



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:01 AM GMT

PDB ID : 2CMZ
Title : CRYSTAL STRUCTURE OF VSV-INDIANA (MUDD-SUMMERS STRAIN)
GLYCOPROTEIN UNDER ITS ACIDIC CONFORMATION
Authors : Roche, S.; Bressanelli, S.
Deposited on : 2006-05-17
Resolution : 2.40 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

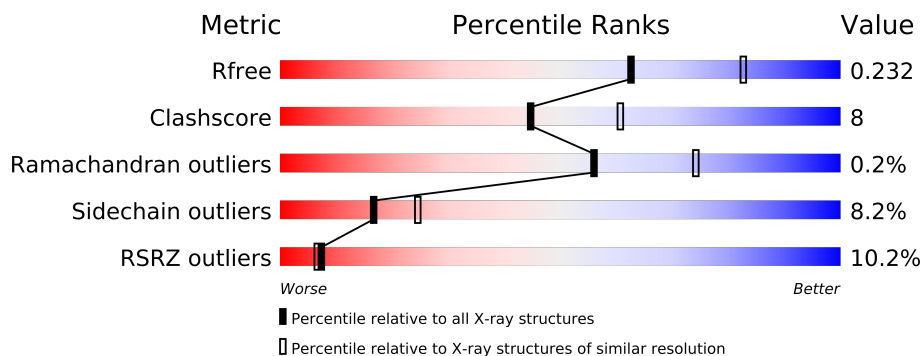
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	423	
1	B	423	
1	C	423	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	PE4	A	1410	-	X
2	PE4	B	1412	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10477 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

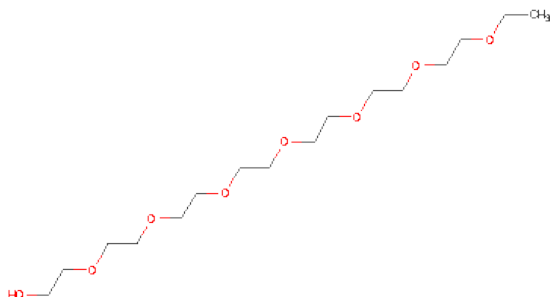
- Molecule 1 is a protein called SPIKE GLYCOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	0
			3233	2061	539	612	21			
1	B	410	Total	C	N	O	S	0	0	0
			3241	2067	540	613	21			
1	C	408	Total	C	N	O	S	0	0	0
			3223	2055	536	611	21			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	ALA	GLY	CONFLICT	UNP P04883
A	41	ILE	LEU	CONFLICT	UNP P04883
A	80	GLN	HIS	CONFLICT	UNP P04883
A	156	TYR	ASP	CONFLICT	UNP P04883
A	184	MET	THR	CONFLICT	UNP P04883
A	395	ASP	GLY	CONFLICT	UNP P04883
B	40	ALA	GLY	CONFLICT	UNP P04883
B	41	ILE	LEU	CONFLICT	UNP P04883
B	80	GLN	HIS	CONFLICT	UNP P04883
B	156	TYR	ASP	CONFLICT	UNP P04883
B	184	MET	THR	CONFLICT	UNP P04883
B	395	ASP	GLY	CONFLICT	UNP P04883
C	40	ALA	GLY	CONFLICT	UNP P04883
C	41	ILE	LEU	CONFLICT	UNP P04883
C	80	GLN	HIS	CONFLICT	UNP P04883
C	156	TYR	ASP	CONFLICT	UNP P04883
C	184	MET	THR	CONFLICT	UNP P04883
C	395	ASP	GLY	CONFLICT	UNP P04883

- Molecule 2 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: C₁₆H₃₄O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	14	6		
2	B	1	Total	C	O	0	0
			19	13	6		
2	B	1	Total	C	O	0	0
			23	15	8		
2	B	1	Total	C	O	0	0
			20	14	6		
2	C	1	Total	C	O	0	0
			23	15	8		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Ca	0	0
			1	1		

- Molecule 4 is water.

