



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:39 AM UTC

PDB ID : 3ROL / pdb_00003rol
Title : Murine class I major histocompatibility complex H-2Kb in complex with post-translationally modified LCMV-derived gp34-41 peptide, comprising a nitrotyrosine at position 3
Authors : Madhurantakam, C.; Duru, A.D.; Leong, C.; Sandalova, T.; Webb, J.R.; Achour, A.
Deposited on : 2011-04-26
Resolution : 2.60 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:

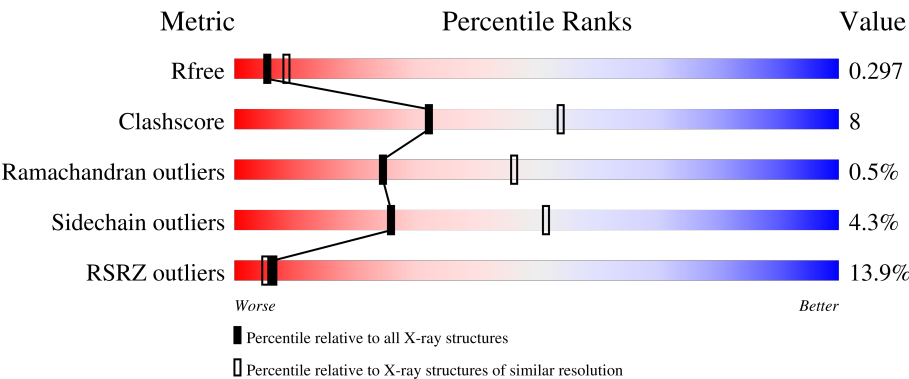
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	275	11% 81%16%..
1	C	275	18% 79%18%..
2	B	99	11% 85%15%
2	D	99	13% 87%12%.

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Mol	Chain	Length	Quality of chain
3	E	8	
3	F	8	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	MPD	D	277	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6447 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, K-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2195	1384	388	414	9			
1	C	272	Total	C	N	O	S	0	0	0
			2207	1393	389	416	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
			821	524	138	152	7			
2	D	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			

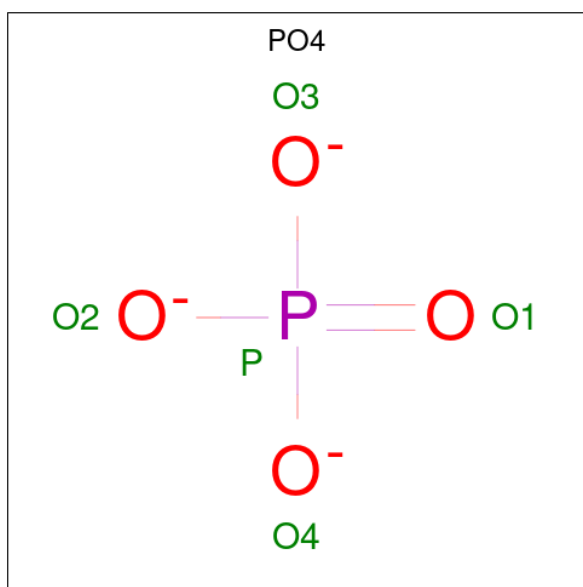
- Molecule 3 is a protein called Pre-glycoprotein polyprotein GP complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	8	Total	C	N	O	S	0	0	0
			66	42	10	13	1			
3	F	8	Total	C	N	O	S	0	0	0
			66	42	10	13	1			

There are 2 discrepancies between the modelled and reference sequences:

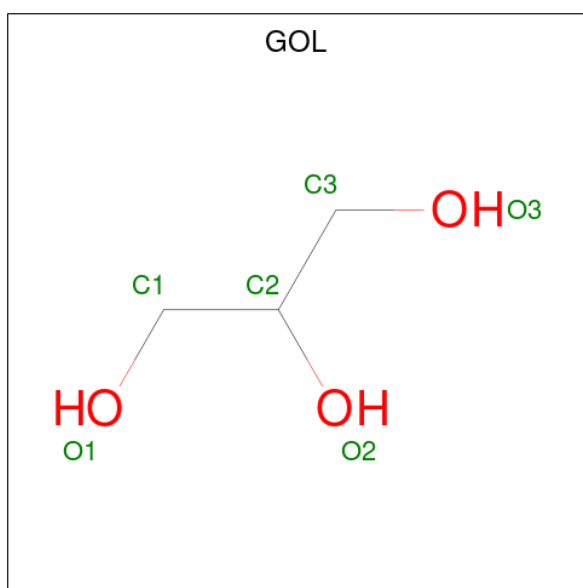
Chain	Residue	Modelled	Actual	Comment	Reference
E	8	MET	CYS	engineered mutation	UNP Q9QDK7
F	8	MET	CYS	engineered mutation	UNP Q9QDK7

