Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 01:24 AM EDT

PDB ID	:	5WK3
Title	:	CRYSTAL STRUCTURE OF THE COMPLEX BETWEEN CCL17 AND M116 FAB
Authors	:	Teplyakov, A.; Obmolova, G.; Gilliland, G.L.
Deposited on	:	2017-07-24
Resolution	:	1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
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:

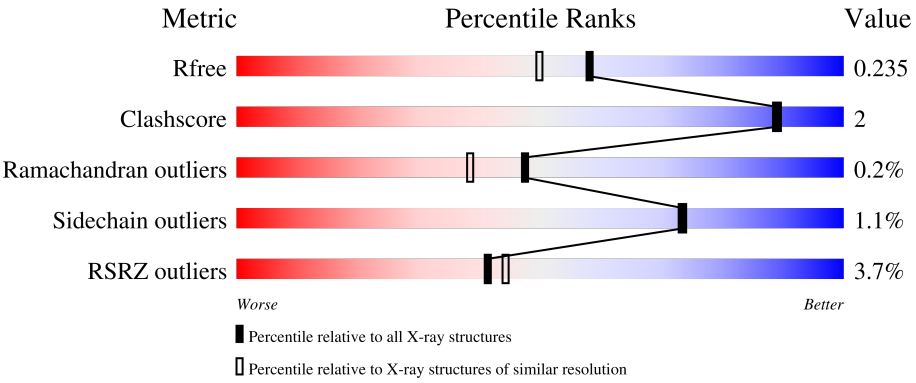
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	P	220	4% 91% 7% ·
1	R	220	2% 93% 6% ·
1	T	220	4% 93% 6% ·
1	V	220	4% 89% 10% ·
2	Q	230	5% 90% 6% ·

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Mol	Chain	Length	Quality of chain
2	S	230	5% 93%
2	U	230	4% 95%
2	W	230	3% 91% 5%
3	A	71	82% 6% 13%
3	B	71	% 80% 8% 11%
3	C	71	% 79% 10% 10%
3	D	71	4% 76% 8% 14%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16264 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 M116 LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	217	Total	C	N	O	S	0	0	0
			1672	1049	279	339	5			
1	R	217	Total	C	N	O	S	0	0	0
			1669	1048	279	337	5			
1	T	218	Total	C	N	O	S	0	0	0
			1673	1050	280	338	5			
1	V	216	Total	C	N	O	S	0	0	0
			1664	1045	278	336	5			

- Molecule 2 is a protein called M116 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	221	Total	C	N	O	S	0	0	0
			1653	1051	268	327	7			
2	S	221	Total	C	N	O	S	0	0	0
			1653	1051	268	327	7			
2	U	221	Total	C	N	O	S	0	0	0
			1653	1051	268	327	7			
2	W	221	Total	C	N	O	S	0	0	0
			1653	1051	268	327	7			

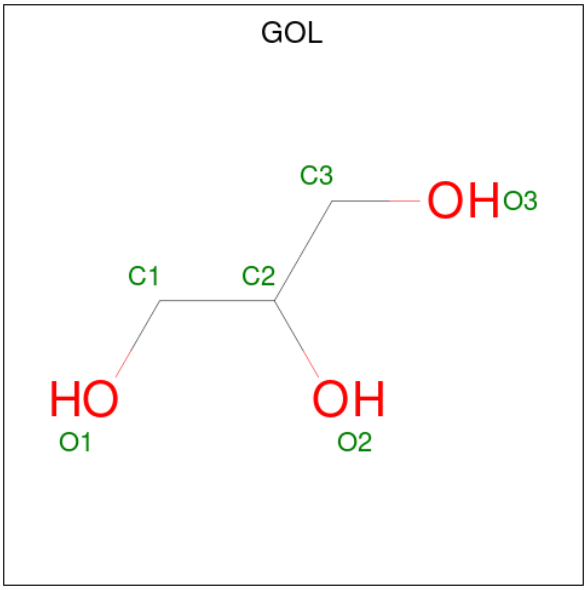
- Molecule 3 is a protein called C-C motif chemokine 17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	62	Total	C	N	O	S	0	0	0
			479	305	83	87	4			
3	B	63	Total	C	N	O	S	0	0	0
			486	306	87	89	4			
3	C	64	Total	C	N	O	S	0	0	0
			503	316	92	91	4			
3	D	61	Total	C	N	O	S	0	0	0
			462	294	82	82	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	THR	GLY	variant	UNP Q92583
B	7	THR	GLY	variant	UNP Q92583
C	7	THR	GLY	variant	UNP Q92583
D	7	THR	GLY	variant	UNP Q92583

