



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:08 AM UTC

PDB ID : 1S9V / pdb_00001s9v
Title : Crystal structure of HLA-DQ2 complexed with deamidated gliadin peptide
Authors : Kim, C.-Y.; Quarsten, H.; Bergseng, E.; Khosla, C.; Sollid, L.M.
Deposited on : 2004-02-05
Resolution : 2.22 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

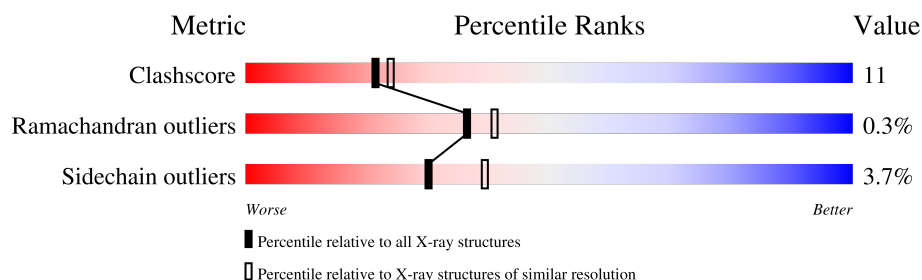
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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))
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	193	69% 22% 7%
1	D	193	69% 19% 8%
2	B	198	66% 21% 5% 9%
2	E	198	65% 24% 9%
3	C	11	82% 18%
3	F	11	82% 18%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6330 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 HLA class II histocompatibility antigen, DQ(3) alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	0	0	0
			1428	920	234	271	3			
1	D	177	Total	C	N	O	S	0	0	0
			1412	910	232	267	3			

- Molecule 2 is a protein called HLA class II histocompatibility antigen, DQ(1) beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	181	Total	C	N	O	S	0	0	0
			1486	938	268	273	7			
2	E	180	Total	C	N	O	S	0	0	0
			1470	929	263	271	7			

- Molecule 3 is a protein called alpha-I gliadin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	11	Total	C	N	O	0	0	0
			78	51	12	15			
3	F	11	Total	C	N	O	0	0	0
			86	58	12	16			

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	88	Total	O	0	0
			88	88		
5	B	71	Total	O	0	0
			71	71		
5	C	4	Total	O	0	0
			4	4		
5	D	102	Total	O	0	0
			102	102		
5	E	86	Total	O	0	0
			86	86		
5	F	3	Total	O	0	0
			3	3		

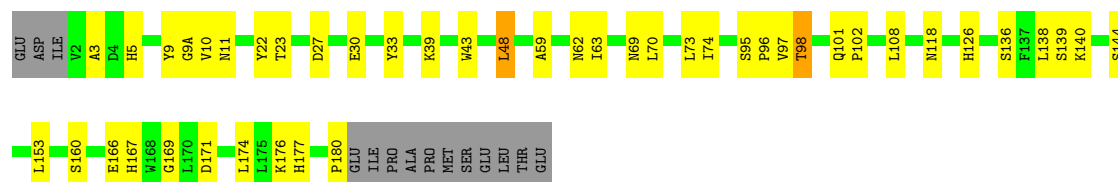
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

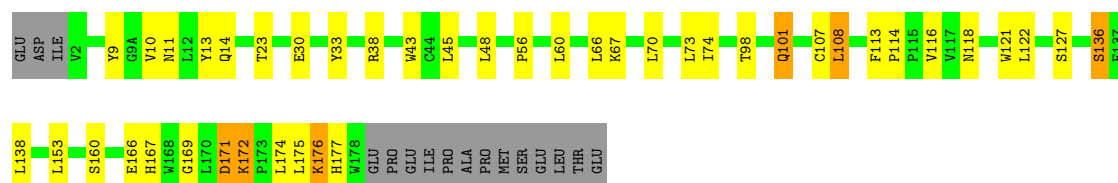
- Molecule 1: HLA class II histocompatibility antigen, DQ(3) alpha chain

Chain A: 



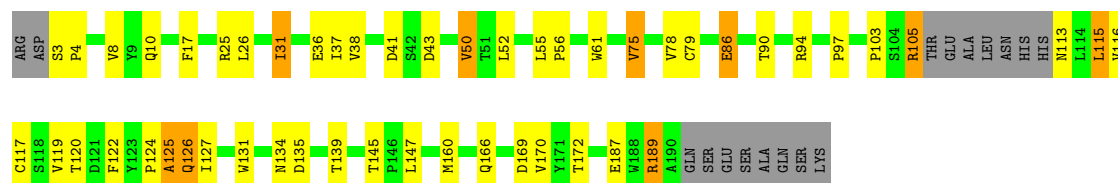
- Molecule 1: HLA class II histocompatibility antigen, DQ(3) alpha chain