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



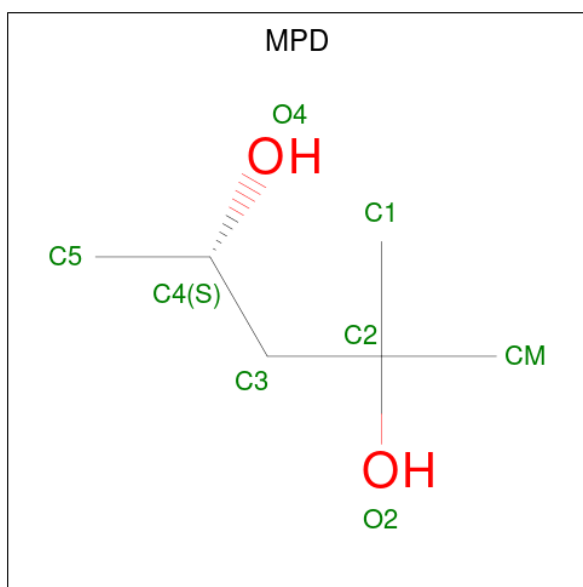
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		

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



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

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			8	6	2		

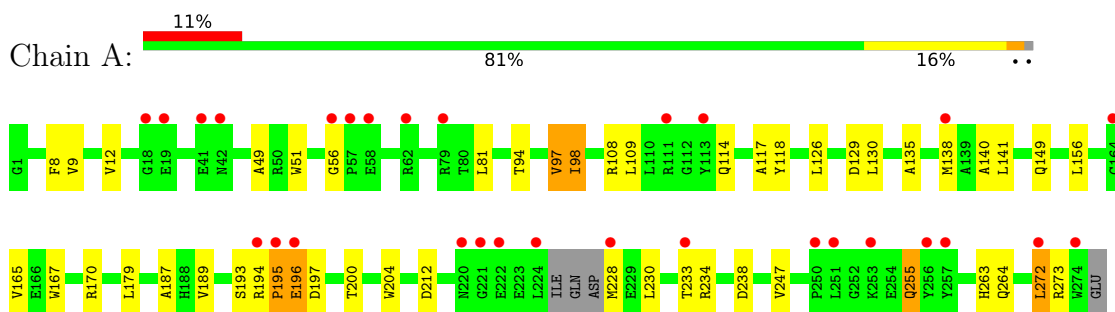
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	72	Total	O	0	0
			72	72		
7	B	23	Total	O	0	0
			23	23		
7	C	93	Total	O	0	0
			93	93		
7	D	55	Total	O	0	0
			55	55		
7	F	4	Total	O	0	0
			4	4		

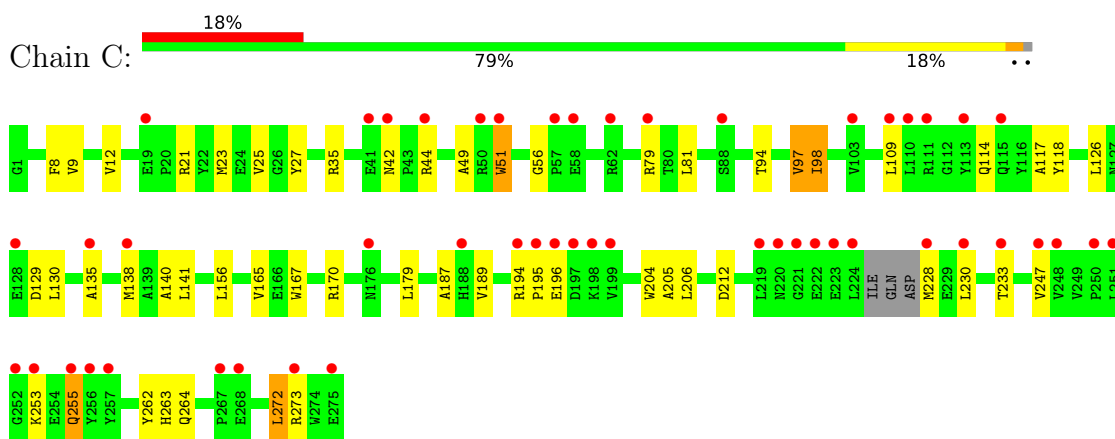
3 Residue-property plots

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.