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Q	1	Total C O 6 3 3	0	0
4	S	1	Total C O 6 3 3	0	0
4	U	1	Total C O 6 3 3	0	0
4	V	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	P	81	Total O 81 81	0	0
5	Q	113	Total O 113 113	0	0
5	R	112	Total O 112 112	0	0

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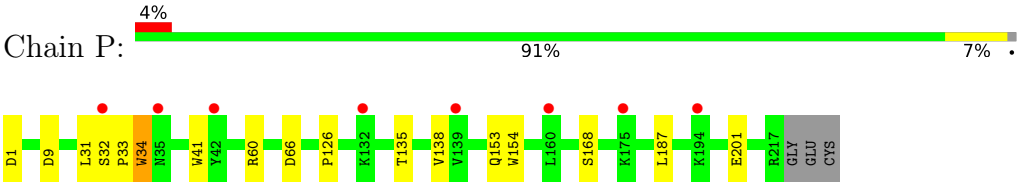
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	S	133	Total O 133 133	0	0
5	T	100	Total O 100 100	0	0
5	U	116	Total O 116 116	0	0
5	V	82	Total O 82 82	0	0
5	W	157	Total O 157 157	0	0
5	A	29	Total O 29 29	0	0
5	B	39	Total O 39 39	0	0
5	C	26	Total O 26 26	0	0
5	D	32	Total O 32 32	0	0

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.

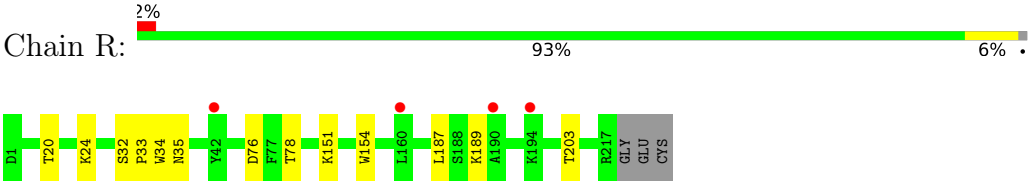
• Molecule 1: M116 LIGHT CHAIN

Chain P:



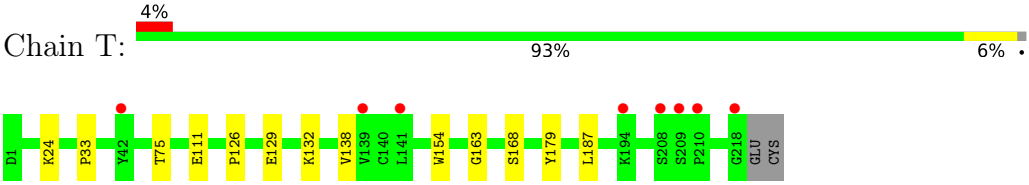
• Molecule 1: M116 LIGHT CHAIN

Chain R:



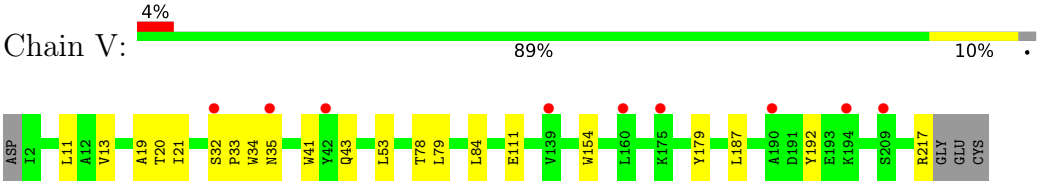
• Molecule 1: M116 LIGHT CHAIN

Chain T:



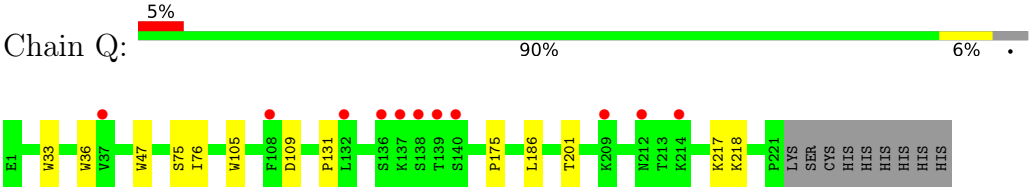
• Molecule 1: M116 LIGHT CHAIN

Chain V:



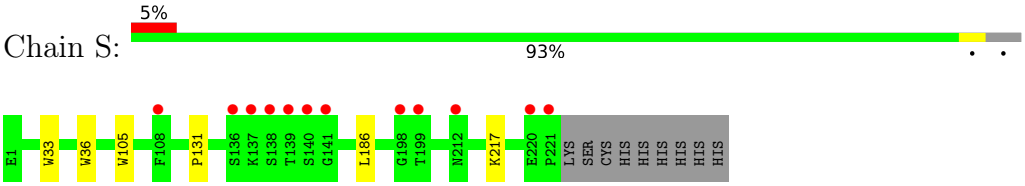
• Molecule 2: M116 HEAVY CHAIN

Chain Q:



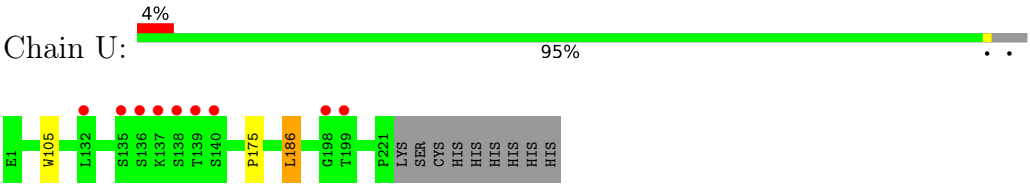
• Molecule 2: M116 HEAVY CHAIN

Chain S:



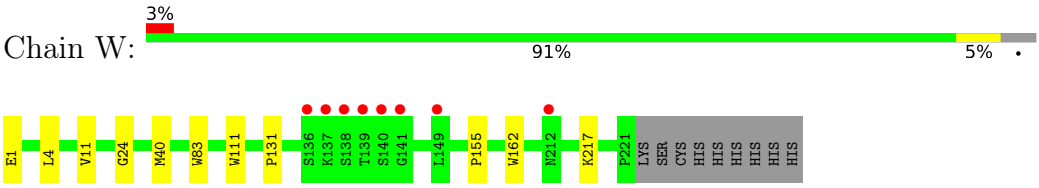
• Molecule 2: M116 HEAVY CHAIN

Chain U:



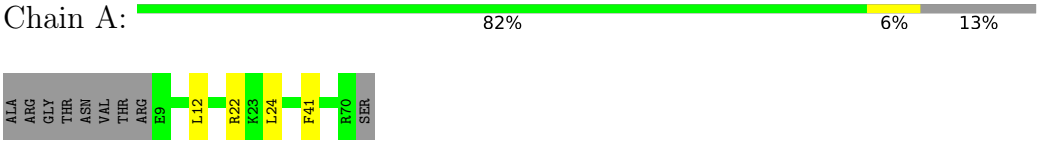
• Molecule 2: M116 HEAVY CHAIN

Chain W:



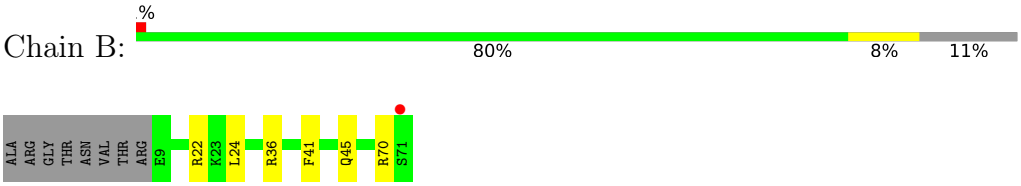
• Molecule 3: C-C motif chemokine 17

Chain A:



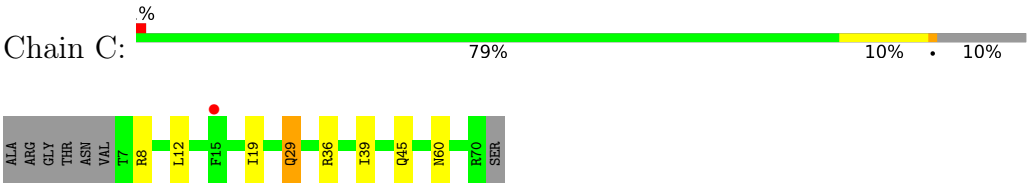
• Molecule 3: C-C motif chemokine 17

Chain B:



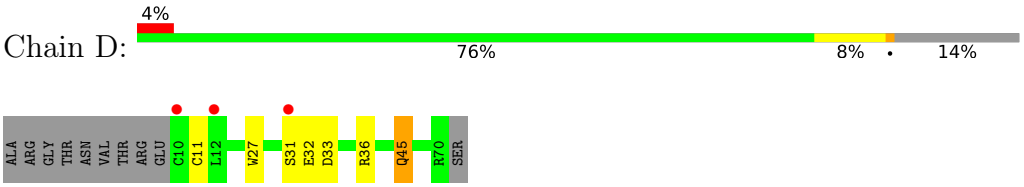
• Molecule 3: C-C motif chemokine 17

Chain C:



• Molecule 3: C-C motif chemokine 17

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	51.51Å 81.93Å 130.50Å 93.96° 99.21° 104.19°	Depositor
Resolution (Å)	15.00 – 1.90 29.38 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.2 (15.00-1.90) 96.2 (29.38-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.180 , 0.231 0.182 , 0.235	Depositor DCC
R_{free} test set	1540 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	23.5	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 50.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16264	wwPDB-VP
Average B, all atoms (Å^2)	34.0	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 26.75 % 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 2.4881e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: GOL

