



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 06:25 AM UTC

PDB ID : 5JWE / pdb_00005jwe
Title : Crystal structure of H-2Db in complex with the LCMV-derived GP92-101 peptide
Authors : Buratto, J.; Badia-Martinez, D.; Norstrom, M.; Sandalova, T.; Achour, A.
Deposited on : 2016-05-12
Resolution : 2.40 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 ⓘ symbol.

The types of validation reports are described at

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

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

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

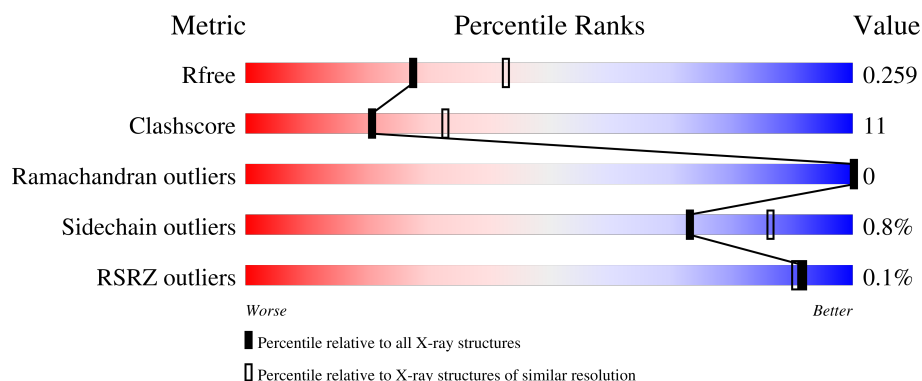
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

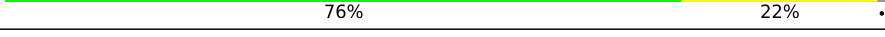
The reported resolution of this entry is 2.40 Å.

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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	276	 77% 22%
1	C	276	 76% 22% .
1	E	276	 78% 19% . .
1	G	276	 76% 22% .
2	B	99	 74% 26%

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Mol	Chain	Length	Quality of chain
2	D	99	 65%35%
2	F	99	 70%29%.•
2	H	99	 82%18%
3	P	10	 90%10%
3	Q	10	 80%20%
3	R	10	 80%20%
3	S	10	 70%30%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12734 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 H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	1	0
			2243	1420	397	417	9			
1	C	276	Total	C	N	O	S	0	1	0
			2234	1414	396	416	8			
1	E	268	Total	C	N	O	S	0	2	0
			2098	1337	363	389	9			
1	G	273	Total	C	N	O	S	0	0	0
			2156	1364	378	405	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			803	513	133	150	7			
2	D	99	Total	C	N	O	S	0	1	0
			814	521	135	150	8			
2	F	99	Total	C	N	O	S	0	1	0
			817	522	138	150	7			
2	H	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	85	ASP	ALA	conflict	UNP P01887
D	85	ASP	ALA	conflict	UNP P01887
F	85	ASP	ALA	conflict	UNP P01887
H	85	ASP	ALA	conflict	UNP P01887

- Molecule 3 is a protein called Pre-glycoprotein polyprotein GP complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	10	Total	C	N	O	S	0	0	0
			80	47	16	16	1			
3	Q	10	Total	C	N	O	S	0	0	0
			80	47	16	16	1			
3	R	10	Total	C	N	O	S	0	0	0
			80	47	16	16	1			
3	S	10	Total	C	N	O	S	0	0	0
			80	47	16	16	1			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



