52(A)	ASN
1	H	52(A)	ASN

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 carbohydrates in this entry.

5.6   Ligand geometry (i)

Of 5 ligands modelled in this entry, 2 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	#$|Z| > 2$
3	KD2	A	301	-	36,38,38	1.97	8 (22%)	52,57,57	1.55	10 (19%)
3	KD2	C	302	-	36,38,38	2.64	12 (33%)	52,57,57	1.50	10 (19%)
3	KD2	H	302	-	36,38,38	1.86	7 (19%)	52,57,57	1.34	8 (15%)

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	KD2	A	301	-	-	0/24/65/65	0/2/2/2
3	KD2	C	302	-	-	0/24/65/65	0/2/2/2
3	KD2	H	302	-	-	0/24/65/65	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302	KD2	PAB-OAC	-6.13	1.33	1.54
3	C	302	KD2	PAZ-OBA	-5.71	1.35	1.54
3	C	302	KD2	PAZ-OBB	-5.69	1.35	1.54
3	C	302	KD2	PAB-OAA	-5.65	1.35	1.54
3	C	302	KD2	PAB-OAD	-4.87	1.35	1.50
3	H	302	KD2	PAB-OAC	-4.80	1.38	1.54
3	A	301	KD2	PAZ-OBB	-4.78	1.38	1.54
3	A	301	KD2	PAB-OAA	-4.57	1.39	1.54
3	A	301	KD2	PAB-OAC	-4.51	1.39	1.54
3	H	302	KD2	PAZ-OBB	-4.29	1.39	1.54
3	C	302	KD2	O6-C6	-4.11	1.36	1.43
3	C	302	KD2	PAZ-OBC	-4.05	1.38	1.50
3	H	302	KD2	PAB-OAA	-4.04	1.40	1.54
3	H	302	KD2	PAZ-OBA	-4.02	1.40	1.54
3	A	301	KD2	PAZ-OBA	-3.91	1.41	1.54
3	A	301	KD2	PAB-OAD	-3.79	1.38	1.50
3	A	301	KD2	PAZ-OBC	-3.67	1.39	1.50
3	H	302	KD2	PAB-OAD	-3.49	1.39	1.50
3	H	302	KD2	O6-CAS	-3.04	1.34	1.40
3	C	302	KD2	O5-C5	-2.90	1.37	1.44
3	A	301	KD2	OAW-CAV	-2.83	1.30	1.42
3	C	302	KD2	O4-C4	-2.50	1.37	1.43
3	C	302	KD2	O6-CAS	-2.39	1.35	1.40
3	H	302	KD2	PAZ-OBC	-2.34	1.43	1.50
3	C	302	KD2	OAT-CAU	-2.19	1.38	1.44
3	A	301	KD2	C1-C2	2.20	1.56	1.53
3	C	302	KD2	C4-C5	2.38	1.58	1.53