Chain D: 



- Molecule 2: HLA class II histocompatibility antigen, DQ(1) beta chain

Chain B: 



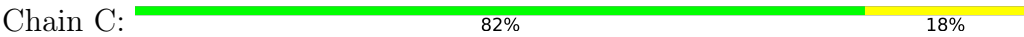
- Molecule 2: HLA class II histocompatibility antigen, DQ(1) beta chain

Chain E: 

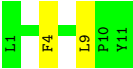
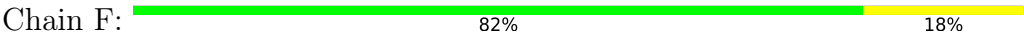




● Molecule 3: alpha-I gliadin



● Molecule 3: alpha-I gliadin



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.11Å 93.75Å 102.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.00 – 2.22	Depositor
% Data completeness (in resolution range)	(Not available) (69.00-2.22)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.221 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6330	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.42	0/1470	0.89	4/2008 (0.2%)
1	D	0.42	0/1453	0.88	3/1984 (0.2%)
2	B	0.39	0/1519	0.93	7/2062 (0.3%)
2	E	0.41	0/1503	0.93	9/2041 (0.4%)
3	C	0.51	0/82	0.88	0/111
3	F	0.52	0/91	0.87	0/124
All	All	0.41	0/6118	0.91	23/8330 (0.3%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	10	VAL	N-CA-C	-8.05	95.51	107.51
1	A	10	VAL	N-CA-C	-6.91	96.95	107.73
1	D	136	SER	N-CA-C	-6.60	101.25	110.35
2	B	145	THR	CA-C-N	-6.58	113.94	120.98
2	B	145	THR	C-N-CA	-6.58	113.94	120.98
2	B	120	THR	N-CA-C	6.10	119.49	109.85
2	B	125	ALA	N-CA-C	6.10	118.01	111.36
2	B	8	VAL	N-CA-C	6.02	117.26	108.53
2	B	31	ILE	N-CA-C	5.76	116.17	108.11
2	E	175	VAL	N-CA-C	5.74	116.15	108.11
2	E	8	VAL	N-CA-C	5.67	116.64	108.48
1	A	144	SER	N-CA-C	-5.61	101.67	110.36
2	E	31	ILE	N-CA-C	5.58	115.98	108.17
2	E	145	THR	CA-C-N	-5.58	115.00	120.52
2	E	145	THR	C-N-CA	-5.58	115.00	120.52
1	A	139	SER	N-CA-C	5.47	117.76	110.53
2	E	145	THR	N-CA-C	-5.33	102.29	110.07
2	E	121	ASP	N-CA-C	5.29	118.70	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	TYR	N-CA-C	-5.29	102.26	109.71
2	B	139	THR	N-CA-C	-5.26	107.51	114.04
1	D	9	TYR	N-CA-C	-5.17	101.87	109.62
2	E	181	GLN	N-CA-C	-5.11	105.71	111.28
2	E	14	MET	N-CA-C	5.03	117.92	110.48

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1428	0	1378	25	0
1	D	1412	0	1365	33	0
2	B	1486	0	1457	45	0
2	E	1470	0	1437	31	0
3	C	78	0	67	2	0
3	F	86	0	75	2	0
4	A	8	0	12	0	0
4	D	8	0	12	0	0
5	A	88	0	0	1	0
5	B	71	0	0	1	0
5	C	4	0	0	0	0
5	D	102	0	0	2	0
5	E	86	0	0	0	0
5	F	3	0	0	0	0
All	All	6330	0	5803	128	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 11.