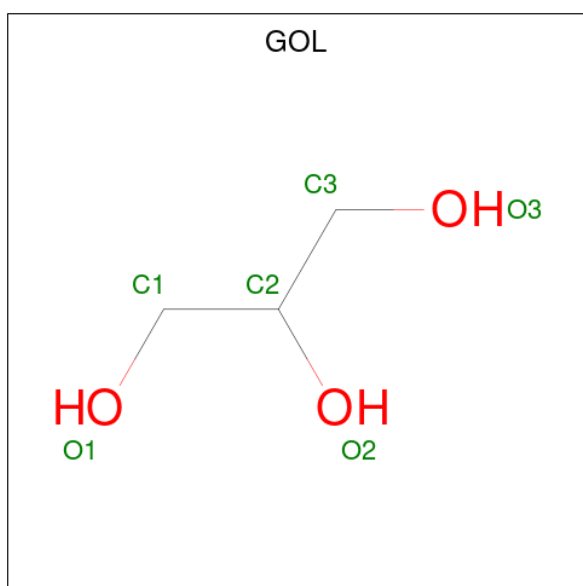
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		
5	G	1	Total	C	O	0	0
			6	3	3		
5	G	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		

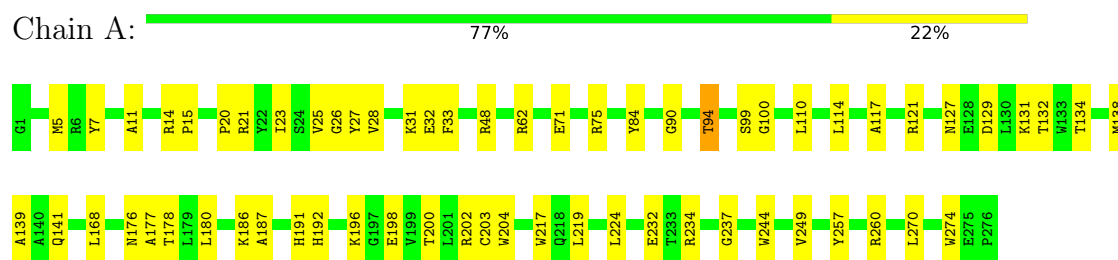
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	48	Total	O	0	0
			48	48		
6	B	23	Total	O	0	0
			23	23		
6	C	59	Total	O	0	0
			59	59		
6	D	24	Total	O	0	0
			24	24		
6	E	35	Total	O	0	0
			35	35		
6	F	28	Total	O	0	0
			28	28		
6	G	27	Total	O	0	0
			27	27		
6	H	25	Total	O	0	0
			25	25		
6	P	2	Total	O	0	0
			2	2		
6	Q	2	Total	O	0	0
			2	2		

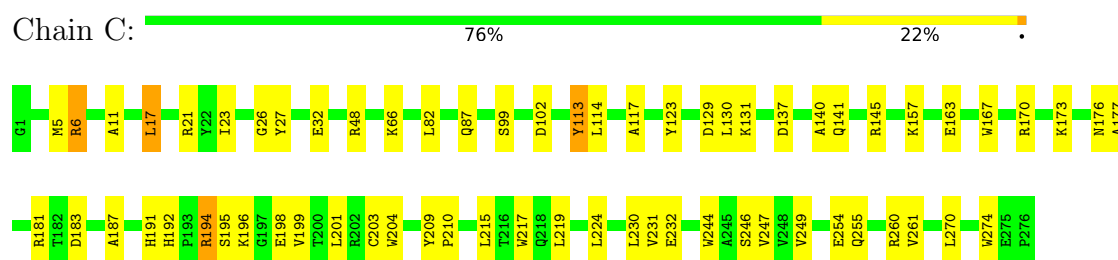
3 Residue-property plots

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.

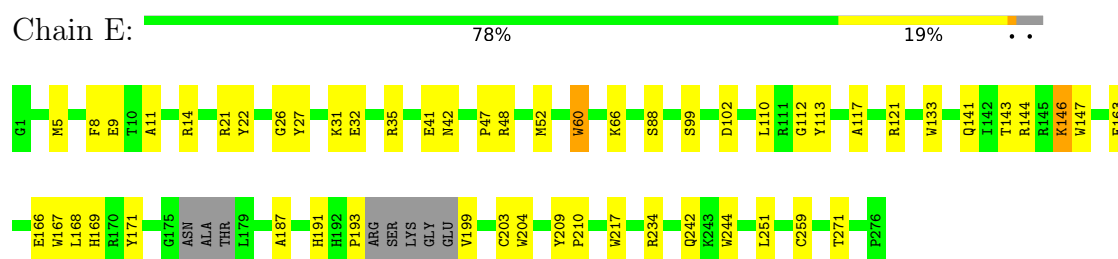
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



