



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:24 AM UTC

PDB ID : 4D9Q / pdb_00004d9q
Title : Inhibiting Alternative Pathway Complement Activation by Targeting the Exosite on Factor D
Authors : Murray, J.M.; Wiesmann, C.
Deposited on : 2012-01-11
Resolution : 2.28 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	:	4-5-2 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

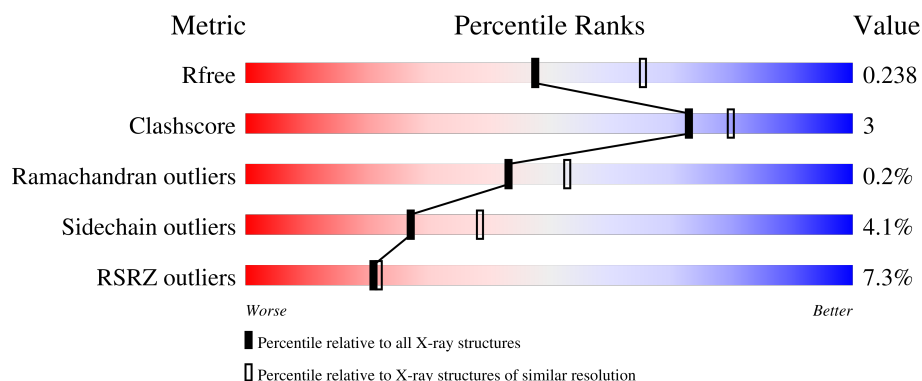
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	228	5% 89% 9% .
1	B	228	18% 85% 14% .
2	D	213	3% 86% 13% .
2	L	213	7% 91% 9% .
3	E	217	6% 88% 7% ..

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Mol	Chain	Length	Quality of chain
3	H	217	 A horizontal bar chart showing the quality of chain H. The bar is divided into three segments: a red segment at the beginning labeled '5%', a large green segment in the middle labeled '88%', and a yellow segment at the end labeled '11%'. A small black dot is located at the far right end of the bar.

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10620 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 Factor D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	2	0
			1726	1063	330	322	11			
1	B	228	Total	C	N	O	S	0	2	0
			1726	1063	330	322	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	VAL	LEU	conflict	UNP F6YBP7
B	47	VAL	LEU	conflict	UNP F6YBP7

- Molecule 2 is a protein called Anti-Factor D, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	213	Total	C	N	O	S	0	0	0
			1624	1011	270	338	5			
2	L	213	Total	C	N	O	S	0	0	0
			1624	1011	270	338	5			

- Molecule 3 is a protein called Anti-Factor D, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	212	Total	C	N	O	S	0	0	0
			1592	1009	260	317	6			
3	H	216	Total	C	N	O	S	0	0	0
			1618	1024	265	323	6			

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

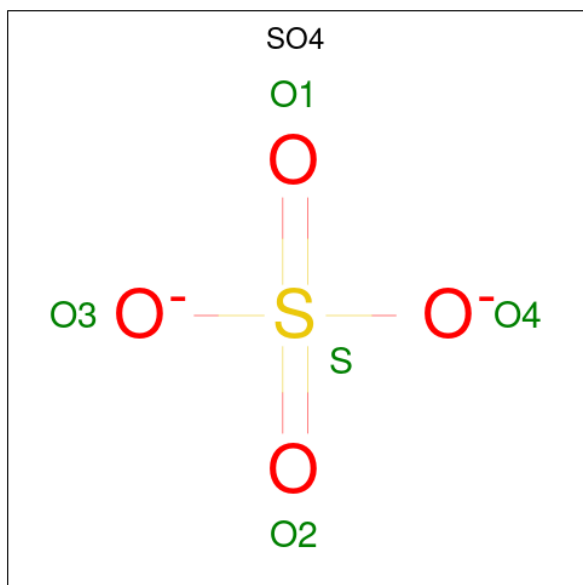
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	B	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	2	Total	Zn	0	0
			2	2		
5	H	1	Total	Zn	0	0
			1	1		
5	L	2	Total	Zn	0	0
			2	2		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	124	Total	O	0	0
			124	124		
7	B	69	Total	O	0	0
			69	69		
7	D	133	Total	O	0	0
			133	133		