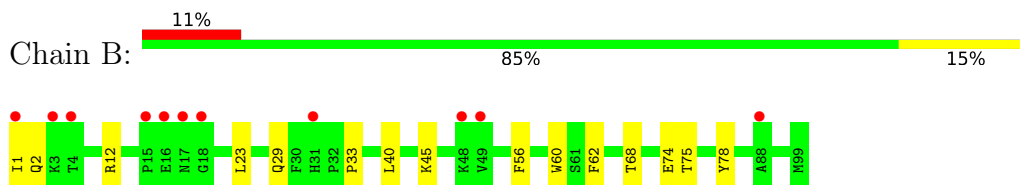
- Molecule 1: H-2 class I histocompatibility antigen, K-B alpha chain



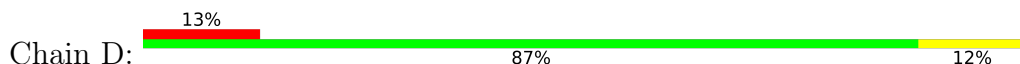
- Molecule 1: H-2 class I histocompatibility antigen, K-B alpha chain

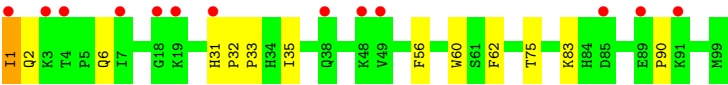


- Molecule 2: Beta-2-microglobulin

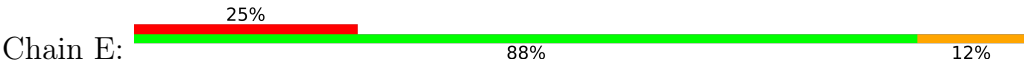


- Molecule 2: Beta-2-microglobulin

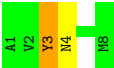
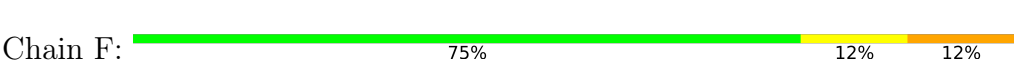




● Molecule 3: Pre-glycoprotein polyprotein GP complex



● Molecule 3: Pre-glycoprotein polyprotein GP complex



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.47Å 88.50Å 119.05Å 90.00° 94.71° 90.00°	Depositor
Resolution (Å)	50.30 – 2.60 50.30 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.30-2.60) 100.0 (50.30-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.27 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.246 , 0.295 0.250 , 0.297	Depositor DCC
R_{free} test set	1654 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	6447	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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 24.62 % 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 3.7039e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, NIY, GOL, PO4

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	0.66	0/2254	0.81	4/3061 (0.1%)
1	C	0.72	0/2267	0.80	2/3079 (0.1%)
2	B	0.70	0/847	0.80	0/1148
2	D	0.74	0/847	0.81	0/1148
3	E	0.61	0/50	0.73	0/65
3	F	0.73	0/50	0.85	0/65
All	All	0.70	0/6315	0.80	6/8566 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	56	GLY	CA-C-N	6.12	127.49	119.84
1	C	56	GLY	C-N-CA	6.12	127.49	119.84
1	A	56	GLY	CA-C-N	5.53	126.76	119.84
1	A	56	GLY	C-N-CA	5.53	126.76	119.84
1	A	234	ARG	CA-C-N	5.26	125.02	119.76
1	A	234	ARG	C-N-CA	5.26	125.02	119.76

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	2195	0	2081	43	0
1	C	2207	0	2090	41	0
2	B	821	0	796	6	0
2	D	821	0	796	10	0
3	E	66	0	59	1	0
3	F	66	0	58	2	0
4	A	5	0	0	0	0
4	C	5	0	0	0	0
5	C	6	0	8	2	0
6	D	8	0	14	6	0
7	A	72	0	0	4	0
7	B	23	0	0	1	0
7	C	93	0	0	6	0
7	D	55	0	0	2	0
7	F	4	0	0	1	0
All	All	6447	0	5902	97	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 8.