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	P	0.47	3/1708 (0.2%)	0.59	0/2323
1	R	0.50	2/1705 (0.1%)	0.62	0/2319
1	T	0.48	1/1709 (0.1%)	0.61	0/2324
1	V	0.48	2/1700 (0.1%)	0.60	0/2312
2	Q	0.58	3/1698 (0.2%)	0.62	0/2317
2	S	0.58	2/1698 (0.1%)	0.63	0/2317
2	U	0.57	1/1698 (0.1%)	0.62	1/2317 (0.0%)
2	W	0.59	3/1698 (0.2%)	0.63	0/2317
3	A	0.50	0/487	0.58	0/658
3	B	0.50	0/494	0.57	0/668
3	C	0.48	0/511	0.65	0/689
3	D	0.54	1/470 (0.2%)	0.65	0/637
All	All	0.53	18/15576 (0.1%)	0.62	1/21198 (0.0%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	33	TRP	CD2-CE2	5.52	1.48	1.41
2	Q	47	TRP	CD2-CE2	5.41	1.47	1.41
2	U	105	TRP	CD2-CE2	5.34	1.47	1.41
1	V	154	TRP	CD2-CE2	5.32	1.47	1.41
3	D	27	TRP	CD2-CE2	5.30	1.47	1.41
2	Q	33	TRP	CD2-CE2	5.28	1.47	1.41
1	P	34	TRP	CD2-CE2	5.24	1.47	1.41
1	V	41	TRP	CD2-CE2	5.19	1.47	1.41
1	P	41	TRP	CD2-CE2	5.16	1.47	1.41
1	R	154	TRP	CD2-CE2	5.14	1.47	1.41
2	W	111	TRP	CD2-CE2	5.10	1.47	1.41
2	W	162	TRP	CD2-CE2	5.08	1.47	1.41
1	R	34	TRP	CD2-CE2	5.04	1.47	1.41
2	S	36	TRP	CD2-CE2	5.04	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	36	TRP	CD2-CE2	5.03	1.47	1.41
2	W	83	TRP	CD2-CE2	5.03	1.47	1.41
1	T	154	TRP	CD2-CE2	5.02	1.47	1.41
1	P	154	TRP	CD2-CE2	5.00	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	U	186	LEU	CA-CB-CG	5.34	127.58	115.30

There are no chirality outliers.

There are no planarity outliers.

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	P	1672	0	1632	8	0
1	R	1669	0	1630	6	0
1	T	1673	0	1633	7	0
1	V	1664	0	1625	13	0
2	Q	1653	0	1602	7	0
2	S	1653	0	1602	2	0
2	U	1653	0	1602	1	0
2	W	1653	0	1602	3	0
3	A	479	0	471	2	0
3	B	486	0	468	2	0
3	C	503	0	497	6	0
3	D	462	0	444	7	0
4	Q	6	0	8	1	0
4	S	6	0	8	0	0
4	U	6	0	8	0	0
4	V	6	0	8	0	0
5	A	29	0	0	0	0
5	B	39	0	0	1	0
5	C	26	0	0	0	0
5	D	32	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	81	0	0	0	0
5	Q	113	0	0	0	0
5	R	112	0	0	0	0
5	S	133	0	0	0	0
5	T	100	0	0	0	0
5	U	116	0	0	0	0
5	V	82	0	0	0	0
5	W	157	0	0	0	0
All	All	16264	0	14840	56	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 2.