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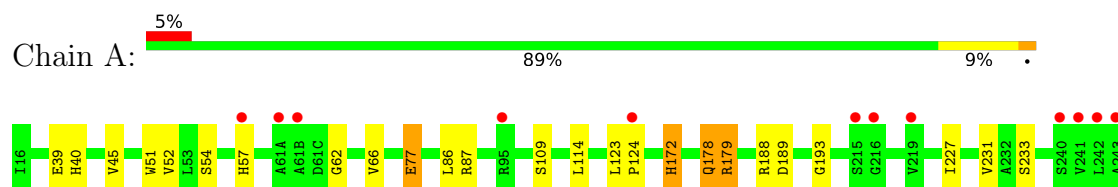
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	113	Total 113	O 113	0	0
7	H	66	Total 66	O 66	0	0
7	L	123	Total 123	O 123	0	0

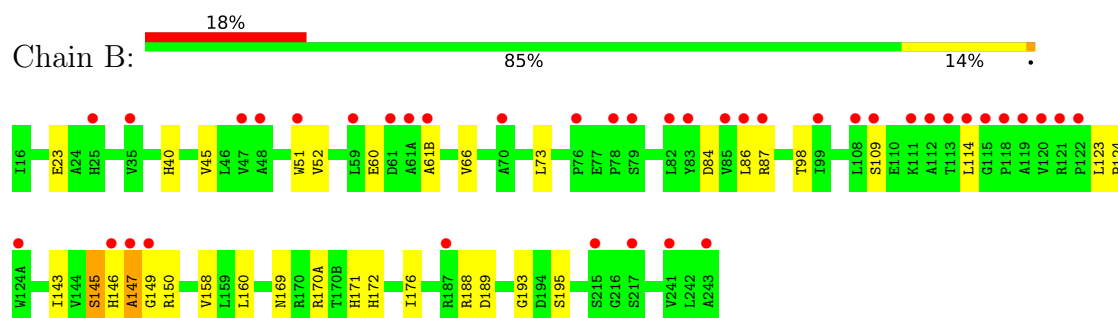
3 Residue-property plots

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.

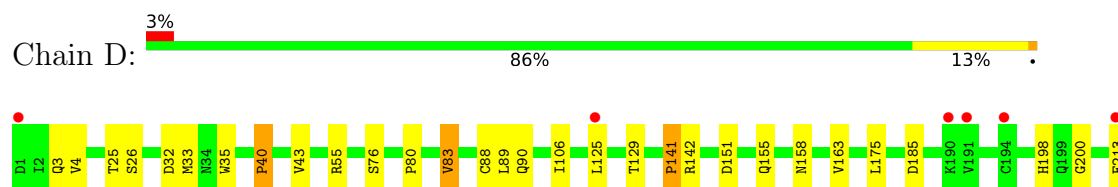
- Molecule 1: Factor D



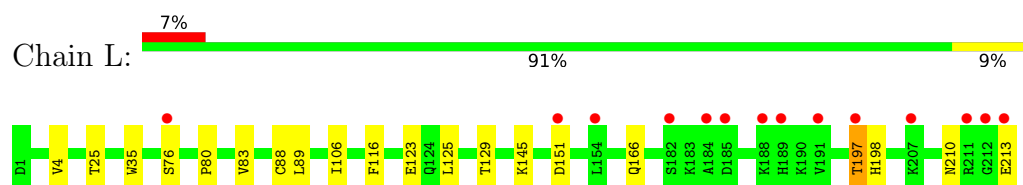
- Molecule 1: Factor D



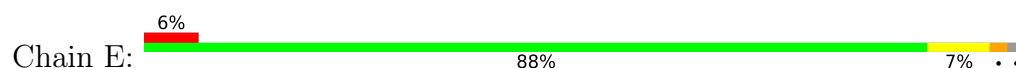
- Molecule 2: Anti-Factor D, light chain