All (97) 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:C:79:ARG:HB3	7:C:348:HOH:O	1.41	1.20
1:C:21:ARG:HD3	6:D:277:MPD:H52	1.51	0.92
2:D:35:ILE:HG22	6:D:277:MPD:CM	2.06	0.85
1:A:189:VAL:HG23	1:A:272:LEU:HD12	1.62	0.81
1:C:21:ARG:HD3	6:D:277:MPD:C5	2.10	0.81
1:C:233:THR:HG22	7:C:352:HOH:O	1.85	0.75
2:D:35:ILE:HG22	6:D:277:MPD:HM1	1.69	0.74
1:A:193:SER:C	1:A:194:ARG:HG2	2.11	0.74
1:C:189:VAL:HG23	1:C:272:LEU:HD12	1.69	0.73
2:D:33:PRO:O	6:D:277:MPD:HM1	1.90	0.71
1:C:117:ALA:HB2	2:D:60:TRP:CE2	2.25	0.70
1:A:193:SER:O	1:A:194:ARG:HG2	1.94	0.67
1:A:126:LEU:HD22	1:A:156:LEU:CD2	2.28	0.63
1:A:129:ASP:OD1	1:A:130:LEU:N	2.31	0.62
1:A:108:ARG:NH1	7:A:341:HOH:O	2.26	0.62
1:C:51:TRP:H	1:C:51:TRP:CD1	2.18	0.61
1:C:49:ALA:HB1	1:C:51:TRP:NE1	2.15	0.60
1:C:35:ARG:NH2	7:C:346:HOH:O	2.34	0.59
1:A:49:ALA:HB1	1:A:51:TRP:NE1	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:TRP:CD1	1:A:51:TRP:H	2.20	0.58
1:C:126:LEU:HD22	1:C:156:LEU:CD2	2.34	0.57
1:A:233:THR:HG22	7:A:279:HOH:O	2.04	0.57
1:A:126:LEU:HD22	1:A:156:LEU:HD23	1.85	0.57
1:A:212:ASP:O	1:A:263:HIS:CD2	2.58	0.57
1:A:8:PHE:CE2	1:A:98:ILE:HD11	2.39	0.57
2:B:33:PRO:HB3	2:B:62:PHE:CZ	2.40	0.55
1:C:135:ALA:HB1	1:C:140:ALA:HB3	1.88	0.55
1:C:129:ASP:OD1	1:C:130:LEU:N	2.40	0.55
1:C:212:ASP:O	1:C:263:HIS:CD2	2.60	0.55
1:C:126:LEU:HD22	1:C:156:LEU:HD23	1.88	0.54
2:D:33:PRO:HB3	2:D:62:PHE:CZ	2.42	0.54
1:A:194:ARG:HD3	1:A:200:THR:OG1	2.07	0.54
2:D:35:ILE:CG2	6:D:277:MPD:CM	2.81	0.54
1:C:42:ASN:ND2	7:C:345:HOH:O	2.40	0.54
1:A:9:VAL:HB	1:A:97:VAL:HB	1.90	0.54
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.44	0.53
1:A:108:ARG:HD2	1:C:262:TYR:CG	2.45	0.52
1:C:135:ALA:HB3	1:C:141:LEU:HD12	1.93	0.51
1:C:35:ARG:HH11	5:C:276:GOL:H2	1.76	0.51
1:C:8:PHE:CE2	1:C:98:ILE:HD11	2.46	0.50
1:A:135:ALA:HB3	1:A:141:LEU:HD12	1.93	0.50
2:B:29:GLN:NE2	7:B:101:HOH:O	2.43	0.50
2:D:6:GLN:NE2	7:D:133:HOH:O	2.44	0.50
1:A:255:GLN:O	1:A:273:ARG:CZ	2.60	0.50
1:C:135:ALA:HB1	1:C:140:ALA:CB	2.42	0.50
1:A:135:ALA:HB1	1:A:140:ALA:HB3	1.93	0.49
1:C:255:GLN:O	1:C:273:ARG:CZ	2.61	0.48
1:C:114:GLN:OE1	3:F:3:NIY:O1	2.31	0.48
1:C:9:VAL:HB	1:C:97:VAL:HB	1.95	0.48
1:C:12:VAL:HG22	1:C:94:THR:HG23	1.95	0.48
1:A:238:ASP:OD2	2:B:12:ARG:NE	2.42	0.48
3:E:3:NIY:O2	3:E:3:NIY:OH	2.15	0.48
1:A:194:ARG:O	7:A:286:HOH:O	2.20	0.47
1:A:49:ALA:HB1	1:A:51:TRP:CE2	2.49	0.47
1:A:196:GLU:O	1:A:197:ASP:HB2	2.14	0.47
1:C:109:LEU:HD13	1:C:165:VAL:CG2	2.45	0.47
2:D:1:ILE:N	7:D:117:HOH:O	2.47	0.47
1:A:212:ASP:O	1:A:263:HIS:HD2	1.97	0.47
