Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 05:52 PM EDT

PDB ID	:	1S9V
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 (i) 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 (i)) were used in the production of this report:

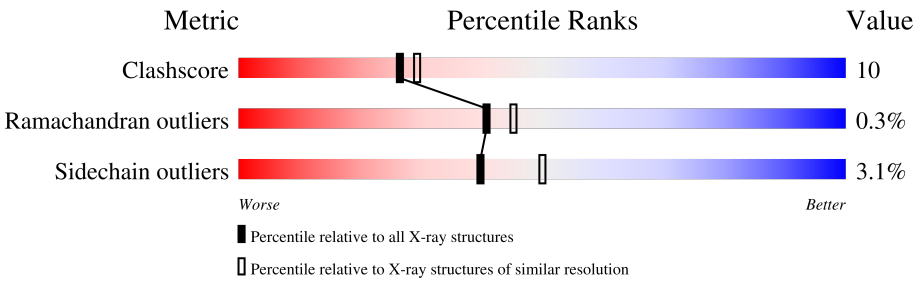
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.22 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	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	193	72% 20% • 7%
1	D	193	70% 19% • 8%
2	B	198	68% 21% • 9%
2	E	198	70% 20% • 9%
3	C	11	82% 18%
3	F	11	82% 18%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	179	1428	920	234	271	3	0	0	0
1	D	177	1412	910	232	267	3	0	0	0

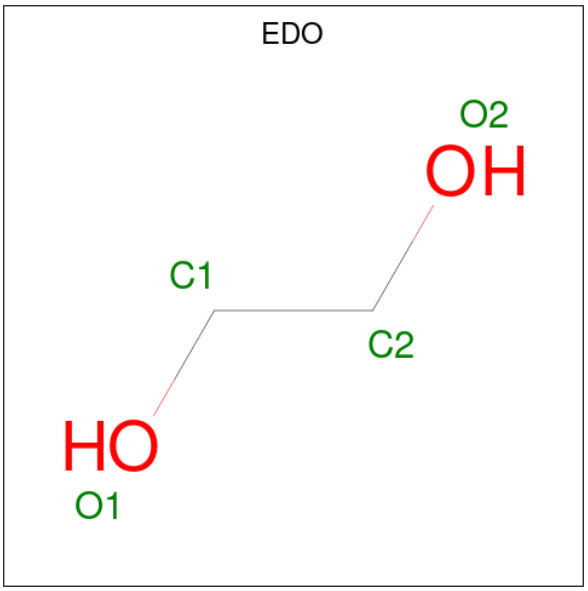
- Molecule 2 is a protein called HLA class II histocompatibility antigen, DQ(1) beta chain.

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

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

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is water.

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

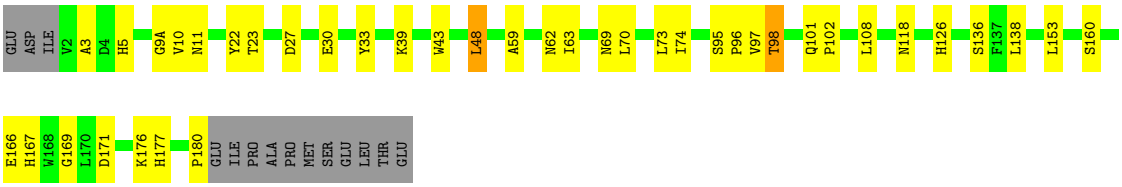
3 Residue-property plots (i)

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.