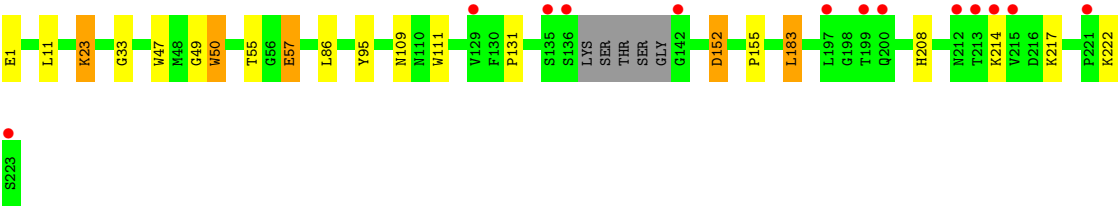


- Molecule 2: Anti-Factor D, light chain

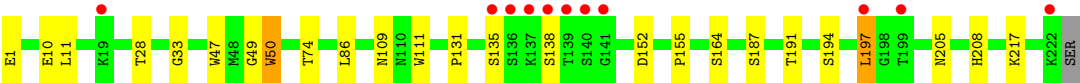
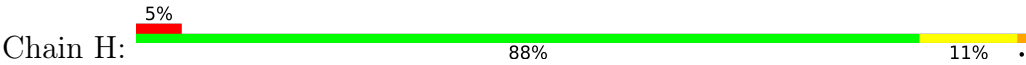


- Molecule 3: Anti-Factor D, heavy chain





● Molecule 3: Anti-Factor D, heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	182.33Å 80.76Å 142.63Å 90.00° 107.19° 90.00°	Depositor
Resolution (Å)	33.38 – 2.28 33.38 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.6 (33.38-2.28) 99.7 (33.38-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.29Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.11.2, BUSTER 2.11.2	Depositor
R, R_{free}	0.189 , 0.230 0.199 , 0.238	Depositor DCC
R_{free} test set	4589 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10620	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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, ZN

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	0.96	4/1771 (0.2%)	1.17	6/2406 (0.2%)
1	B	0.96	5/1771 (0.3%)	1.18	2/2406 (0.1%)
2	D	0.86	0/1656	1.11	6/2252 (0.3%)
2	L	0.84	0/1656	1.10	4/2252 (0.2%)
3	E	0.81	0/1631	1.10	1/2224 (0.0%)
3	H	0.76	0/1658	1.11	2/2261 (0.1%)
All	All	0.87	9/10143 (0.1%)	1.13	21/13801 (0.2%)

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	B	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	171	HIS	CG-ND1	-7.16	1.30	1.38
1	B	172	HIS	CD2-NE2	-6.73	1.30	1.37
1	B	172	HIS	CG-ND1	-6.68	1.30	1.38
1	A	172	HIS	CD2-NE2	-6.31	1.30	1.37
1	A	188	ARG	C-O	-5.77	1.17	1.23
1	B	170(A)	ARG	C-O	-5.66	1.17	1.24
1	B	171	HIS	CD2-NE2	-5.31	1.32	1.37
1	A	172	HIS	CG-ND1	-5.16	1.32	1.38
1	A	54	SER	C-O	-5.14	1.19	1.24

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	76	SER	N-CA-C	7.66	120.71	111.82
2	D	76	SER	N-CA-C	6.70	119.59	111.82
1	A	62	GLY	N-CA-C	6.52	119.50	112.33
1	B	189	ASP	CA-CB-CG	6.44	119.04	112.60
3	H	191	THR	CB-CA-C	6.38	120.75	109.72
1	A	77	GLU	CB-CA-C	-5.98	101.79	109.92
2	D	83	VAL	N-CA-CB	5.94	117.32	110.49
2	D	151	ASP	CA-CB-CG	5.81	118.41	112.60
1	A	189	ASP	CA-CB-CG	5.81	118.41	112.60
2	D	141	PRO	CA-C-N	5.37	127.74	120.38
2	D	141	PRO	C-N-CA	5.37	127.74	120.38
3	E	152	ASP	N-CA-C	5.34	117.16	110.91
2	L	151	ASP	CA-CB-CG	5.33	117.93	112.60
1	B	51	TRP	N-CA-C	5.23	117.42	108.90
2	D	40	PRO	N-CA-C	5.18	123.13	112.47
1	A	51	TRP	N-CA-C	5.06	117.14	108.90
1	A	231	VAL	CA-C-N	5.04	127.29	120.38
1	A	231	VAL	C-N-CA	5.04	127.29	120.38
2	L	198	HIS	CA-C-N	5.02	127.26	120.38
2	L	198	HIS	C-N-CA	5.02	127.26	120.38
3	H	152	ASP	N-CA-C	5.01	116.77	110.91

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	147	ALA	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	1726	0	1709	8	0
1	B	1726	0	1709	10	0
2	D	1624	0	1582	15	0
2	L	1624	0	1582	10	0
3	E	1592	0	1550	11	0
3	H	1618	0	1579	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	12	0	16	0	0
4	B	18	0	24	0	0
4	D	12	0	16	1	0
4	E	12	0	16	0	0
4	H	6	0	8	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	D	2	0	0	0	0
5	H	1	0	0	0	0
5	L	2	0	0	0	0
6	A	10	0	0	0	0
6	B	5	0	0	0	0
7	A	124	0	0	1	0
7	B	69	0	0	0	0
7	D	133	0	0	1	0
7	E	113	0	0	1	0
7	H	66	0	0	0	0
7	L	123	0	0	0	0
All	All	10620	0	9791	63	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 3.