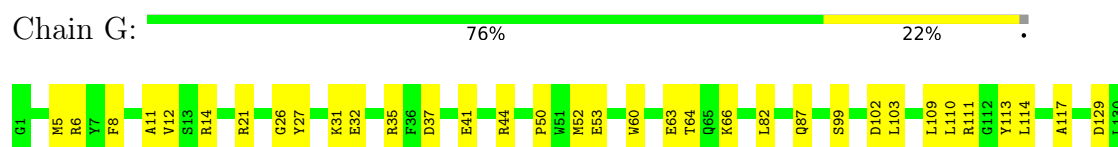
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

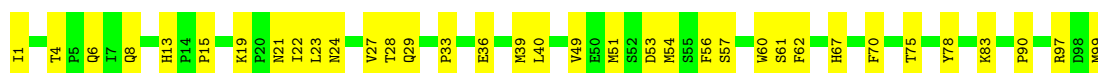




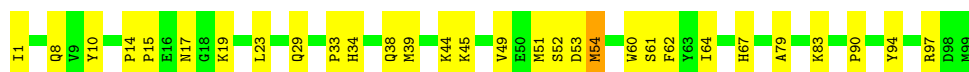
- Molecule 2: Beta-2-microglobulin



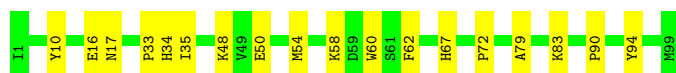
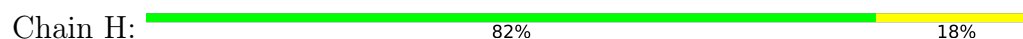
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



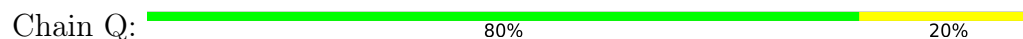
- Molecule 2: Beta-2-microglobulin



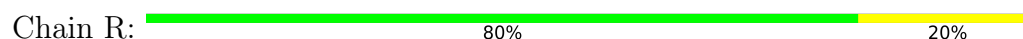
- Molecule 3: Pre-glycoprotein polypeptide GP complex



- Molecule 3: Pre-glycoprotein polypeptide GP complex



- Molecule 3: Pre-glycoprotein polypeptide GP complex





- Molecule 3: Pre-glycoprotein polyprotein GP complex

Chain S:  70% 30%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.50Å 176.30Å 85.60Å 90.00° 119.80° 90.00°	Depositor
Resolution (Å)	19.45 – 2.40 19.45 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.45-2.40) 98.2 (19.45-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.41Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.199 , 0.259 0.200 , 0.259	Depositor DCC
R_{free} test set	4220 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.024 for -h-l,k,h 0.024 for l,k,-h-l 0.478 for h,-k,-h-l 0.027 for -h-l,-k,l 0.028 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12734	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4

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	0.43	0/2313	0.70	0/3144
1	C	0.56	4/2304 (0.2%)	0.71	3/3134 (0.1%)
1	E	0.45	0/2167	0.78	5/2954 (0.2%)
1	G	0.49	2/2220 (0.1%)	0.67	0/3024
2	B	0.39	0/829	0.66	0/1128
2	D	0.41	0/843	0.65	0/1145
2	F	0.45	0/847	0.73	0/1151
2	H	0.49	0/847	0.74	1/1148 (0.1%)
3	P	0.31	0/82	0.72	0/109
3	Q	0.28	0/82	0.73	0/109
3	R	0.34	0/82	0.55	0/109
3	S	0.35	0/82	0.68	0/109
All	All	0.47	6/12698 (0.0%)	0.71	9/17264 (0.1%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	194	ARG	NE-CZ	-9.64	1.22	1.33
1	G	181	ARG	NE-CZ	-9.10	1.23	1.33
1	G	181	ARG	CZ-NH2	-8.91	1.21	1.33
1	C	194	ARG	CZ-NH2	-8.48	1.22	1.33
1	C	113	TYR	CB-CG	-6.06	1.38	1.51