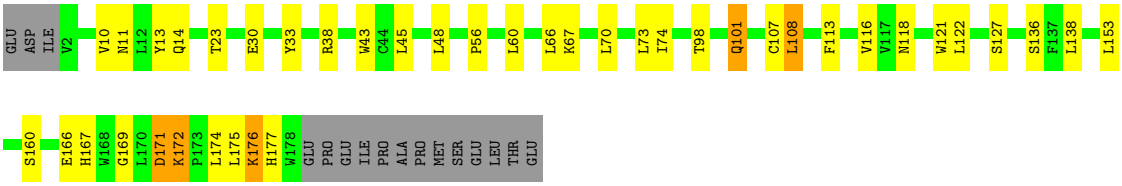
• Molecule 1: HLA class II histocompatibility antigen, DQ(3) alpha chain

Chain A:



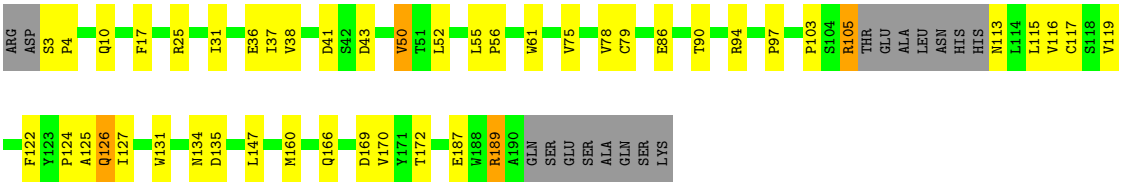
• Molecule 1: HLA class II histocompatibility antigen, DQ(3) alpha chain

Chain D:



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

Chain B:

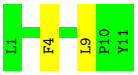


• Molecule 2: HLA class II histocompatibility antigen, DQ(1) beta chain

Chain E:

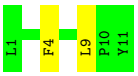
• Molecule 3: alpha-I gliadin

Chain C: 82% 18%



• Molecule 3: alpha-I gliadin

Chain F: 82% 18%



4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

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	0.36	0/1470	0.66	1/2008 (0.0%)
1	D	0.37	0/1453	0.63	1/1984 (0.1%)
2	B	0.35	0/1519	0.62	0/2062
2	E	0.35	0/1503	0.64	0/2041
3	C	0.50	0/82	0.59	0/111
3	F	0.47	0/91	0.60	0/124
All	All	0.36	0/6118	0.64	2/8330 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	10	VAL	N-CA-C	-5.74	95.51	111.00
1	A	10	VAL	N-CA-C	-5.21	96.95	111.00

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	29	0
2	B	1486	0	1457	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1470	0	1437	29	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	121	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 10.

All (121) 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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:25:ARG:HD3	2:B:43:ASP:CG	2.26	0.56
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:86:GLU:HG3	2:B:90:THR:HB	1.90	0.52
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:126:GLN:H	2:B:126:GLN:CD	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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
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
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:25:ARG:HD3	2:E:43:ASP:CG	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:GLU:HG2	2:B:50:VAL:CG1	2.35	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
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
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
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%)	25	25
1	D	175/193 (91%)	171 (98%)	4 (2%)	0	100	100
2	B	177/198 (89%)	164 (93%)	12 (7%)	1 (1%)	25	25
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%)	41	45

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%)	158 (97%)	5 (3%)	40	50
1	D	161/176 (92%)	154 (96%)	7 (4%)	29	35
2	B	165/181 (91%)	160 (97%)	5 (3%)	41	51
2	E	163/181 (90%)	159 (98%)	4 (2%)	47	58
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%)	648 (97%)	21 (3%)	40	50

All (21) 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	153	LEU
1	A	171	ASP
2	B	50	VAL
2	B	52	LEU
2	B	105	ARG
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

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Mol	Chain	Res	Type
1	D	172	LYS
1	D	176	LYS
2	E	50	VAL
2	E	87	LEU
2	E	172	THR
2	E	189	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	11	ASN
1	A	14	GLN
1	A	71	ASN
1	A	101	GLN
2	B	84	GLN
2	B	92	GLN
2	B	113	ASN
2	B	126	GLN
2	B	134	ASN
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	113	ASN
2	E	166	GLN
2	E	174	HIS
2	E	181	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	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
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

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	501	-	-	0/1/1/1	-
4	EDO	D	502	-	-	0/1/1/1	-
4	EDO	A	504	-	-	0/1/1/1	-
4	EDO	D	503	-	-	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 (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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.