All (63) 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:155:GLN:HE21	2:D:158:ASN:HD21	1.31	0.75
1:B:169:ASN:HD21	1:B:176:ILE:H	1.36	0.73
1:A:77:GLU:HG3	7:A:522:HOH:O	1.90	0.71
3:E:109:ASN:HD21	3:E:111:TRP:HE1	1.41	0.69
1:A:123:LEU:HD12	1:A:124:PRO:HD2	1.76	0.68
3:E:55:THR:OG1	3:E:57:GLU:HG2	1.93	0.68
1:B:123:LEU:HD12	1:B:124:PRO:HD2	1.77	0.67
2:L:145:LYS:HB3	2:L:197:THR:HG23	1.77	0.66
3:H:109:ASN:HD21	3:H:111:TRP:HE1	1.41	0.65
3:H:135:SER:H	3:H:138:SER:HB3	1.61	0.65
3:H:164:SER:H	3:H:205:ASN:HD21	1.46	0.64
2:L:83:VAL:HG23	2:L:106:ILE:HD12	1.86	0.58
1:B:143:ILE:HD12	1:B:146:HIS:O	2.06	0.56
1:A:86:LEU:HD13	1:A:109:SER:HA	1.89	0.55
2:D:83:VAL:HG13	2:D:106:ILE:HD12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:VAL:HG21	1:A:66:VAL:HG11	1.89	0.55
3:H:138:SER:HA	2:L:116:PHE:HD1	1.72	0.54
1:B:52:VAL:HG21	1:B:66:VAL:HG11	1.89	0.53
3:E:33:GLY:HA3	3:E:50:TRP:CZ3	2.44	0.52
1:B:158:VAL:HG21	1:B:188:ARG:HG3	1.90	0.51
3:E:152:ASP:HB3	3:E:183:LEU:HD23	1.93	0.51
1:B:146:HIS:CG	1:B:147:ALA:N	2.79	0.51
3:H:11:LEU:HB2	3:H:155:PRO:HG3	1.91	0.51
1:B:160:LEU:CD2	1:B:188:ARG:HB3	2.41	0.51
2:D:55:ARG:NH1	7:D:402:HOH:O	2.33	0.51
2:D:141:PRO:O	2:D:198:HIS:HE1	1.94	0.51
3:H:47:TRP:CZ3	3:H:49:GLY:HA2	2.47	0.50
2:D:198:HIS:CD2	2:D:200:GLY:H	2.31	0.49
3:H:33:GLY:HA3	3:H:50:TRP:CZ3	2.47	0.49
2:L:80:PRO:HA	2:L:106:ILE:CD1	2.44	0.48
2:L:83:VAL:HG11	2:L:166:GLN:HB3	1.94	0.48
2:D:80:PRO:HA	2:D:106:ILE:CD1	2.44	0.48
1:A:172:HIS:CE1	1:A:227:ILE:HD11	2.49	0.48
3:H:194:SER:O	3:H:197:LEU:HD22	2.14	0.47
2:L:80:PRO:HA	2:L:106:ILE:HD13	1.97	0.47
3:E:47:TRP:CZ3	3:E:49:GLY:HA2	2.50	0.47
3:E:11:LEU:HB2	3:E:155:PRO:HG3	1.97	0.46
3:H:131:PRO:HD3	3:H:217:LYS:HE2	1.98	0.46
2:L:35:TRP:CZ3	2:L:88:CYS:HB3	2.51	0.45
1:B:146:HIS:CD2	1:B:147:ALA:N	2.85	0.44
2:D:80:PRO:HA	2:D:106:ILE:HD13	2.00	0.44
2:L:4:VAL:HG22	2:L:25:THR:HG22	1.98	0.43
3:E:131:PRO:HD3	3:E:217:LYS:HE2	2.00	0.43
2:D:142:ARG:HD2	2:D:163:VAL:HG11	2.00	0.43
1:A:40:HIS:HE1	1:A:193:GLY:O	2.02	0.43
2:D:163:VAL:HG22	2:D:175:LEU:HD12	2.01	0.43
2:D:3:GLN:HB3	2:D:26:SER:HB3	2.00	0.43
1:B:145:SER:O	1:B:149:GLY:HA3	2.20	0.42
2:D:33:MET:SD	2:D:88:CYS:HB2	2.60	0.42
2:L:210:ASN:HB2	2:L:213:GLU:HB2	2.02	0.42
3:H:155:PRO:O	3:H:208:HIS:HE1	2.03	0.42
2:D:35:TRP:CZ3	2:D:88:CYS:HB3	2.55	0.41
3:E:155:PRO:O	3:E:208:HIS:HE1	2.04	0.41
2:D:32:ASP:OD1	4:D:301:GOL:O1	2.39	0.41
1:A:178:GLN:HE22	3:H:28:THR:HG21	1.86	0.41
3:E:23:LYS:NZ	7:E:469:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:109:ASN:HD21	3:H:111:TRP:NE1	2.11	0.41
1:B:40:HIS:HE1	1:B:193:GLY:O	2.04	0.41
3:E:109:ASN:HD21	3:E:111:TRP:NE1	2.13	0.41
3:H:217:LYS:NZ	2:L:123:GLU:OE2	2.51	0.41
2:D:43:VAL:HG22	3:E:95:TYR:HE1	1.86	0.40
1:A:179:ARG:HD2	1:A:233[A]:SER:HB3	2.03	0.40
2:D:4:VAL:HG22	2:D:25:THR:HG22	2.03	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	A	228/228 (100%)	222 (97%)	6 (3%)	0	100	100
1	B	228/228 (100%)	217 (95%)	10 (4%)	1 (0%)	30	36
2	D	211/213 (99%)	204 (97%)	6 (3%)	1 (0%)	24	29
2	L	211/213 (99%)	205 (97%)	6 (3%)	0	100	100
3	E	208/217 (96%)	201 (97%)	7 (3%)	0	100	100
3	H	214/217 (99%)	205 (96%)	9 (4%)	0	100	100
All	All	1300/1316 (99%)	1254 (96%)	44 (3%)	2 (0%)	43	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	61(B)	ALA
2	D	40	PRO