All (56) 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)
1:P:31:LEU:HG	1:P:34:TRP:CD1	2.20	0.77
1:R:189:LYS:HE2	1:T:163:GLY:HA3	1.67	0.76
1:V:11:LEU:HD21	1:V:21:ILE:HG22	1.71	0.71
1:V:13:VAL:HG23	1:V:84:LEU:HD22	1.76	0.67
1:V:13:VAL:CG2	1:V:84:LEU:HD22	2.25	0.66
2:S:131:PRO:HD3	2:S:217:LYS:HE2	1.77	0.66
1:R:33:PRO:HG2	5:B:127:HOH:O	1.96	0.66
1:V:11:LEU:CD2	1:V:21:ILE:HG22	2.26	0.65
1:P:60:ARG:HH11	1:P:66:ASP:HA	1.63	0.64
2:Q:75:SER:OG	3:C:8:ARG:NH2	2.31	0.62
3:D:11:CYS:O	3:D:36:ARG:CD	2.51	0.58
1:V:11:LEU:HD21	1:V:21:ILE:CG2	2.34	0.58
1:R:24:LYS:HG2	1:R:76:ASP:OD1	2.06	0.56
1:T:168:SER:OG	2:U:175:PRO:HD2	2.05	0.56
2:Q:76:ILE:HG23	3:C:8:ARG:NH2	2.22	0.54
1:V:43:GLN:HB2	1:V:53:LEU:HD11	1.90	0.54
3:D:11:CYS:O	3:D:36:ARG:HD2	2.07	0.53
1:P:31:LEU:HG	1:P:34:TRP:HD1	1.75	0.52
1:P:126:PRO:HD3	1:P:138:VAL:HG22	1.92	0.51
2:W:131:PRO:HD3	2:W:217:LYS:HE2	1.92	0.51
1:R:20:THR:HG23	1:R:78:THR:CG2	2.40	0.51
1:V:192:TYR:CZ	1:V:217:ARG:HG3	2.47	0.50
1:P:153:GLN:HB3	1:P:201:GLU:HB3	1.93	0.49
3:B:24:LEU:HD22	3:B:41:PHE:HB3	1.94	0.49
1:P:32:SER:HB3	1:P:33:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:13:VAL:HG21	1:V:19:ALA:HB2	1.96	0.48
3:D:36:ARG:HD2	5:D:119:HOH:O	2.12	0.47
1:T:111:GLU:CD	1:T:179:TYR:HH	2.17	0.47
1:V:20:THR:HG23	1:V:78:THR:CG2	2.44	0.47
3:C:29:GLN:HG2	3:C:39:ILE:HD13	1.96	0.47
3:C:12:LEU:O	3:C:36:ARG:HG3	2.14	0.46
1:P:34:TRP:CD1	1:P:34:TRP:N	2.84	0.45
1:P:168:SER:OG	2:Q:175:PRO:HD2	2.17	0.45
3:D:11:CYS:O	3:D:36:ARG:HD3	2.16	0.44
1:V:21:ILE:HD11	1:V:79:LEU:HD23	1.98	0.44
3:C:19:ILE:H	3:C:19:ILE:HD12	1.82	0.44
2:Q:201:THR:HG23	2:Q:218:LYS:HE3	1.99	0.44
2:S:105:TRP:CZ3	3:B:22:ARG:HD3	2.53	0.44
1:R:151:LYS:HB3	1:R:203:THR:HB	1.99	0.43
1:V:111:GLU:OE1	1:V:179:TYR:OH	2.22	0.43
2:Q:131:PRO:HD3	2:Q:217:LYS:HE2	1.99	0.43
2:Q:105:TRP:CZ3	3:A:22:ARG:HD3	2.53	0.43
1:T:126:PRO:HD3	1:T:138:VAL:HG22	2.01	0.43
2:W:11:VAL:HG21	2:W:155:PRO:HG3	2.01	0.42
3:D:45:GLN:HG2	5:D:104:HOH:O	2.19	0.42
1:V:32:SER:HB2	1:V:33:PRO:HD3	2.01	0.42
2:W:4:LEU:HD23	2:W:24:GLY:HA2	2.01	0.42
2:Q:109:ASP:HB3	4:Q:301:GOL:H12	2.02	0.41
1:T:33:PRO:HB3	3:C:60:ASN:ND2	2.35	0.41
1:T:129:GLU:HA	1:T:132:LYS:HE2	2.02	0.41
3:A:24:LEU:HD22	3:A:41:PHE:HB3	2.03	0.41
1:T:24:LYS:HA	1:T:75:THR:O	2.20	0.41
3:D:31:SER:O	3:D:33:ASP:N	2.44	0.41
1:R:32:SER:HB2	1:R:33:PRO:HD3	2.03	0.40
3:D:36:ARG:HH11	3:D:36:ARG:HG2	1.87	0.40
1:V:33:PRO:HB2	1:V:34:TRP:CE3	2.56	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	P	215/220 (98%)	208 (97%)	7 (3%)	0	100 100
1	R	215/220 (98%)	209 (97%)	5 (2%)	1 (0%)	29 18
1	T	216/220 (98%)	209 (97%)	7 (3%)	0	100 100
1	V	214/220 (97%)	208 (97%)	6 (3%)	0	100 100
2	Q	219/230 (95%)	218 (100%)	1 (0%)	0	100 100
2	S	219/230 (95%)	217 (99%)	2 (1%)	0	100 100
2	U	219/230 (95%)	216 (99%)	3 (1%)	0	100 100
2	W	219/230 (95%)	217 (99%)	2 (1%)	0	100 100
3	A	60/71 (84%)	58 (97%)	2 (3%)	0	100 100
3	B	61/71 (86%)	59 (97%)	1 (2%)	1 (2%)	9 2
3	C	62/71 (87%)	60 (97%)	2 (3%)	0	100 100
3	D	59/71 (83%)	57 (97%)	1 (2%)	1 (2%)	9 2
All	All	1978/2084 (95%)	1936 (98%)	39 (2%)	3 (0%)	47 38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	35	ASN
3	D	32	GLU
3	B	70	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	P	192/194 (99%)	188 (98%)	4 (2%)	53 48
1	R	191/194 (98%)	190 (100%)	1 (0%)	88 89
1	T	191/194 (98%)	190 (100%)	1 (0%)	88 89
1	V	191/194 (98%)	189 (99%)	2 (1%)	76 76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	Q	185/197 (94%)	184 (100%)	1 (0%)	88 89
2	S	185/197 (94%)	184 (100%)	1 (0%)	88 89
2	U	185/197 (94%)	184 (100%)	1 (0%)	88 89
2	W	185/197 (94%)	183 (99%)	2 (1%)	73 73
3	A	51/63 (81%)	50 (98%)	1 (2%)	55 51
3	B	51/63 (81%)	49 (96%)	2 (4%)	32 23
3	C	54/63 (86%)	52 (96%)	2 (4%)	34 25
3	D	47/63 (75%)	46 (98%)	1 (2%)	53 48
All	All	1708/1816 (94%)	1689 (99%)	19 (1%)	73 73