1:C:187:ALA:HA	1:C:204:TRP:O	2.15	0.47
1:C:205:ALA:O	1:C:206:LEU:HD23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ARG:HD2	1:C:262:TYR:CB	2.46	0.46
1:A:109:LEU:HD13	1:A:165:VAL:CG2	2.45	0.46
1:C:230:LEU:C	1:C:230:LEU:HD12	2.41	0.46
1:A:135:ALA:HB1	1:A:140:ALA:CB	2.45	0.46
2:B:40:LEU:HD23	2:B:45:LYS:HA	1.98	0.46
1:A:187:ALA:HA	1:A:204:TRP:O	2.16	0.46
1:A:51:TRP:CH2	1:A:179:LEU:HD11	2.50	0.45
1:C:49:ALA:HB1	1:C:51:TRP:CE2	2.50	0.45
1:A:109:LEU:HD13	1:A:165:VAL:HG23	1.98	0.45
1:A:194:ARG:CB	1:A:195:PRO:CD	2.95	0.45
3:F:4:ASN:ND2	7:F:27:HOH:O	2.27	0.45
1:C:212:ASP:O	1:C:263:HIS:HD2	1.99	0.45
1:A:149:GLN:OE1	7:A:329:HOH:O	2.21	0.44
1:C:167:TRP:CZ3	1:C:170:ARG:HD3	2.52	0.43
1:C:44:ARG:HD2	7:C:318:HOH:O	2.16	0.43
1:A:230:LEU:HD12	1:A:230:LEU:C	2.44	0.43
1:A:167:TRP:CZ3	1:A:170:ARG:HD3	2.53	0.43
1:C:129:ASP:O	1:C:130:LEU:HB2	2.18	0.43
1:C:23:MET:HE1	5:C:276:GOL:O2	2.17	0.43
1:A:81:LEU:HD23	1:A:118:TYR:CG	2.54	0.43
1:A:135:ALA:CB	1:A:141:LEU:HD12	2.49	0.43
1:A:194:ARG:HB3	1:A:195:PRO:HD2	2.01	0.43
1:C:167:TRP:CE3	1:C:170:ARG:HD3	2.55	0.42
1:A:98:ILE:O	1:A:114:GLN:HA	2.20	0.41
1:A:12:VAL:HG22	1:A:94:THR:HG23	2.02	0.41
2:D:31:HIS:ND1	2:D:32:PRO:HA	2.35	0.41
1:C:51:TRP:CH2	1:C:179:LEU:HD11	2.56	0.41
1:C:81:LEU:HD23	1:C:118:TYR:CG	2.55	0.41
1:C:253:LYS:NZ	7:C:335:HOH:O	2.52	0.41
1:A:167:TRP:CE3	1:A:170:ARG:HD3	2.55	0.41
1:C:25:VAL:HG12	1:C:27:TYR:CE1	2.56	0.41
1:A:98:ILE:O	1:A:98:ILE:HG22	2.21	0.41
1:C:230:LEU:C	1:C:230:LEU:CD1	2.94	0.41
2:D:83:LYS:HG2	2:D:90:PRO:HG3	2.03	0.41
1:A:135:ALA:HB3	1:A:141:LEU:CD1	2.51	0.41
2:B:23:LEU:HD21	2:B:78:TYR:HB3	2.03	0.40
1:A:8:PHE:CZ	1:A:98:ILE:HD11	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	267/275 (97%)	255 (96%)	10 (4%)	2 (1%)	18	38
1	C	268/275 (98%)	257 (96%)	9 (3%)	2 (1%)	18	38
2	B	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
2	D	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
3	E	5/8 (62%)	5 (100%)	0	0	100	100
3	F	5/8 (62%)	5 (100%)	0	0	100	100
All	All	739/764 (97%)	711 (96%)	24 (3%)	4 (0%)	24	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	GLN
1	C	195	PRO
1	C	264	GLN
1	A	195	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	227/233 (97%)	219 (96%)	8 (4%)	32	59
1	C	228/233 (98%)	218 (96%)	10 (4%)	25	50
2	B	94/94 (100%)	88 (94%)	6 (6%)	16	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	94/94 (100%)	90 (96%)	4 (4%)	26	51
3	E	5/5 (100%)	5 (100%)	0	100	100
3	F	5/5 (100%)	5 (100%)	0	100	100
All	All	653/664 (98%)	625 (96%)	28 (4%)	26	51