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	186/184 (101%)	179 (96%)	7 (4%)	29	42
1	B	186/184 (101%)	173 (93%)	13 (7%)	14	17
2	D	190/190 (100%)	184 (97%)	6 (3%)	34	49
2	L	190/190 (100%)	186 (98%)	4 (2%)	47	63
3	E	179/183 (98%)	171 (96%)	8 (4%)	24	35
3	H	182/183 (100%)	175 (96%)	7 (4%)	29	42
All	All	1113/1114 (100%)	1068 (96%)	45 (4%)	27	40

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	A	45	VAL
1	A	57	HIS
1	A	87	ARG
1	A	114	LEU
1	A	178	GLN
1	A	179	ARG
1	B	23	GLU
1	B	45	VAL
1	B	60	GLU
1	B	73	LEU
1	B	84	ASP
1	B	86	LEU
1	B	87	ARG
1	B	98	THR
1	B	109	SER
1	B	114	LEU
1	B	145	SER
1	B	150	ARG
1	B	195	SER
2	D	89	LEU
2	D	90	GLN

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Mol	Chain	Res	Type
2	D	125	LEU
2	D	129	THR
2	D	185	ASP
2	D	213	GLU
3	E	1	GLU
3	E	23	LYS
3	E	50	TRP
3	E	57	GLU
3	E	86	LEU
3	E	183	LEU
3	E	214	LYS
3	E	222	LYS
3	H	1	GLU
3	H	10	GLU
3	H	50	TRP
3	H	74	THR
3	H	86	LEU
3	H	187	SER
3	H	197	LEU
2	L	89	LEU
2	L	125	LEU
2	L	129	THR
2	L	197	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	40	HIS
1	A	107	GLN
1	A	156	GLN
1	A	157	HIS
1	A	178	GLN
1	B	34	GLN
1	B	37	ASN
1	B	40	HIS
1	B	157	HIS
1	B	169	ASN
2	D	37	GLN
2	D	38	GLN
2	D	52	ASN
2	D	79	GLN