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	1	ASP
1	P	9	ASP
1	P	135	THR
1	P	187	LEU
2	Q	186	LEU
1	R	187	LEU
2	S	186	LEU
1	T	187	LEU
2	U	186	LEU
1	V	35	ASN
1	V	187	LEU
2	W	1	GLU
2	W	40	MET
3	A	12	LEU
3	B	36	ARG
3	B	45	GLN
3	C	29	GLN
3	C	45	GLN
3	D	45	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	195	HIS
1	T	205	GLN

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Mol	Chain	Res	Type
3	A	45	GLN
3	A	60	ASN
3	B	45	GLN
3	B	60	ASN
3	C	45	GLN
3	C	60	ASN
3	D	60	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 monosaccharides in this entry.

5.6 Ligand geometry

4 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	$\#\|Z\| > 2$
4	GOL	Q	301	-	5,5,5	0.30	0	5,5,5	0.63	0
4	GOL	V	1001	-	5,5,5	0.35	0	5,5,5	0.34	0
4	GOL	S	301	-	5,5,5	0.33	0	5,5,5	0.24	0
4	GOL	U	301	-	5,5,5	0.31	0	5,5,5	0.21	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	Q	301	-	-	4/4/4/4	-
4	GOL	V	1001	-	-	1/4/4/4	-
4	GOL	S	301	-	-	0/4/4/4	-
4	GOL	U	301	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Q	301	GOL	O1-C1-C2-C3
4	Q	301	GOL	O2-C2-C3-O3
4	Q	301	GOL	C1-C2-C3-O3
4	Q	301	GOL	O1-C1-C2-O2
4	V	1001	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Q	301	GOL	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, 95^{th} 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	P	217/220 (98%)	0.16	8 (3%)	41	44	17, 36, 63, 83	0
1	R	217/220 (98%)	0.02	4 (1%)	68	71	18, 31, 60, 73	0
1	T	218/220 (99%)	0.09	8 (3%)	41	44	20, 33, 61, 75	0
1	V	216/220 (98%)	0.06	9 (4%)	36	39	19, 34, 60, 90	0
2	Q	221/230 (96%)	0.19	11 (4%)	28	32	17, 33, 57, 165	0
2	S	221/230 (96%)	0.15	12 (5%)	25	29	16, 30, 64, 150	0
2	U	221/230 (96%)	0.06	9 (4%)	37	40	18, 30, 63, 139	0
2	W	221/230 (96%)	-0.06	8 (3%)	42	45	15, 26, 47, 163	0
3	A	62/71 (87%)	-0.50	0	100	100	18, 28, 41, 50	0
3	B	63/71 (88%)	-0.34	1 (1%)	72	74	19, 29, 50, 67	0
3	C	64/71 (90%)	-0.15	1 (1%)	72	74	21, 31, 63, 73	0
3	D	61/71 (85%)	-0.11	3 (4%)	29	33	17, 30, 55, 76	0
All	All	2002/2084 (96%)	0.04	74 (3%)	41	44	15, 31, 61, 165	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	W	140	SER	17.5
2	Q	138	SER	13.9
2	U	136	SER	12.5
2	W	138	SER	12.1
2	U	140	SER	12.1
2	Q	136	SER	11.7
2	S	139	THR	11.5
2	S	138	SER	10.8
2	Q	140	SER	10.5
2	W	139	THR	9.4
2	U	138	SER	9.3