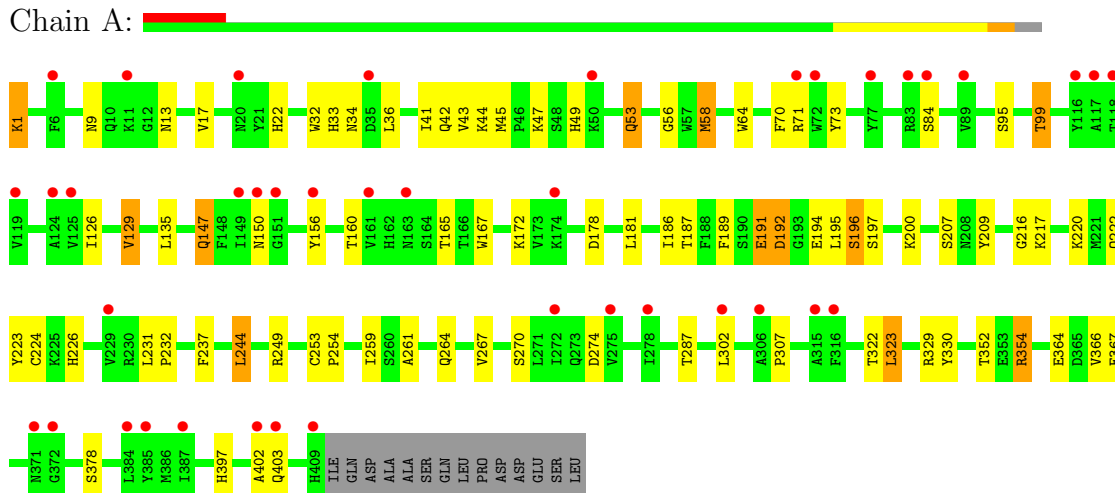
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	203	Total	O	0	0
			203	203		
4	B	219	Total	O	0	0
			219	219		
4	C	252	Total	O	0	0
			252	252		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

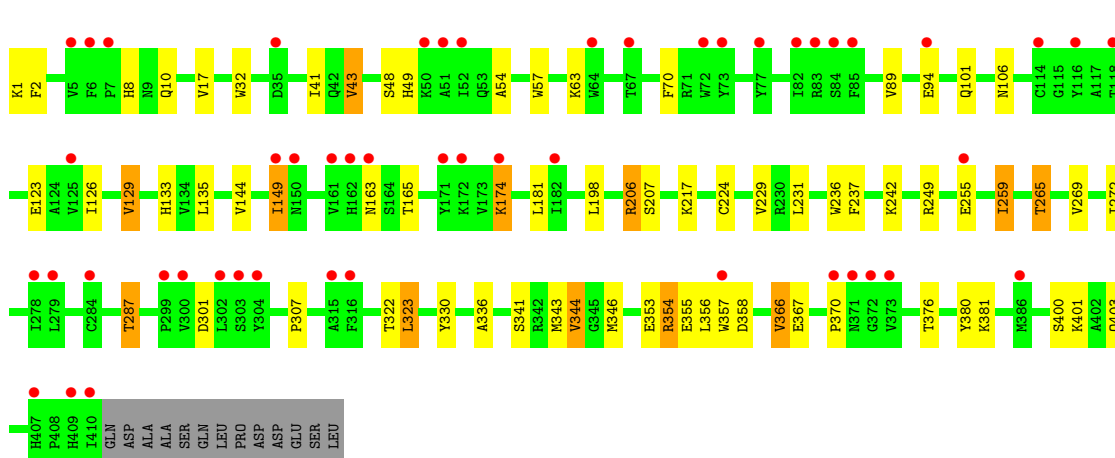
• Molecule 1: SPIKE GLYCOPROTEIN

Chain A:



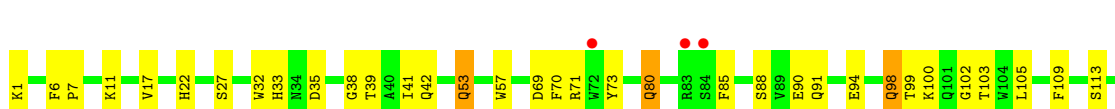
• Molecule 1: SPIKE GLYCOPROTEIN

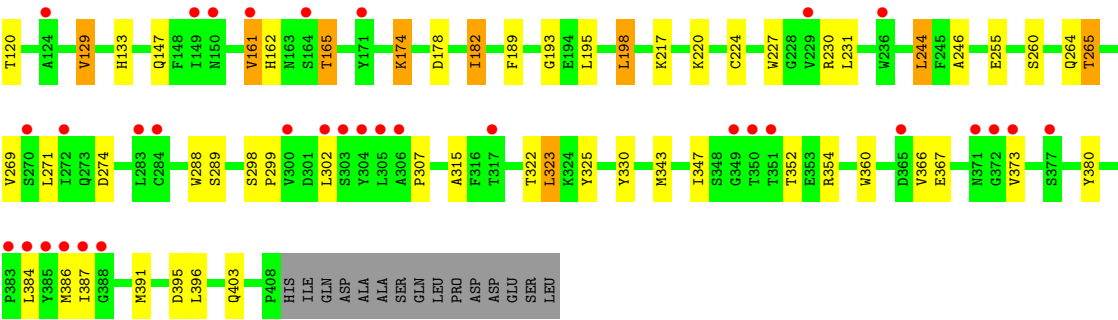
Chain B:



• Molecule 1: SPIKE GLYCOPROTEIN

Chain C:





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	71.27Å 224.20Å 375.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.40 24.96 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (25.00-2.40) 99.9 (24.96-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.196 , 0.233 0.197 , 0.232	Depositor DCC
R_{free} test set	5888 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 117758 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10477	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PE4, CA

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	0.70	3/3332 (0.1%)	0.72	0/4537
1	B	0.64	0/3340	0.70	1/4548 (0.0%)
1	C	0.76	3/3321 (0.1%)	0.75	4/4522 (0.1%)
All	All	0.70	6/9993 (0.1%)	0.72	5/13607 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	TYR	C-O	8.61	1.39	1.23
1	C	73	TYR	C-N	7.09	1.45	1.33
1	A	73	TYR	C-N	6.63	1.45	1.33
1	C	98	GLN	CG-CD	5.56	1.63	1.51
1	C	100	LYS	CB-CG	5.04	1.66	1.52
1	A	71	ARG	C-O	5.00	1.32	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	198	LEU	CB-CG-CD2	-6.57	99.83	111.00
1	C	274	ASP	CB-CG-OD1	6.51	124.16	118.30
1	C	230	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	358	ASP	CB-CG-OD1	-5.36	113.48	118.30
1	C	230	ARG	NE-CZ-NH2	-5.15	117.73	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3233	0	3082	56	0
1	B	3241	0	3093	59	0
1	C	3223	0	3075	60	0
2	A	20	0	24	5	0
2	B	62	0	75	6	0
2	C	23	0	29	5	0
3	C	1	0	0	0	0
4	A	203	0	0	4	0
4	B	219	0	0	7	0
4	C	252	0	0	8	0
All	All	10477	0	9378	162	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (162) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:341:SER:H	2:B:1412:PE4:H131	1.09	1.12
1:B:1:LYS:HD3	1:C:38:GLY:HA3	1.52	0.91
1:B:1:LYS:HE3	1:B:2:PHE:CE1	2.06	0.90
1:B:343:MET:CE	1:B:380:TYR:HB3	2.02	0.88
1:B:17:VAL:HG21	1:B:323:LEU:HD13	1.57	0.86
1:A:43:VAL:CG1	1:A:237:PHE:HB2	2.06	0.84
1:B:341:SER:N	2:B:1412:PE4:H131	1.93	0.83
1:B:272:ILE:HD13	1:C:271:LEU:HB3	1.60	0.82
1:A:220:LYS:NZ	2:A:1410:PE4:H132	2.01	0.76
1:B:174:LYS:H	1:B:174:LYS:HE3	1.51	0.75
1:C:1:LYS:HE3	1:C:1:LYS:O	1.88	0.73
1:B:1:LYS:HD3	1:C:38:GLY:CA	2.20	0.71
1:C:133:HIS:HB2	4:C:2065:HOH:O	1.91	0.71
1:C:343:MET:HE1	1:C:380:TYR:HB3	1.71	0.70