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	VAL
1	A	98	ILE
1	A	138	MET
1	A	196	GLU
1	A	228	MET
1	A	247	VAL
1	A	255	GLN
1	A	272	LEU
2	B	1	ILE
2	B	2	GLN
2	B	56	PHE
2	B	68	THR
2	B	74	GLU
2	B	75	THR
1	C	51	TRP
1	C	97	VAL
1	C	98	ILE
1	C	138	MET
1	C	194	ARG
1	C	196	GLU
1	C	228	MET
1	C	247	VAL
1	C	255	GLN
1	C	272	LEU
2	D	1	ILE
2	D	2	GLN
2	D	56	PHE
2	D	75	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	GLN
1	A	174	ASN
1	A	218	GLN
1	A	255	GLN
2	B	6	GLN
2	B	17	ASN
1	C	114	GLN
1	C	115	GLN
1	C	174	ASN
1	C	218	GLN
1	C	255	GLN
2	D	6	GLN
2	D	17	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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$
3	NIY	F	3	3	14,15,16	4.03	3 (21%)	11,20,22	1.03	1 (9%)
3	NIY	E	3	3	14,15,16	4.18	2 (14%)	11,20,22	1.05	1 (9%)

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	NIY	F	3	3	-	2/7/10/12	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NIY	E	3	3	-	2/7/10/12	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	3	NIY	O2-NN	13.96	1.46	1.22
3	F	3	NIY	O2-NN	13.04	1.45	1.22
3	F	3	NIY	CE1-NN	-6.63	1.33	1.45
3	E	3	NIY	CE1-NN	-6.16	1.34	1.45
3	F	3	NIY	CB-CA	-2.15	1.49	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	3	NIY	CD2-CE2-CZ	-2.47	118.03	120.50
3	F	3	NIY	CD2-CE2-CZ	-2.44	118.06	120.50

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	3	NIY	CD1-CE1-NN-O2
3	F	3	NIY	CZ-CE1-NN-O2
3	E	3	NIY	CA-CB-CG-CD2
3	E	3	NIY	CA-CB-CG-CD1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	3	NIY	1	0
3	E	3	NIY	1	0

5.5 Carbohydrates

There are no oligosaccharides 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	PO4	C	278	-	4,4,4	1.00	0	6,6,6	1.03	1 (16%)
5	GOL	C	276	-	5,5,5	0.48	0	5,5,5	0.63	0
6	MPD	D	277	-	7,7,7	0.36	0	9,10,10	0.37	0
4	PO4	A	276	-	4,4,4	0.90	0	6,6,6	0.57	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
6	MPD	D	277	-	-	0/5/5/5	-
5	GOL	C	276	-	-	3/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	278	PO4	O3-P-O2	2.13	114.54	107.91