All (128) 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:B:116:VAL:HG22	2:B:160:MET:HG2	1.51	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:GLU:HG2	2:B:50:VAL:HG11	1.50	0.93
2:E:132:PHE:HB2	2:E:172:THR:HG23	1.59	0.85
2:E:37:ILE:HG13	2:E:38:VAL:HG23	1.59	0.84
2:B:126:GLN:NE2	2:B:126:GLN:H	1.85	0.74
1:A:11:ASN:HD21	1:A:62:ASN:HD22	1.36	0.73
1:A:11:ASN:ND2	1:A:62:ASN:HD22	1.89	0.71
1:D:167:HIS:CD2	1:D:169:GLY:H	2.11	0.67
2:B:124:PRO:CG	2:B:126:GLN:HE22	2.10	0.65
2:B:125:ALA:HB1	2:B:147:LEU:HD21	1.80	0.64
2:E:10:GLN:HB2	2:E:31:ILE:HB	1.80	0.63
1:D:160:SER:HB2	1:D:177:HIS:HE1	1.65	0.62
1:A:160:SER:HB2	1:A:177:HIS:HE1	1.65	0.62
2:B:124:PRO:HB2	2:B:126:GLN:HE22	1.66	0.61
2:B:25:ARG:HD3	2:B:43:ASP:CG	2.26	0.61
1:D:118:ASN:HB3	1:D:166:GLU:HB2	1.80	0.61
2:E:125:ALA:HB1	2:E:147:LEU:HD21	1.82	0.61
1:A:167:HIS:CD2	1:A:169:GLY:H	2.18	0.61
2:B:189:ARG:NE	2:B:189:ARG:H	1.99	0.61
2:B:172:THR:HG22	2:B:187:GLU:HG2	1.83	0.61
2:E:97:PRO:HB3	2:E:122:PHE:HB3	1.84	0.59
1:A:118:ASN:HB2	1:A:166:GLU:HB2	1.84	0.59
1:A:59:ALA:O	1:A:63:ILE:HG12	2.03	0.59
2:B:94:ARG:HH11	2:B:94:ARG:HG3	1.68	0.59
1:D:56:PRO:O	1:D:60:LEU:HD23	2.03	0.58
2:B:37:ILE:HG13	2:B:38:VAL:HG23	1.87	0.57
1:D:167:HIS:HD2	1:D:169:GLY:H	1.54	0.56
1:A:23:THR:HG22	1:A:33:TYR:CB	2.35	0.56
1:D:66:LEU:HD22	2:E:9:TYR:CE2	2.41	0.56
2:B:124:PRO:HG2	2:B:126:GLN:HE22	1.70	0.56
2:E:36:GLU:HG2	2:E:50:VAL:HG11	1.87	0.56
2:B:124:PRO:CB	2:B:126:GLN:HE22	2.18	0.56
2:E:116:VAL:HG22	2:E:160:MET:HG2	1.89	0.55
2:B:97:PRO:HB3	2:B:122:PHE:HB3	1.90	0.54
2:E:25:ARG:HD2	2:E:41:ASP:OD1	2.06	0.54
1:A:101:GLN:NE2	5:A:515:HOH:O	2.40	0.54
1:D:98:THR:HB	5:D:511:HOH:O	2.07	0.53
2:B:124:PRO:HG2	2:B:126:GLN:NE2	2.24	0.53
2:E:55:LEU:HB3	2:E:56:PRO:HD3	1.90	0.52
2:E:67:ILE:HD13	2:E:70:ARG:NH1	2.25	0.52
2:B:126:GLN:H	2:B:126:GLN:CD	2.18	0.52
2:B:86:GLU:HG3	2:B:90:THR:HB	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:88:ARG:HH11	2:E:88:ARG:HG2	1.75	0.51
2:E:67:ILE:HD13	2:E:70:ARG:HH12	1.74	0.51
1:A:30:GLU:HB2	1:A:138:LEU:HD11	1.93	0.50
2:E:94:ARG:HH11	2:E:94:ARG:HG3	1.76	0.50
2:B:103:PRO:HB3	2:B:115:LEU:HD12	1.94	0.49
2:E:189:ARG:HD3	2:E:189:ARG:H	1.76	0.49
1:A:43:TRP:CE3	1:A:48:LEU:HB3	2.47	0.49
1:D:171:ASP:HB2	1:D:172:LYS:HD3	1.95	0.49
1:A:70:LEU:O	1:A:74:ILE:HG13	2.13	0.48
2:B:10:GLN:HB2	2:B:31:ILE:HB	1.95	0.48
2:B:61:TRP:CZ2	3:C:9:LEU:HB2	2.47	0.48
2:B:134:ASN:HD21	2:B:170:VAL:H	1.62	0.48
1:A:69:ASN:O	1:A:73:LEU:HD23	2.13	0.48
1:A:101:GLN:NE2	1:A:102:PRO:HD2	2.28	0.48
1:A:23:THR:HG22	1:A:33:TYR:HB3	1.95	0.48
1:D:30:GLU:HB2	1:D:138:LEU:HD11	1.96	0.47
2:B:117:CYS:HB2	2:B:131:TRP:CZ2	2.50	0.47
2:B:125:ALA:HB1	2:B:147:LEU:CD2	2.44	0.47
2:B:134:ASN:ND2	2:B:170:VAL:H	2.13	0.47
1:A:101:GLN:HE21	1:A:102:PRO:HD2	1.79	0.47
2:B:25:ARG:HD2	2:B:41:ASP:OD1	2.15	0.47
2:B:31:ILE:HD13	2:B:36:GLU:HA	1.95	0.47
2:E:117:CYS:HB2	2:E:131:TRP:CZ2	2.49	0.47
1:D:172:LYS:HD3	1:D:172:LYS:N	2.30	0.47
2:E:25:ARG:HD3	2:E:43:ASP:CG	2.40	0.46
1:D:98:THR:O	1:D:101:GLN:HB3	2.14	0.46
2:B:119:VAL:HG11	2:B:127:ILE:HD11	1.98	0.46
1:A:98:THR:HG23	1:A:101:GLN:HB3	1.97	0.46
2:B:166:GLN:HB2	2:B:169:ASP:OD2	2.15	0.46
1:D:122:LEU:HD13	1:D:127:SER:HA	1.97	0.46