1:A:47:LYS:O	1:A:49:HIS:HD2	1.75	0.69
1:A:58:MET:HE1	1:A:160:THR:HG21	1.73	0.69
1:A:220:LYS:HZ3	2:A:1410:PE4:H132	1.55	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:265:THR:HB	4:B:2123:HOH:O	1.94	0.68
1:A:43:VAL:HG13	1:A:237:PHE:HB2	1.74	0.67
1:B:206:ARG:NH1	1:B:207:SER:O	2.27	0.66
1:A:17:VAL:HG21	1:A:323:LEU:HD13	1.78	0.65
1:C:193:GLY:HA2	4:C:2118:HOH:O	1.97	0.65
1:C:366:VAL:CG1	1:C:367:GLU:N	2.59	0.64
1:B:366:VAL:HG13	1:B:367:GLU:H	1.62	0.64
1:C:343:MET:HE2	1:C:380:TYR:CD2	2.32	0.64
1:A:9:ASN:H	1:A:354:ARG:NH2	1.95	0.64
1:A:1:LYS:HG2	4:A:2172:HOH:O	1.97	0.64
1:B:174:LYS:HE3	1:B:174:LYS:N	2.12	0.63
1:A:264:GLN:HB3	1:C:265:THR:HG22	1.80	0.62
1:C:17:VAL:HG21	1:C:323:LEU:HD13	1.82	0.62
1:C:366:VAL:HG13	1:C:367:GLU:H	1.65	0.61
1:B:381:LYS:HB3	2:B:1413:PE4:H131	1.83	0.60
1:A:95:SER:O	1:A:99:THR:HG23	2.02	0.60
1:A:41:ILE:CG2	1:A:186:ILE:HG13	2.31	0.60
1:A:216:GLY:O	1:A:217:LYS:HB2	2.02	0.60
1:B:1:LYS:HB3	4:B:2178:HOH:O	2.01	0.60
1:B:307:PRO:HG2	1:B:330:TYR:CE1	2.37	0.60
1:B:357:TRP:CE2	1:B:370:PRO:HD3	2.38	0.59
1:A:187:THR:HG21	1:C:1:LYS:HD2	1.84	0.59
2:B:1411:PE4:H21	4:B:2217:HOH:O	2.02	0.59
1:C:99:THR:O	1:C:102:GLY:N	2.35	0.59
1:B:354:ARG:HG2	1:B:356:LEU:HD23	1.84	0.58
1:C:366:VAL:CG1	1:C:367:GLU:H	2.16	0.58
1:A:9:ASN:H	1:A:354:ARG:HH22	1.52	0.58
1:C:195:LEU:HB3	1:C:244:LEU:HD11	1.84	0.58
1:B:206:ARG:HD3	1:B:207:SER:N	2.18	0.57
1:B:287:THR:HB	1:B:301:ASP:HB3	1.85	0.57
1:C:343:MET:HE3	1:C:373:VAL:HG11	1.85	0.57
1:B:343:MET:CE	1:B:380:TYR:CB	2.81	0.57
1:A:33:HIS:CE1	1:C:384:LEU:HD11	2.39	0.57
1:C:260:SER:HA	1:C:403:GLN:O	2.06	0.56
1:B:343:MET:HE2	1:B:380:TYR:CB	2.36	0.56
1:A:43:VAL:HG11	1:A:237:PHE:HB2	1.86	0.55
1:B:49:HIS:H	1:B:403:GLN:NE2	2.04	0.55
1:A:186:ILE:HG22	1:A:207:SER:HB2	1.88	0.55
1:C:322:THR:HB	4:C:2214:HOH:O	2.05	0.55
1:B:366:VAL:CG1	1:B:367:GLU:N	2.69	0.54
1:C:387:ILE:O	1:C:391:MET:HG3	2.07	0.54
1:C:80:GLN:HG3	1:C:109:PHE:CE2	2.43	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:80:GLN:HG3	1:C:109:PHE:CD2	2.43	0.54
1:B:48:SER:HB2	4:B:2118:HOH:O	2.07	0.54
1:A:194:GLU:HG3	1:A:196:SER:OG	2.07	0.53
1:C:227:TRP:CZ2	2:C:1409:PE4:H91	2.43	0.53
1:A:43:VAL:HG12	1:A:44:LYS:N	2.24	0.53
1:B:236:TRP:HB3	1:B:259:ILE:HD13	1.90	0.53