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Mol	Chain	Res	Type
2	D	90	GLN
2	D	137	ASN
2	D	155	GLN
2	D	198	HIS
2	D	199	GLN
3	E	35	ASN
3	E	39	GLN
3	E	82	GLN
3	E	109	ASN
3	E	179	GLN
3	E	207	ASN
3	E	208	HIS
3	H	31	ASN
3	H	35	ASN
3	H	43	GLN
3	H	109	ASN
3	H	179	GLN
3	H	205	ASN
3	H	208	HIS
2	L	52	ASN
2	L	79	GLN
2	L	137	ASN
2	L	199	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 7 are monoatomic - leaving 13 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
4	GOL	E	301	-	5,5,5	0.18	0	5,5,5	0.57	0
4	GOL	B	303	-	5,5,5	0.13	0	5,5,5	0.50	0
4	GOL	H	301	-	5,5,5	0.15	0	5,5,5	0.46	0
4	GOL	B	302	-	5,5,5	0.16	0	5,5,5	0.28	0
6	SO4	B	305	-	4,4,4	0.26	0	6,6,6	0.24	0
4	GOL	E	302	-	5,5,5	0.12	0	5,5,5	0.27	0
4	GOL	B	301	-	5,5,5	0.11	0	5,5,5	0.26	0
6	SO4	A	304	-	4,4,4	0.33	0	6,6,6	0.24	0
4	GOL	A	301	-	5,5,5	0.26	0	5,5,5	0.50	0
4	GOL	A	302	-	5,5,5	0.09	0	5,5,5	0.37	0
4	GOL	D	302	-	5,5,5	0.23	0	5,5,5	0.54	0
6	SO4	A	305	-	4,4,4	0.28	0	6,6,6	0.13	0
4	GOL	D	301	-	5,5,5	0.25	0	5,5,5	0.90	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	E	301	-	-	4/4/4/4	-
4	GOL	B	303	-	-	1/4/4/4	-
4	GOL	H	301	-	-	2/4/4/4	-
4	GOL	B	302	-	-	0/4/4/4	-
4	GOL	E	302	-	-	1/4/4/4	-
4	GOL	B	301	-	-	0/4/4/4	-
4	GOL	A	301	-	-	1/4/4/4	-
4	GOL	A	302	-	-	1/4/4/4	-
4	GOL	D	302	-	-	0/4/4/4	-
4	GOL	D	301	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	301	GOL	C1-C2-C3-O3
4	H	301	GOL	C1-C2-C3-O3
4	E	301	GOL	C1-C2-C3-O3
4	D	301	GOL	O2-C2-C3-O3
4	H	301	GOL	O2-C2-C3-O3
4	D	301	GOL	O1-C1-C2-O2
4	E	301	GOL	O2-C2-C3-O3
4	E	301	GOL	O1-C1-C2-O2
4	E	302	GOL	O1-C1-C2-O2
4	A	301	GOL	O1-C1-C2-C3
4	B	303	GOL	O1-C1-C2-C3
4	A	302	GOL	C1-C2-C3-O3
4	E	301	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	D	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, 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	228/228 (100%)	0.28	12 (5%) 32 33	28, 40, 73, 99	2 (0%)
1	B	228/228 (100%)	0.98	40 (17%) 4 4	24, 53, 86, 98	2 (0%)
2	D	213/213 (100%)	0.24	6 (2%) 55 56	22, 40, 71, 105	0
2	L	213/213 (100%)	0.33	14 (6%) 24 25	25, 42, 75, 114	0
3	E	212/217 (97%)	0.23	13 (6%) 27 28	24, 43, 74, 109	0
3	H	216/217 (99%)	0.57	11 (5%) 33 34	25, 51, 80, 114	0
All	All	1310/1316 (99%)	0.44	96 (7%) 21 22	22, 46, 79, 114	4 (0%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	61(A)	ALA	6.2
3	H	137	LYS	6.0
3	H	138	SER	5.5
1	B	146	HIS	5.1
3	H	139	THR	5.0
1	A	219	VAL	4.9
1	B	78	PRO	4.9
3	H	136	SER	4.8
1	B	61(B)	ALA	4.5
1	B	120	VAL	4.2
3	E	223	SER	4.1
3	H	141	GLY	4.1
1	B	48	ALA	3.9
1	B	187	ARG	3.8
1	A	242	LEU	3.8
2	L	184	ALA	3.7
3	E	136	SER	3.7
3	H	140	SER	3.7
1	B	114	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
2	L	188	LYS	3.5
3	E	199	THR	3.5
1	A	243	ALA	3.4
1	B	59	LEU	3.4
1	B	215	SER	3.3
1	A	216	GLY	3.3
1	B	112	ALA	3.3
1	B	147	ALA	3.2
1	B	70	ALA	3.1
2	D	191	VAL	3.1
3	H	222	LYS	3.0
2	D	213	GLU	3.0
1	B	243	ALA	2.9
2	D	1	ASP	2.9
1	B	118	PRO	2.9
1	B	82	LEU	2.9
1	B	121	ARG	2.9
2	L	151	ASP	2.9
1	B	119	ALA	2.9
2	L	191	VAL	2.8
1	B	113	THR	2.8
1	A	241	VAL	2.7
2	L	212	GLY	2.7
1	B	111	LYS	2.7
1	B	86	LEU	2.7
2	L	189	HIS	2.6
1	B	47	VAL	2.6
1	B	76	PRO	2.6
3	H	135	SER	2.6
1	B	109	SER	2.5
1	B	87	ARG	2.5
1	A	57	HIS	2.5
3	H	199	THR	2.5
2	L	76	SER	2.5
1	A	95	ARG	2.5
3	E	221	PRO	2.5
1	A	215	SER	2.4
1	B	35	VAL	2.4
1	B	85	VAL	2.4
1	B	99	ILE	2.4
1	A	61(B)	ALA	2.4
1	B	79	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	124	PRO	2.3
2	D	125	LEU	2.3
3	E	200	GLN	2.3
2	L	185	ASP	2.3
1	B	241	VAL	2.3
1	B	83	TYR	2.3
1	B	61	ASP	2.3
2	D	194	CYS	2.2
2	L	197	THR	2.2
2	D	190	LYS	2.2
2	L	211	ARG	2.2
2	L	213	GLU	2.2
3	H	197	LEU	2.2
3	E	213	THR	2.2
1	B	51	TRP	2.2
2	L	154	LEU	2.2
3	E	212	ASN	2.2
3	H	19	LYS	2.2
3	E	197	LEU	2.1
3	E	214	LYS	2.1
1	B	115	GLY	2.1
2	L	207	LYS	2.1
3	E	215	VAL	2.1
1	B	217	SER	2.1
2	L	182	SER	2.1
3	E	135	SER	2.1
1	B	122	PRO	2.1
3	E	142	GLY	2.1
1	A	240[A]	SER	2.0
1	B	25	HIS	2.0
3	E	129	VAL	2.0
1	B	149	GLY	2.0
1	B	124(A)	TRP	2.0
1	A	61(A)	ALA	2.0
1	B	108	LEU	2.0