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	146	LYS	CA-CB-CG	8.83	131.75	114.10
1	E	146	LYS	CG-CD-CE	-8.70	91.30	111.30
1	E	60	TRP	CA-CB-CG	-7.29	99.76	113.60
1	C	113	TYR	CB-CA-C	-6.34	98.56	109.65
1	E	146	LYS	CD-CE-NZ	6.14	131.55	111.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2243	0	2102	52	0
1	C	2234	0	2085	54	0
1	E	2098	0	1894	42	1
1	G	2156	0	1956	51	0
2	B	803	0	758	29	0
2	D	814	0	776	33	0
2	F	817	0	779	24	0
2	H	821	0	796	15	0
3	P	80	0	68	1	0
3	Q	80	0	68	2	0
3	R	80	0	68	2	0
3	S	80	0	68	3	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0
4	D	10	0	0	1	0
4	F	15	0	0	0	0
4	G	5	0	0	0	0
4	H	20	0	0	0	0
5	A	6	0	8	3	0
5	B	18	0	24	4	0
5	C	6	0	8	0	0
5	D	24	0	32	4	0
5	E	6	0	8	1	0
5	F	6	0	8	0	0
5	G	12	0	16	4	0
5	H	12	0	16	1	0
6	A	48	0	0	2	0
6	B	23	0	0	1	0
6	C	59	0	0	2	1
6	D	24	0	0	0	0
6	E	35	0	0	0	0
6	F	28	0	0	0	0
6	G	27	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	25	0	0	0	0
6	P	2	0	0	0	0
6	Q	2	0	0	0	0
All	All	12734	0	11538	267	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 11.

The worst 5 of 267 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:D:21:ASN:HD22	2:D:22:ILE:H	1.13	0.95
2:F:17:ASN:ND2	2:F:97:ARG:HH12	1.68	0.92
1:A:20:PRO:O	6:A:401:HOH:O	1.94	0.85
1:E:187:ALA:HA	1:E:204:TRP:O	1.81	0.80
1:G:21:ARG:HH12	5:G:303:GOL:H2	1.45	0.80

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:E:88:SER:N	6:C:401:HOH:O[2_555]	2.18	0.02

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	275/276 (100%)	271 (98%)	4 (2%)	0	100	100
1	C	275/276 (100%)	268 (98%)	7 (2%)	0	100	100
1	E	264/276 (96%)	256 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	269/276 (98%)	265 (98%)	4 (2%)	0	100	100
2	B	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
2	D	98/99 (99%)	97 (99%)	1 (1%)	0	100	100
2	F	98/99 (99%)	97 (99%)	1 (1%)	0	100	100
2	H	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
3	P	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
3	Q	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
3	R	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
3	S	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
All	All	1505/1540 (98%)	1472 (98%)	33 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	227/234 (97%)	224 (99%)	3 (1%)	61	80
1	C	225/234 (96%)	224 (100%)	1 (0%)	84	92
1	E	200/234 (86%)	198 (99%)	2 (1%)	68	84
1	G	209/234 (89%)	209 (100%)	0	100	100
2	B	90/94 (96%)	89 (99%)	1 (1%)	65	82
2	D	91/94 (97%)	89 (98%)	2 (2%)	45	67
2	F	92/94 (98%)	91 (99%)	1 (1%)	65	82
2	H	94/94 (100%)	94 (100%)	0	100	100
3	P	9/9 (100%)	9 (100%)	0	100	100
3	Q	9/9 (100%)	9 (100%)	0	100	100
3	R	9/9 (100%)	9 (100%)	0	100	100
3	S	9/9 (100%)	9 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1264/1348 (94%)	1254 (99%)	10 (1%)	73 86