1:B:265:THR:HG22	1:C:264:GLN:HG3	1.91	0.52
1:C:366:VAL:HG12	1:C:367:GLU:N	2.24	0.52
1:B:249:ARG:HA	2:B:1411:PE4:C13	2.40	0.52
1:A:45:MET:HG2	1:A:237:PHE:HB3	1.92	0.52
1:A:220:LYS:HE3	2:A:1410:PE4:H91	1.92	0.52
1:B:1:LYS:HD2	1:C:189:PHE:CE2	2.45	0.52
1:B:346:MET:HE3	4:B:2182:HOH:O	2.11	0.51
1:C:27:SER:HA	1:C:33:HIS:CD2	2.45	0.51
1:B:366:VAL:HG13	1:B:367:GLU:N	2.26	0.50
1:C:69:ASP:OD2	1:C:71:ARG:NH1	2.45	0.50
1:B:272:ILE:CD1	1:C:271:LEU:HB3	2.37	0.49
1:C:217:LYS:HE3	4:C:2130:HOH:O	2.11	0.49
1:C:22:HIS:HD2	1:C:288:TRP:CE3	2.30	0.49
1:A:58:MET:HE2	1:A:165:THR:HG22	1.95	0.49
1:C:220:LYS:HZ3	2:C:1409:PE4:H62	1.76	0.49
1:C:39:THR:HG22	4:C:2118:HOH:O	2.12	0.49
1:A:307:PRO:HG2	1:A:330:TYR:CE1	2.47	0.48
1:A:366:VAL:CG1	1:A:367:GLU:N	2.75	0.48
1:A:99:THR:HG21	1:A:129:VAL:HG12	1.96	0.48
1:C:246:ALA:HA	2:C:1409:PE4:C5	2.43	0.48
1:C:298:SER:HB2	1:C:299:PRO:HD2	1.95	0.48
1:A:274:ASP:OD2	1:C:395:ASP:OD2	2.32	0.48
1:C:246:ALA:HA	2:C:1409:PE4:H52	1.95	0.48
1:B:43:VAL:HG13	1:B:237:PHE:HB2	1.96	0.48
1:C:57:TRP:CE3	1:C:129:VAL:HG13	2.49	0.47
1:A:95:SER:O	1:A:99:THR:CG2	2.61	0.47
1:A:220:LYS:HZ2	2:A:1410:PE4:H132	1.78	0.47
1:C:343:MET:CE	1:C:373:VAL:HG11	2.45	0.47
1:C:6:PHE:CD1	1:C:7:PRO:HD2	2.50	0.47
1:A:156:TYR:CE1	1:A:172:LYS:HG2	2.50	0.47
1:B:376:THR:O	2:B:1412:PE4:H42	2.15	0.47
1:B:57:TRP:HB3	1:B:129:VAL:HG22	1.96	0.47
1:B:135:LEU:HB2	1:B:144:VAL:HB	1.97	0.47
1:A:47:LYS:O	1:A:49:HIS:CD2	2.61	0.46
1:B:229:VAL:O	1:B:236:TRP:HA	2.16	0.46
1:A:232:PRO:HG2	4:A:2096:HOH:O	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:53:GLN:CB	4:C:2065:HOH:O	2.63	0.46
1:C:6:PHE:CG	1:C:7:PRO:HD2	2.50	0.46
1:B:403:GLN:O	1:B:403:GLN:HG3	2.15	0.46
1:A:178:ASP:HA	1:A:181:LEU:HD12	1.97	0.46
1:B:343:MET:HE2	1:B:380:TYR:CG	2.51	0.46
1:B:106:ASN:OD1	1:B:126:ILE:HD13	2.17	0.45
1:B:217:LYS:HD2	1:B:217:LYS:N	2.31	0.45
1:A:253:CYS:HA	1:A:254:PRO:HD2	1.72	0.45
1:B:344:VAL:HG22	1:B:353:GLU:HG2	1.97	0.45
1:A:223:TYR:HB2	1:A:259:ILE:HD13	1.99	0.45
1:B:265:THR:O	1:B:269:VAL:HG23	2.17	0.45
1:B:343:MET:HE1	1:B:380:TYR:HB3	1.93	0.45
1:B:149:ILE:HG13	1:B:149:ILE:H	1.67	0.45
1:C:343:MET:HE3	1:C:360:TRP:HH2	1.82	0.45
1:B:49:HIS:H	1:B:403:GLN:HE22	1.65	0.45
1:C:174:LYS:HD3	1:C:178:ASP:OD1	2.16	0.45