2:B:94:ARG:HG3	2:B:94:ARG:NH1	2.29	0.46
1:A:126:HIS:CD2	2:E:73:ALA:HA	2.51	0.45
2:B:103:PRO:HB2	2:B:113:ASN:HD21	1.82	0.45
2:B:126:GLN:NE2	2:B:126:GLN:N	2.59	0.45
1:D:108:LEU:HD13	5:D:545:HOH:O	2.17	0.45
1:D:174:LEU:HD23	1:D:175:LEU:N	2.31	0.45
1:D:113:PHE:HA	1:D:114:PRO:C	2.41	0.45
1:D:23:THR:HG22	1:D:33:TYR:CB	2.47	0.45
2:B:75:VAL:O	2:B:79:CYS:HB2	2.16	0.45
1:D:11:ASN:HB3	1:D:66:LEU:HD11	1.98	0.45
2:E:76:ASP:OD1	2:E:80:ARG:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:HIS:HD2	1:A:27:ASP:OD2	1.99	0.44
1:D:38:ARG:HG2	1:D:38:ARG:HH11	1.82	0.44
2:E:125:ALA:HB1	2:E:147:LEU:CD2	2.47	0.44
1:D:121:TRP:C	1:D:122:LEU:HD22	2.42	0.44
2:E:166:GLN:HB2	2:E:169:ASP:OD2	2.18	0.44
2:B:38:VAL:HG11	2:B:61:TRP:HZ3	1.81	0.44
2:E:38:VAL:HG22	2:E:54:GLY:HA3	2.00	0.44
2:B:105:ARG:NE	2:B:105:ARG:H	2.16	0.43
1:D:23:THR:HG22	1:D:33:TYR:HB3	1.99	0.43
1:D:107:CYS:HB2	1:D:121:TRP:CH2	2.54	0.43
1:A:95:SER:HB3	1:A:96:PRO:HD2	2.00	0.43
1:D:14:GLN:HE22	1:D:116:VAL:HG23	1.84	0.43
2:E:78:VAL:HG13	3:F:4:PHE:O	2.19	0.43
1:D:43:TRP:CE3	1:D:48:LEU:HB3	2.54	0.43
1:D:70:LEU:O	1:D:74:ILE:HG13	2.18	0.43
2:B:41:ASP:OD1	2:B:43:ASP:HB2	2.19	0.43
2:E:26:LEU:C	2:E:26:LEU:HD23	2.43	0.43
1:A:136:SER:O	1:A:138:LEU:HD22	2.18	0.42
1:D:176:LYS:NZ	1:D:176:LYS:HB2	2.35	0.42
1:D:13:TYR:CZ	1:D:67:LYS:HG3	2.55	0.42
1:A:97:VAL:HG11	1:A:180:PRO:HB3	2.01	0.42
2:E:180:LEU:HB3	2:E:182:SER:O	2.20	0.42
1:A:176:LYS:HD2	1:A:176:LYS:HA	1.92	0.41
2:B:3:SER:HA	2:B:4:PRO:HD3	1.90	0.41
2:B:36:GLU:HG2	2:B:50:VAL:CG1	2.35	0.41
2:B:26:LEU:C	2:B:26:LEU:HD23	2.45	0.41
1:D:73:LEU:HD23	2:E:32:TYR:CD1	2.55	0.41
2:B:36:GLU:CG	2:B:50:VAL:HG11	2.36	0.41
2:B:55:LEU:HB3	2:B:56:PRO:HD3	2.01	0.41
1:D:136:SER:O	1:D:138:LEU:HD22	2.21	0.41
2:B:189:ARG:H	2:B:189:ARG:CZ	2.33	0.41
1:D:98:THR:OG1	1:D:101:GLN:HB3	2.21	0.41
1:D:113:PHE:CE2	2:E:34:ARG:HG3	2.55	0.41
2:B:78:VAL:HG13	3:C:4:PHE:O	2.20	0.41
1:D:176:LYS:HB2	1:D:176:LYS:HZ3	1.85	0.41
2:E:61:TRP:CZ2	3:F:9:LEU:HB2	2.56	0.41
1:A:11:ASN:HD21	1:A:22:TYR:HE1	1.69	0.40
2:B:119:VAL:HG11	2:B:127:ILE:CD1	2.49	0.40
2:E:98:THR:OG1	2:E:120:THR:OG1	2.39	0.40
1:A:3:ALA:HB1	2:B:17:PHE:O	2.21	0.40
1:A:39:LYS:O	1:A:39:LYS:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:LEU:C	1:D:175:LEU:HD22	2.47	0.40
2:B:172:THR:HG23	5:B:199:HOH:O	2.20	0.40
2:E:82:ASN:O	2:E:86:GLU:HG2	2.21	0.40
1:D:73:LEU:HD23	2:E:32:TYR:HB2	2.04	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	177/193 (92%)	174 (98%)	2 (1%)	1 (1%)	21	22
1	D	175/193 (91%)	171 (98%)	4 (2%)	0	100	100
2	B	177/198 (89%)	164 (93%)	12 (7%)	1 (1%)	21	22
2	E	176/198 (89%)	171 (97%)	5 (3%)	0	100	100
3	C	9/11 (82%)	9 (100%)	0	0	100	100
3	F	9/11 (82%)	9 (100%)	0	0	100	100
All	All	723/804 (90%)	698 (96%)	23 (3%)	2 (0%)	36	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	135	ASP
1	A	9(A)	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	163/176 (93%)	156 (96%)	7 (4%)	26	33
1	D	161/176 (92%)	154 (96%)	7 (4%)	26	33
2	B	165/181 (91%)	157 (95%)	8 (5%)	23	28
2	E	163/181 (90%)	160 (98%)	3 (2%)	51	66
3	C	8/11 (73%)	8 (100%)	0	100	100
3	F	9/11 (82%)	9 (100%)	0	100	100
All	All	669/736 (91%)	644 (96%)	25 (4%)	30	39