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	GOL	D	302	6/6	0.74	0.20	55,62,66,69	0
4	GOL	A	302	6/6	0.75	0.26	76,77,78,79	0
4	GOL	D	301	6/6	0.78	0.18	38,51,52,54	0
4	GOL	B	303	6/6	0.78	0.17	64,69,70,73	0
4	GOL	H	301	6/6	0.79	0.21	59,62,63,64	0
6	SO4	A	305	5/5	0.82	0.26	127,127,128,129	0
4	GOL	E	301	6/6	0.83	0.19	44,60,65,65	0
4	GOL	E	302	6/6	0.86	0.17	49,57,60,62	0
5	ZN	L	302	1/1	0.88	0.12	96,96,96,96	0
4	GOL	B	302	6/6	0.88	0.16	58,64,68,70	0
6	SO4	B	305	5/5	0.89	0.09	82,84,84,87	0
5	ZN	D	304	1/1	0.90	0.10	83,83,83,83	0
5	ZN	A	303	1/1	0.92	0.14	124,124,124,124	0
5	ZN	L	301	1/1	0.96	0.11	41,41,41,41	0
4	GOL	A	301	6/6	0.96	0.07	32,32,33,34	0
6	SO4	A	304	5/5	0.97	0.10	53,53,53,57	0
4	GOL	B	301	6/6	0.97	0.07	30,31,34,35	0
5	ZN	H	302	1/1	0.97	0.07	73,73,73,73	0
5	ZN	D	303	1/1	0.98	0.08	33,33,33,33	0
5	ZN	B	304	1/1	0.98	0.03	36,36,36,36	0

6.5 Other polymers ⓘ

There are no such residues in this entry.