1:A:43:VAL:CG1	1:A:44:LYS:N	2.80	0.44
1:A:41:ILE:HG23	1:A:186:ILE:HG13	1.98	0.44
1:A:209:TYR:HA	1:A:267:VAL:HG22	1.99	0.44
1:A:261:ALA:O	1:A:402:ALA:HB1	2.17	0.44
1:B:1:LYS:HD3	1:C:38:GLY:N	2.31	0.44
1:A:189:PHE:CE2	1:C:1:LYS:HD3	2.52	0.44
1:A:220:LYS:HD2	2:A:1410:PE4:H121	2.00	0.44
1:B:1:LYS:O	1:B:1:LYS:HG2	2.16	0.44
1:C:22:HIS:CD2	4:C:2028:HOH:O	2.70	0.44
1:A:147:GLN:OE1	1:B:101:GLN:HG2	2.18	0.44
1:C:161:VAL:HG12	1:C:162:HIS:ND1	2.33	0.44
1:C:307:PRO:HG2	1:C:330:TYR:CE1	2.53	0.44
1:A:197:SER:HB3	1:A:200:LYS:HE3	1.98	0.44
1:C:88:SER:OG	1:C:91:GLN:HG3	2.18	0.43
1:B:63:LYS:HD3	1:B:123:GLU:HG2	2.00	0.43
1:A:191:GLU:HG3	1:A:192:ASP:N	2.33	0.43
1:A:56:GLY:HA3	1:A:167:TRP:CZ2	2.53	0.43
1:A:195:LEU:HB3	1:A:244:LEU:HD11	2.00	0.43
1:C:94:GLU:O	1:C:98:GLN:HG3	2.19	0.43
1:B:1:LYS:HD2	1:C:189:PHE:HE2	1.83	0.42
1:A:64:TRP:CG	1:A:126:ILE:HD12	2.54	0.42
1:C:182:ILE:C	1:C:182:ILE:HD13	2.40	0.42
1:B:1:LYS:HB3	1:B:1:LYS:HE2	1.93	0.42
1:B:269:VAL:HG21	1:B:400:SER:HB3	2.01	0.42
1:C:113:SER:O	1:C:120:THR:OG1	2.37	0.42
1:A:397:HIS:HB2	4:A:2061:HOH:O	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1:LYS:HE2	1:B:336:ALA:O	2.20	0.42
1:C:162:HIS:HB2	1:C:165:THR:CG2	2.49	0.42
2:C:1409:PE4:H52	4:C:2161:HOH:O	2.19	0.42
1:B:54:ALA:O	1:B:133:HIS:HA	2.20	0.42
1:A:41:ILE:HG23	1:A:186:ILE:CG1	2.50	0.41
1:A:41:ILE:HG22	1:A:186:ILE:O	2.20	0.41
1:A:53:GLN:HE21	1:A:53:GLN:HB3	1.70	0.41
1:C:269:VAL:HG13	1:C:396:LEU:HD22	2.01	0.41
1:A:64:TRP:CD1	1:A:126:ILE:HD12	2.55	0.41
1:B:10:GLN:NE2	1:B:355:GLU:HB3	2.35	0.41
1:A:34:ASN:C	1:A:36:LEU:H	2.23	0.41
1:A:222:GLN:HA	1:A:226:HIS:O	2.20	0.41
1:C:265:THR:O	1:C:269:VAL:HG23	2.21	0.41
1:B:48:SER:CB	4:B:2118:HOH:O	2.66	0.41
1:A:22:HIS:CD2	4:A:2018:HOH:O	2.73	0.41
1:B:265:THR:HG23	4:B:2119:HOH:O	2.21	0.40
1:C:315:ALA:O	1:C:325:TYR:HA	2.21	0.40
1:A:58:MET:O	1:A:129:VAL:HA	2.22	0.40
1:B:272:ILE:HD13	1:C:271:LEU:CB	2.43	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	407/423 (96%)	388 (95%)	17 (4%)	2 (0%)	38	53
1	B	408/423 (96%)	397 (97%)	11 (3%)	0	100	100
1	C	406/423 (96%)	392 (97%)	14 (3%)	0	100	100
All	All	1221/1269 (96%)	1177 (96%)	42 (3%)	2 (0%)	56	74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	352	THR