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	276	GOL	C1-C2-C3-O3
5	C	276	GOL	O2-C2-C3-O3
5	C	276	GOL	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	276	GOL	2	0
6	D	277	MPD	6	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	271/275 (98%)	0.98	29 (10%) 11 9	23, 38, 51, 65	0
1	C	272/275 (98%)	1.17	50 (18%) 3 3	23, 38, 52, 65	0
2	B	99/99 (100%)	0.91	11 (11%) 10 8	23, 34, 46, 52	0
2	D	99/99 (100%)	1.07	13 (13%) 7 5	23, 34, 46, 52	0
3	E	7/8 (87%)	1.44	2 (28%) 1 1	38, 40, 42, 43	0
3	F	7/8 (87%)	0.09	0 100 100	21, 22, 26, 27	0
All	All	755/764 (98%)	1.05	105 (13%) 6 5	21, 37, 50, 65	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1	ILE	5.5
1	C	195	PRO	4.8
1	C	220	ASN	4.7
2	B	1	ILE	4.7
1	A	195	PRO	4.3
1	C	251	LEU	4.2
1	C	275	GLU	4.1
1	A	224	LEU	4.0
1	C	256	TYR	3.8
2	D	18	GLY	3.8
1	A	138	MET	3.7
1	A	58	GLU	3.7
1	C	224	LEU	3.6
2	B	48	LYS	3.5
2	D	48	LYS	3.5
1	C	222	GLU	3.4
1	A	42	ASN	3.4
1	C	221	GLY	3.4
1	C	58	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	18	GLY	3.2
1	C	199	VAL	3.2
1	A	253	LYS	3.2
1	A	222	GLU	3.1
2	D	89	GLU	3.1
1	C	257	TYR	3.1
1	C	248	VAL	3.0
1	A	113	TYR	3.0
1	C	228	MET	3.0
1	A	220	ASN	2.9
1	A	221	GLY	2.9
2	B	49	VAL	2.9
2	D	19	LYS	2.8
1	C	115	GLN	2.8
1	C	138	MET	2.8
1	C	196	GLU	2.8
2	D	3	LYS	2.7
1	C	252	GLY	2.7
1	C	111	ARG	2.7
1	A	111	ARG	2.7
1	C	253	LYS	2.7
2	B	17	ASN	2.6
1	C	268	GLU	2.6
1	C	57	PRO	2.6
2	D	49	VAL	2.5
1	A	196	GLU	2.5
1	C	51	TRP	2.5
2	B	3	LYS	2.5
1	A	272	LEU	2.5
1	C	62	ARG	2.5
1	A	274	TRP	2.5
2	D	38	GLN	2.5
1	C	273	ARG	2.4
1	A	228	MET	2.4
1	C	79	ARG	2.4
1	A	41	GLU	2.4
1	C	247	VAL	2.4
1	C	42	ASN	2.4
1	C	188	HIS	2.4
1	C	41	GLU	2.4
1	C	250	PRO	2.4
1	C	255	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	4	THR	2.4
3	E	1	ALA	2.4
1	C	88	SER	2.3
1	A	194	ARG	2.3
1	C	135	ALA	2.3
1	C	198	LYS	2.3
2	D	91	LYS	2.2
1	C	128	GLU	2.2
1	C	176	ASN	2.2
1	A	56	GLY	2.2
3	E	2	VAL	2.2
1	C	19	GLU	2.2
1	C	44	ARG	2.2
1	A	164	CYS	2.2
1	A	18	GLY	2.2
1	C	110	LEU	2.2
1	C	197	ASP	2.2
2	B	16	GLU	2.1
1	C	233	THR	2.1
2	B	4	THR	2.1
1	A	250	PRO	2.1
1	A	256	TYR	2.1
1	A	62	ARG	2.1
1	A	233	THR	2.1
1	C	113	TYR	2.1
1	C	223	GLU	2.1
1	C	267	PRO	2.1
2	B	15	PRO	2.1
1	C	109	LEU	2.1
1	C	230	LEU	2.1
1	A	257	TYR	2.1
1	C	50	ARG	2.1
1	C	194	ARG	2.1
1	A	251	LEU	2.1
1	C	219	LEU	2.1
2	B	31	HIS	2.1
1	C	103	VAL	2.1
2	D	85	ASP	2.0
1	A	19	GLU	2.0
2	B	88	ALA	2.0
1	A	57	PRO	2.0
2	D	31	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	7	ILE	2.0
1	A	79	ARG	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NIY	F	3	15/16	0.83	0.16	22,25,34,36	0
3	NIY	E	3	15/16	0.85	0.16	38,39,43,44	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MPD	D	277	8/8	0.83	0.20	34,35,37,38	0
5	GOL	C	276	6/6	0.90	0.13	22,27,28,29	0
4	PO4	A	276	5/5	0.92	0.20	57,57,58,59	0
4	PO4	C	278	5/5	0.96	0.15	42,42,44,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.