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	251	LEU
1	E	271	THR
2	F	54	MET
2	B	75	THR
1	C	17	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	34	HIS
2	H	67	HIS
3	R	7	HIS
1	C	96	GLN
1	C	87	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](#)

28 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	$\# Z > 2$
5	GOL	B	103	-	5,5,5	0.34	0	5,5,5	0.73	0
4	SO4	F	101	-	4,4,4	0.23	0	6,6,6	0.18	0
5	GOL	G	303	-	5,5,5	0.31	0	5,5,5	0.46	0
5	GOL	D	104	-	5,5,5	0.35	0	5,5,5	0.27	0
4	SO4	B	101	-	4,4,4	0.43	0	6,6,6	0.23	0
5	GOL	D	106	-	5,5,5	0.36	0	5,5,5	0.30	0
5	GOL	H	105	-	5,5,5	0.37	0	5,5,5	0.39	0
5	GOL	G	302	-	5,5,5	0.41	0	5,5,5	0.55	0
5	GOL	D	103	-	5,5,5	0.41	0	5,5,5	0.73	0
5	GOL	F	104	-	5,5,5	0.43	0	5,5,5	0.52	0
4	SO4	H	101	-	4,4,4	0.25	0	6,6,6	0.17	0
4	SO4	F	102	-	4,4,4	0.27	0	6,6,6	0.13	0
5	GOL	D	105	-	5,5,5	0.40	0	5,5,5	0.65	0
5	GOL	H	106	-	5,5,5	0.36	0	5,5,5	0.48	0
5	GOL	B	104	-	5,5,5	0.47	0	5,5,5	0.32	0
4	SO4	D	101	-	4,4,4	0.23	0	6,6,6	0.17	0
5	GOL	A	302	-	5,5,5	0.54	0	5,5,5	1.04	0
5	GOL	E	301	-	5,5,5	0.33	0	5,5,5	0.33	0
4	SO4	H	103	-	4,4,4	0.21	0	6,6,6	0.18	0
5	GOL	C	301	-	5,5,5	0.34	0	5,5,5	0.52	0
4	SO4	G	301	-	4,4,4	0.25	0	6,6,6	0.05	0
4	SO4	H	102	-	4,4,4	0.23	0	6,6,6	0.12	0
4	SO4	F	103	-	4,4,4	0.24	0	6,6,6	0.15	0
4	SO4	H	104	-	4,4,4	0.25	0	6,6,6	0.12	0
4	SO4	B	102	-	4,4,4	0.24	0	6,6,6	0.21	0
4	SO4	D	102	-	4,4,4	0.25	0	6,6,6	0.17	0
5	GOL	B	105	-	5,5,5	0.57	0	5,5,5	0.68	0
4	SO4	A	301	-	4,4,4	0.25	0	6,6,6	0.18	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
5	GOL	B	104	-	-	3/4/4/4	-
5	GOL	H	106	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	103	-	-	3/4/4/4	-
5	GOL	A	302	-	-	4/4/4/4	-
5	GOL	E	301	-	-	3/4/4/4	-
5	GOL	G	303	-	-	2/4/4/4	-
5	GOL	G	302	-	-	4/4/4/4	-
5	GOL	D	103	-	-	4/4/4/4	-
5	GOL	F	104	-	-	2/4/4/4	-
5	GOL	D	104	-	-	0/4/4/4	-
5	GOL	B	105	-	-	0/4/4/4	-
5	GOL	C	301	-	-	2/4/4/4	-
5	GOL	D	105	-	-	2/4/4/4	-
5	GOL	D	106	-	-	2/4/4/4	-
5	GOL	H	105	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	302	GOL	O1-C1-C2-C3
5	C	301	GOL	O1-C1-C2-O2
5	D	103	GOL	O1-C1-C2-C3
5	D	103	GOL	C1-C2-C3-O3
5	D	105	GOL	O1-C1-C2-C3

There are no ring outliers.