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	358/370 (97%)	329 (92%)	29 (8%)	17	25
1	B	359/370 (97%)	331 (92%)	28 (8%)	18	27
1	C	357/370 (96%)	326 (91%)	31 (9%)	15	22
All	All	1074/1110 (97%)	986 (92%)	88 (8%)	17	24

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LYS
1	A	32	TRP
1	A	42	GLN
1	A	53	GLN
1	A	58	MET
1	A	70	PHE
1	A	84	SER
1	A	99	THR
1	A	129	VAL
1	A	135	LEU
1	A	147	GLN
1	A	150	ASN
1	A	191	GLU
1	A	192	ASP
1	A	196	SER
1	A	224	CYS
1	A	231	LEU
1	A	244	LEU
1	A	249	ARG
1	A	270	SER
1	A	287	THR
1	A	302	LEU

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Mol	Chain	Res	Type
1	A	322	THR
1	A	323	LEU
1	A	329	ARG
1	A	354	ARG
1	A	364	GLU
1	A	378	SER
1	A	403	GLN
1	B	8	HIS
1	B	32	TRP
1	B	41	ILE
1	B	43	VAL
1	B	70	PHE
1	B	89	VAL
1	B	94	GLU
1	B	129	VAL
1	B	149	ILE
1	B	163	ASN
1	B	165	THR
1	B	174	LYS
1	B	181	LEU
1	B	198	LEU
1	B	206	ARG
1	B	224	CYS
1	B	231	LEU
1	B	242	LYS
1	B	255	GLU
1	B	259	ILE
1	B	265	THR
1	B	287	THR
1	B	322	THR
1	B	323	LEU
1	B	344	VAL
1	B	354	ARG
1	B	366	VAL
1	B	401	LYS
1	C	11	LYS
1	C	32	TRP
1	C	35	ASP
1	C	41	ILE
1	C	42	GLN
1	C	53	GLN
1	C	70	PHE

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Mol	Chain	Res	Type
1	C	80	GLN
1	C	85	PHE
1	C	90	GLU
1	C	103	THR
1	C	105	LEU
1	C	129	VAL
1	C	147	GLN
1	C	161	VAL
1	C	165	THR
1	C	174	LYS
1	C	182	ILE
1	C	198	LEU
1	C	224	CYS
1	C	231	LEU
1	C	244	LEU
1	C	255	GLU
1	C	265	THR
1	C	289	SER
1	C	302	LEU
1	C	323	LEU
1	C	347	ILE
1	C	352	THR
1	C	354	ARG
1	C	386	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	33	HIS
1	A	42	GLN
1	A	49	HIS
1	A	53	GLN
1	A	163	ASN
1	A	180	ASN
1	B	8	HIS
1	B	9	ASN
1	B	22	HIS
1	B	33	HIS
1	B	60	HIS
1	B	163	ASN
1	B	168	HIS

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Mol	Chain	Res	Type
1	B	403	GLN
1	C	9	ASN
1	C	22	HIS
1	C	33	HIS
1	C	163	ASN
1	C	180	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\# Z > 2$
2	PE4	A	1410	-	19,19,23	1.69	2 (10%)	16,18,22	0.32	0
2	PE4	B	1411	-	17,18,23	1.06	1 (5%)	15,17,22	0.49	0
2	PE4	B	1412	-	21,22,23	0.64	0	20,21,22	0.50	0
2	PE4	B	1413	-	19,19,23	1.84	2 (10%)	16,18,22	0.27	0
2	PE4	C	1409	-	21,22,23	0.54	0	20,21,22	0.41	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
2	PE4	A	1410	-	-	0/17/17/21	0/0/0/0
2	PE4	B	1411	-	-	0/16/16/21	0/0/0/0
2	PE4	B	1412	-	-	0/20/20/21	0/0/0/0
2	PE4	B	1413	-	-	0/17/17/21	0/0/0/0
2	PE4	C	1409	-	-	0/20/20/21	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1413	PE4	C1-C2	-6.99	1.52	1.55
2	A	1410	PE4	C1-C2	-6.59	1.52	1.55
2	B	1411	PE4	C1-C2	-3.60	1.53	1.55
2	B	1413	PE4	C14-C13	-3.23	1.53	1.55
2	A	1410	PE4	C14-C13	2.23	1.56	1.55