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	98	THR
1	A	108	LEU
1	A	140	LYS
1	A	153	LEU
1	A	171	ASP
1	A	174	LEU
2	B	50	VAL
2	B	52	LEU
2	B	75	VAL
2	B	86	GLU
2	B	105	ARG
2	B	115	LEU
2	B	126	GLN
2	B	189	ARG
1	D	45	LEU
1	D	101	GLN
1	D	108	LEU
1	D	153	LEU
1	D	171	ASP
1	D	172	LYS
1	D	176	LYS
2	E	50	VAL
2	E	87	LEU
2	E	172	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	11	ASN
1	A	14	GLN
1	A	31	GLN
1	A	71	ASN
1	A	101	GLN
1	A	126	HIS
1	A	177	HIS
2	B	64	GLN
2	B	84	GLN
2	B	92	GLN
2	B	113	ASN
2	B	126	GLN
2	B	134	ASN
2	B	150	ASN
2	B	156	GLN
2	B	166	GLN
1	D	5	HIS
1	D	14	GLN
1	D	71	ASN
1	D	111	ASN
1	D	167	HIS
1	D	177	HIS
2	E	92	GLN
2	E	166	GLN
2	E	174	HIS
2	E	181	GLN
3	F	6	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no 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	EDO	A	504	-	3,3,3	0.50	0	2,2,2	0.30	0
4	EDO	D	503	-	3,3,3	0.43	0	2,2,2	0.42	0
4	EDO	A	501	-	3,3,3	0.36	0	2,2,2	0.42	0
4	EDO	D	502	-	3,3,3	0.36	0	2,2,2	0.43	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	EDO	A	504	-	-	0/1/1/1	-
4	EDO	D	503	-	-	0/1/1/1	-
4	EDO	A	501	-	-	0/1/1/1	-
4	EDO	D	502	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.