11 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	303	GOL	2	0
5	D	106	GOL	1	0
5	G	302	GOL	2	0
5	D	103	GOL	2	0
5	D	105	GOL	1	0
5	H	106	GOL	1	0
5	B	104	GOL	1	0
5	A	302	GOL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	301	GOL	1	0
4	D	102	SO4	1	0
5	B	105	GOL	3	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	A	276/276 (100%)	-1.41	0	100	100	36, 59, 96, 172	1 (0%)
1	C	276/276 (100%)	-1.42	0	100	100	36, 58, 97, 156	1 (0%)
1	E	268/276 (97%)	-1.24	0	100	100	28, 74, 122, 193	2 (0%)
1	G	273/276 (98%)	-1.22	1 (0%)	88	86	39, 77, 136, 184	0
2	B	99/99 (100%)	-1.48	0	100	100	38, 60, 87, 125	0
2	D	99/99 (100%)	-1.45	0	100	100	38, 60, 93, 149	1 (1%)
2	F	99/99 (100%)	-1.52	0	100	100	35, 53, 82, 105	1 (1%)
2	H	99/99 (100%)	-1.50	0	100	100	37, 54, 84, 108	0
3	P	10/10 (100%)	-1.46	0	100	100	50, 60, 68, 70	0
3	Q	10/10 (100%)	-1.45	0	100	100	50, 61, 74, 79	0
3	R	10/10 (100%)	-1.28	0	100	100	64, 75, 96, 104	0
3	S	10/10 (100%)	-1.36	0	100	100	66, 78, 92, 96	0
All	All	1529/1540 (99%)	-1.37	1 (0%)	92	90	28, 64, 112, 193	6 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	254	GLU	2.3

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 ⓘ

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
4	SO4	A	301	5/5	0.96	0.06	149,149,150,153	0
4	SO4	G	301	5/5	0.97	0.05	133,136,136,139	0
4	SO4	H	104	5/5	0.97	0.04	135,137,139,139	0
4	SO4	F	103	5/5	0.98	0.04	122,122,126,133	0
4	SO4	B	101	5/5	0.98	0.03	125,130,132,134	0
4	SO4	H	103	5/5	0.98	0.05	87,94,100,101	5
4	SO4	D	102	5/5	0.98	0.04	115,119,121,122	5
5	GOL	A	302	6/6	0.98	0.04	48,49,61,64	0
5	GOL	B	104	6/6	0.98	0.06	77,98,105,106	0
5	GOL	G	303	6/6	0.98	0.04	80,85,89,90	0
4	SO4	H	102	5/5	0.99	0.04	93,103,108,109	0
4	SO4	F	101	5/5	0.99	0.04	113,115,119,120	0
4	SO4	F	102	5/5	0.99	0.06	105,112,114,114	0
4	SO4	D	101	5/5	0.99	0.04	113,120,122,125	0
5	GOL	B	103	6/6	0.99	0.05	73,76,78,78	0
4	SO4	B	102	5/5	0.99	0.06	124,128,131,133	5
5	GOL	B	105	6/6	0.99	0.04	61,67,82,91	0
5	GOL	C	301	6/6	0.99	0.04	70,75,79,89	0
5	GOL	D	105	6/6	0.99	0.06	65,84,86,89	0
5	GOL	D	106	6/6	0.99	0.04	83,92,95,103	0
5	GOL	E	301	6/6	0.99	0.04	49,53,59,64	0
5	GOL	F	104	6/6	0.99	0.04	56,72,78,78	0
5	GOL	G	302	6/6	0.99	0.04	61,65,67,80	0
4	SO4	H	101	5/5	0.99	0.04	100,106,113,114	0
5	GOL	H	105	6/6	0.99	0.04	73,86,89,91	0
5	GOL	H	106	6/6	0.99	0.04	90,96,100,104	0
5	GOL	D	103	6/6	1.00	0.02	42,54,58,65	0
5	GOL	D	104	6/6	1.00	0.04	62,90,98,99	0

6.5 Other polymers ⓘ

There are no such residues in this entry.