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	409/423 (96%)	0.65	40 (9%) 8 7	47, 64, 78, 90	0
1	B	410/423 (96%)	0.73	50 (12%) 5 4	45, 64, 75, 87	0
1	C	408/423 (96%)	0.55	36 (8%) 10 9	57, 67, 79, 85	0
All	All	1227/1269 (96%)	0.65	126 (10%) 7 6	45, 65, 78, 90	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	410	ILE	5.3
1	A	409	HIS	5.1
1	B	72	TRP	4.1
1	A	402	ALA	4.0
1	B	370	PRO	3.9
1	B	149	ILE	3.9
1	A	161	VAL	3.8
1	A	84	SER	3.7
1	A	403	GLN	3.6
1	A	72	TRP	3.6
1	A	83	ARG	3.5
1	B	51	ALA	3.5
1	A	174	LYS	3.4
1	C	385	TYR	3.4
1	C	303	SER	3.4
1	C	349	GLY	3.3
1	C	149	ILE	3.3
1	B	171	TYR	3.3
1	B	303	SER	3.2
1	C	351	THR	3.2
1	C	72	TRP	3.2
1	B	409	HIS	3.2
1	C	386	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	371	ASN	3.1
1	B	161	VAL	3.0
1	B	85	PHE	3.0
1	C	171	TYR	3.0
1	B	6	PHE	2.9
1	A	77	TYR	2.9
1	A	156	TYR	2.9
1	A	50	LYS	2.9
1	A	150	ASN	2.9
1	B	373	VAL	2.9
1	B	371	ASN	2.9
1	A	35	ASP	2.9
1	C	150	ASN	2.9
1	C	373	VAL	2.9
1	B	7	PRO	2.8
1	B	172	LYS	2.8
1	A	149	ILE	2.8
1	B	52	ILE	2.8
1	B	255	GLU	2.8
1	C	388	GLY	2.7
1	A	229	VAL	2.7
1	B	182	ILE	2.7
1	B	84	SER	2.7
1	A	371	ASN	2.7
1	C	236	TRP	2.7
1	A	302	LEU	2.7
1	A	117	ALA	2.7
1	B	302	LEU	2.7
1	A	125	VAL	2.7
1	B	174	LYS	2.7
1	C	84	SER	2.6
1	C	302	LEU	2.6
1	B	284	CYS	2.6
1	B	163	ASN	2.6
1	A	163	ASN	2.6
1	B	150	ASN	2.6
1	C	377	SER	2.6
1	C	124	ALA	2.6
1	B	64	TRP	2.6
1	B	386	MET	2.5
1	B	83	ARG	2.5
1	B	372	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	316	PHE	2.5
1	B	407	HIS	2.5
1	C	304	TYR	2.4
1	C	161	VAL	2.4
1	B	357	TRP	2.4
1	A	119	VAL	2.4
1	C	306	ALA	2.4
1	B	316	PHE	2.4
1	A	151	GLY	2.4
1	B	162	HIS	2.4
1	A	116	TYR	2.4
1	B	278	ILE	2.4
1	B	77	TYR	2.4
1	C	164	SER	2.3
1	B	5	VAL	2.3
1	B	125	VAL	2.3
1	A	275	VAL	2.3
1	C	83	ARG	2.3
1	A	11	LYS	2.3
1	A	272	ILE	2.3
1	B	73	TYR	2.3
1	B	116	TYR	2.3
1	B	94	GLU	2.3
1	C	300	VAL	2.3
1	A	387	ILE	2.3
1	C	229	VAL	2.3
1	C	387	ILE	2.3
1	A	118	THR	2.2
1	C	384	LEU	2.2
1	B	114	CYS	2.2
1	C	270	SER	2.2
1	B	299	PRO	2.2
1	A	315	ALA	2.2
1	A	385	TYR	2.2
1	B	50	LYS	2.2
1	A	20	ASN	2.2
1	B	35	ASP	2.2
1	C	372	GLY	2.2
1	C	272	ILE	2.2
1	A	124	ALA	2.2
1	A	89	VAL	2.2
1	B	315	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	383	PRO	2.1
1	B	279	LEU	2.1
1	B	304	TYR	2.1
1	C	317	THR	2.1
1	A	278	ILE	2.1
1	A	306	ALA	2.1
1	C	305	LEU	2.1
1	B	118	THR	2.1
1	A	384	LEU	2.1
1	C	283	LEU	2.1
1	A	372	GLY	2.1
1	C	284	CYS	2.1
1	B	67	THR	2.0
1	B	300	VAL	2.0
1	C	350	THR	2.0
1	C	365	ASP	2.0
1	B	82	ILE	2.0
1	A	6	PHE	2.0
1	A	71	ARG	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	PE4	A	1410	20/24	0.31	3.02	64,69,77,78	0
2	PE4	B	1412	23/24	0.24	2.40	94,96,99,100	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	PE4	C	1409	23/24	0.18	1.03	60,69,85,87	0
2	PE4	B	1413	20/24	0.23	0.73	98,102,107,107	0
2	PE4	B	1411	19/24	0.17	-0.34	64,66,74,75	0
3	CA	C	1410	1/1	0.05	-8.50	61,61,61,61	0

6.5 Other polymers

There are no such residues in this entry.