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Mol	Chain	Res	Type	RSRZ
2	U	139	THR	8.5
2	S	140	SER	8.4
2	S	137	LYS	7.6
2	W	137	LYS	7.5
2	U	137	LYS	7.2
2	Q	137	LYS	6.7
2	S	136	SER	6.2
2	W	136	SER	6.1
2	S	198	GLY	5.9
2	Q	139	THR	5.2
2	U	135	SER	4.6
1	R	160	LEU	4.4
2	S	141	GLY	4.2
1	P	160	LEU	4.0
1	P	132	LYS	3.8
1	V	194	LYS	3.6
1	V	35	ASN	3.5
3	D	10	CYS	3.4
3	B	71	SER	3.3
1	T	218	GLY	3.3
2	Q	108	PHE	3.3
2	U	198	GLY	3.2
1	T	194	LYS	3.1
2	Q	214	LYS	3.1
1	T	209	SER	3.0
1	R	194	LYS	3.0
1	P	35	ASN	2.9
2	Q	212	ASN	2.9
1	T	139	VAL	2.9
2	Q	209	LYS	2.9
1	T	208	SER	2.8
2	S	221	PRO	2.7
1	V	190	ALA	2.6
1	T	141	LEU	2.6
3	D	12	LEU	2.6
1	V	160	LEU	2.5
3	C	15	PHE	2.5
2	S	199	THR	2.5
1	T	210	PRO	2.5
1	P	194	LYS	2.5
1	V	42	TYR	2.5
2	S	220	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	V	175	LYS	2.4
2	W	141	GLY	2.4
1	R	190	ALA	2.3
2	S	108	PHE	2.3
1	V	32	SER	2.3
2	Q	132	LEU	2.3
2	S	212	ASN	2.3
2	U	132	LEU	2.3
1	P	42	TYR	2.2
1	V	139	VAL	2.2
2	W	212	ASN	2.2
1	R	42	TYR	2.2
2	U	199	THR	2.2
3	D	31	SER	2.2
2	W	149	LEU	2.1
1	P	139	VAL	2.1
1	P	175	LYS	2.1
2	Q	37	VAL	2.1
1	T	42	TYR	2.0
1	V	209	SER	2.0
1	P	32	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 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, 95^{th} 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
4	GOL	S	301	6/6	0.92	0.13	34,36,42,44	0
4	GOL	U	301	6/6	0.93	0.11	32,37,44,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	Q	301	6/6	0.94	0.11	32,38,50,51	0
4	GOL	V	1001	6/6	0.95	0.14	30,34,37,42	0

6.5 Other polymers (i)

There are no such residues in this entry.