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	KD2	OAY-PAZ-OBC	-3.55	99.01	107.48
3	A	301	KD2	CAV-CAU-CAX	-3.30	103.54	113.25
3	A	301	KD2	O1-PAB-OAD	-3.20	99.83	107.48
3	H	302	KD2	O1-PAB-OAD	-2.86	100.64	107.48
3	C	302	KD2	OAC-PAB-O1	-2.63	98.76	106.62
3	A	301	KD2	OAA-PAB-O1	-2.59	98.87	106.62
3	A	301	KD2	CAS-CBF-NBG	-2.46	106.37	111.01
3	C	302	KD2	O1-PAB-OAD	-2.43	101.67	107.48
3	C	302	KD2	C4-C3-C2	-2.24	106.97	110.37
3	H	302	KD2	CAS-CBF-NBG	-2.19	106.89	111.01
3	C	302	KD2	OBK-CAJ-CAK	-2.19	118.05	122.07
3	H	302	KD2	C1-O5-C5	2.00	117.67	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	KD2	OAT-CAU-CAV	2.01	111.59	106.38
3	C	302	KD2	OAA-PAB-OAD	2.08	117.40	110.63
3	C	302	KD2	OAC-PAB-OAA	2.08	115.08	107.44
3	A	301	KD2	OAY-CAX-CBD	2.14	112.76	108.48
3	A	301	KD2	OAA-PAB-OAD	2.15	117.66	110.63
3	H	302	KD2	OAC-PAB-OAA	2.16	115.36	107.44
3	H	302	KD2	OAT-CAU-CAV	2.19	112.05	106.38
3	H	302	KD2	OAY-CAX-CAU	2.27	113.16	108.53
3	H	302	KD2	OAA-PAB-OAD	2.27	118.04	110.63
3	H	302	KD2	O5-C5-C4	2.59	114.60	109.67
3	C	302	KD2	C1-O5-C5	2.77	119.17	113.74
3	A	301	KD2	OAC-PAB-OAA	2.82	117.79	107.44
3	A	301	KD2	CAS-OAT-CAU	2.96	119.55	113.74
3	C	302	KD2	O1-C1-C2	3.25	114.41	108.42
3	A	301	KD2	OAT-CAU-CAV	3.45	115.31	106.38
3	C	302	KD2	O5-C1-O1	4.17	116.87	111.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	KD2	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 (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	A	218/222 (98%)	0.36	10 (4%)	36	47	19, 35, 62, 75	0
1	C	217/222 (97%)	0.62	19 (8%)	12	20	21, 39, 63, 74	0
1	H	222/222 (100%)	0.45	15 (6%)	20	30	18, 37, 57, 74	0
2	B	212/218 (97%)	0.88	28 (13%)	4	8	22, 43, 70, 97	0
2	D	211/218 (96%)	0.63	22 (10%)	8	13	22, 40, 65, 87	0
2	L	212/218 (97%)	0.48	10 (4%)	35	46	19, 35, 61, 89	0
All	All	1292/1320 (97%)	0.57	104 (8%)	15	24	18, 38, 65, 97	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	202	THR	6.9
2	L	203	SER	6.3
2	L	212	ASN	5.6
2	L	198	HIS	5.1
1	H	160	SER	4.9
2	B	183	LYS	4.8
2	B	203	SER	4.7
1	A	128	CYS	4.7
2	D	203	SER	4.6
2	D	198	HIS	4.4
2	L	128	GLY	3.9
2	D	184	ASP	3.9
2	B	133	VAL	3.9
2	B	188	ARG	3.9
1	A	171	GLN	3.8
2	B	132	VAL	3.8
2	B	157	ASN	3.7
2	D	197	THR	3.7
1	C	172	SER	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	198	HIS	3.6
2	B	197	THR	3.6
2	D	156	GLN	3.5
1	H	159	LEU	3.5
1	H	129	GLY	3.4
1	C	209	LYS	3.4
2	B	182	THR	3.3
2	B	184	ASP	3.3
2	D	169	LYS	3.3
2	L	184	ASP	3.3
1	H	128	CYS	3.2
2	B	127	SER	3.2
2	B	143	ASP	3.2
1	H	158	SER	3.2
2	D	126	THR	3.2
1	C	165	THR	3.1
1	A	172	SER	3.1
1	A	212	PRO	3.1
2	D	157	ASN	3.1
1	C	128	CYS	3.1
2	L	133	VAL	2.9
2	D	205	ILE	2.9
1	H	187	THR	2.9
2	B	153	SER	2.8
2	B	28	TYR	2.8
2	L	28	TYR	2.8
1	C	130	ASP	2.7
2	B	148	TRP	2.7
1	A	187	THR	2.7
2	D	160	LEU	2.7
2	B	158	GLY	2.6
1	C	171	GLN	2.6
1	C	190	SER	2.6
2	B	117	ILE	2.6
1	C	186	SER	2.6
1	C	213	SER	2.6
2	D	46	LEU	2.6
1	H	212	PRO	2.6
2	D	28	TYR	2.6
1	C	50	LEU	2.6
1	H	186	SER	2.6
1	C	35	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	212	PRO	2.4
1	A	170	LEU	2.4
2	D	143	ASP	2.4
2	B	134	CYS	2.4
2	B	110	ASP	2.3
2	B	204	PRO	2.3
2	D	133	VAL	2.3
2	B	145	ASN	2.3
2	B	15	LEU	2.3
2	B	179	LEU	2.3
1	A	1	GLU	2.3
1	A	100(E)	MET	2.2
1	C	184	PRO	2.2
1	A	173	GLY	2.2
2	D	204	PRO	2.2
1	A	161	SER	2.2
1	H	172	SER	2.2
2	L	127	SER	2.2
2	D	47	LEU	2.2
2	D	73	LEU	2.2
1	C	207	ASP	2.2
1	C	74	ALA	2.2
1	C	100(D)	ALA	2.2
2	D	109	ALA	2.2
1	H	144	GLY	2.2
2	L	117	ILE	2.2
1	H	171	GLN	2.2
2	B	156	GLN	2.2
2	D	185	GLU	2.2
1	C	200	PRO	2.1
1	H	113	SER	2.1
1	C	187	THR	2.1
2	B	126	THR	2.1
1	C	211	GLU	2.1
1	H	161	SER	2.1
1	H	139	GLY	2.1
2	L	157	ASN	2.1
2	B	160	LEU	2.1
2	D	211	ARG	2.0
2	D	145	ASN	2.0
1	H	50	LEU	2.0
2	B	175	MET	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	177	SER	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 carbohydrates 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. 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
3	KD2	A	301	37/37	0.93	0.10	-0.56	20,20,20,20	0
3	KD2	C	302	37/37	0.95	0.10	-0.88	20,20,20,20	0
3	KD2	H	302	37/37	0.96	0.09	-1.00	20,20,20,20	0
4	CL	H	301	1/1	0.99	0.10	-1.24	26,26,26,26	0
4	CL	C	301	1/1	1.00	0.08	-	23,23,23,23	1

6.5 Other polymers (i)

There are no such residues in this entry.