



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:12 pm BST

PDB ID : 1D5X
Title : X-RAY CRYSTAL STRUCTURE OF HLA-DR4 COMPLEXED WITH
DIPEPTIDE MIMETIC AND SEB
Authors : Swain, A.; Crowther, R.; Kammlott, U.
Deposited on : 1999-10-12
Resolution : 2.45 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

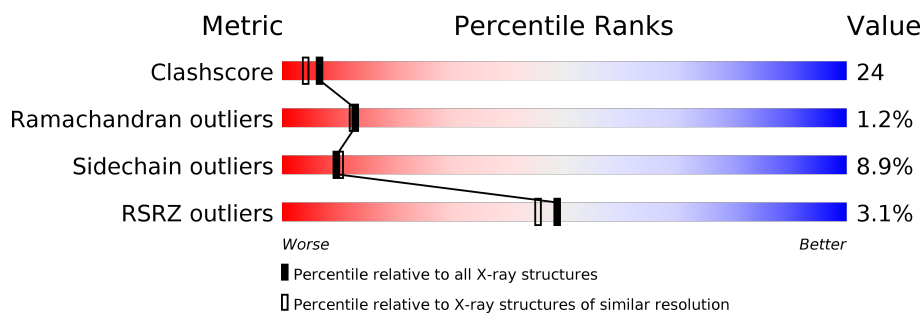
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 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	181	<div> <div>%</div> <div> <div></div> <div>59%</div> <div>36%</div> <div>..</div> </div> </div>
2	B	192	<div> <div>3%</div> <div> <div></div> <div>49%</div> <div>43%</div> <div>.. 5%</div> </div> </div>
3	C	239	<div> <div>4%</div> <div> <div></div> <div>54%</div> <div>33%</div> <div>6%</div> <div>7%</div> </div> </div>
4	D	6	<div> <div> <div></div> <div>67%</div> <div>33%</div> </div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4910 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	0	0	0
			1474	954	239	276	5			

- Molecule 2 is a protein called HLA CLASS II HISTOCOMPATIBILITY ANTIGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	183	Total	C	N	O	S	0	0	0
			1509	954	265	285	5			

- Molecule 3 is a protein called ENTEROTOXIN TYPE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	223	Total	C	N	O	S	0	0	0
			1863	1196	298	359	10			

- Molecule 4 is a protein called DIPEPTIDE MIMETIC INHIBITOR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	6	Total	C	N	O	0	0	0
			54	37	9	8			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total	O	0	0
			7	7		
5	C	3	Total	O	0	0
			3	3		

- Molecule 1: HLA CLASS II HISTOCOMPATIBILITY ANTIGEN



- Molecule 4: DIPEPTIDE MIMETIC INHIBITOR

Chain D:  67% 33%

7803	7803	7803	7803
A804	A804	A804	A804
R805	R805	R805	R805
A806	A806	A806	A806
7807	7807	7807	7807
S808	S808	S808	S808

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.84Å 104.25Å 107.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.45 19.77 – 2.44	Depositor EDS
% Data completeness (in resolution range)	93.3 (20.00-2.45) 92.8 (19.77-2.44)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.44Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.237 , 0.268 0.239 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4910	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAA, HAQ, SEL, ALC, ACE

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	0.73	0/1519	0.87	2/2070 (0.1%)
2	B	0.68	1/1549 (0.1%)	0.88	4/2104 (0.2%)
3	C	0.80	3/1906 (0.2%)	0.85	3/2564 (0.1%)
4	D	0.81	0/10	0.85	0/11
All	All	0.74	4/4984 (0.1%)	0.87	9/6749 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	61	TYR	CZ-OH	15.90	1.64	1.37
3	C	61	TYR	CE1-CZ	11.13	1.53	1.38
3	C	61	TYR	CE2-CZ	6.92	1.47	1.38
2	B	104	ALA	C-N	-5.60	1.21	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	104	ALA	CA-C-N	-8.85	97.72	117.20
3	C	61	TYR	CZ-CE2-CD2	7.94	126.94	119.80
3	C	61	TYR	CE1-CZ-CE2	-7.62	107.61	119.80
2	B	166	ARG	NE-CZ-NH2	6.55	123.58	120.30
1	A	44	ARG	NE-CZ-NH1	-5.79	117.41	120.30
2	B	103	PRO	C-N-CA	-5.69	107.47	121.70
1	A	11	GLU	OE1-CD-OE2	-5.64	116.53	123.30
3	C	200	MET	N-CA-CB	-5.53	100.66	110.60
2	B	27	LEU	CA-CB-CG	5.44	127.81	115.30

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	1474	0	1407	66	0
2	B	1509	0	1416	83	0
3	C	1863	0	1804	88	0
4	D	54	0	56	1	0
5	A	7	0	0	0	0
5	C	3	0	0	0	0
All	All	4910	0	4683	224	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 24.

All (224) 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)
3:C:61:TYR:OH	3:C:61:TYR:CZ	1.64	1.48
2:B:150:ASN:HD22	2:B:154:THR:HG22	1.18	1.08
1:A:108:PHE:CE2	1:A:110:ASP:CB	2.42	1.02
3:C:14:SER:HB3	3:C:201:MET:CE	1.91	1.01
1:A:108:PHE:CE2	1:A:110:ASP:HB2	1.96	0.99
3:C:31:ASN:HD21	3:C:58:LEU:HD21	1.33	0.92
2:B:97:PRO:HB3	2:B:122:PHE:HB3	1.53	0.90
3:C:7:LYS:NZ	3:C:9:ASP:HB2	1.87	0.88
2:B:170:VAL:HG22	2:B:189:ARG:NE	1.89	0.87
1:A:41:THR:HG22	1:A:56:ALA:HB2	1.56	0.87
2:B:152:ASP:OD1	2:B:154:THR:HB	1.75	0.87
3:C:20:LEU:H	3:C:20:LEU:HD23	1.39	0.87
3:C:14:SER:HB3	3:C:201:MET:HE3	1.55	0.85
1:A:108:PHE:HE2	1:A:110:ASP:CB	1.83	0.85
1:A:113:THR:HG22	1:A:114:PRO:HA	1.60	0.84
3:C:57:LYS:HD2	3:C:58:LEU:HD23	1.59	0.83
2:B:114:LEU:HD23	2:B:162:GLU:HA	1.61	0.82
3:C:31:ASN:ND2	3:C:58:LEU:HD21	1.94	0.82
2:B:150:ASN:ND2	2:B:154:THR:HG22	1.98	0.78
1:A:89:VAL:HG21	1:A:165:VAL:HG11	1.64	0.78
3:C:21:MET:HG3	3:C:179:ASN:HA	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:129:VAL:HG22	2:B:175:VAL:HG22	1.67	0.77
3:C:83:ASP:HB2	3:C:119:THR:HG22	1.67	0.74
3:C:7:LYS:HZ2	3:C:9:ASP:HB2	1.52	0.73
2:B:19:ASN:O	2:B:22:GLU:HG3	1.88	0.73
1:A:108:PHE:CE2	1:A:110:ASP:HB3	2.25	0.71
1:A:134:GLU:OE1	1:A:149:HIS:NE2	2.25	0.69
2:B:121:GLY:HA2	2:B:154:THR:HG23	1.74	0.69
3:C:7:LYS:HZ3	3:C:9:ASP:HB2	1.57	0.69
2:B:132:PHE:HD1	2:B:137:GLU:HA	1.58	0.69
2:B:170:VAL:HA	2:B:189:ARG:HG2	1.76	0.68
1:A:4:GLU:OE2	2:B:16:HIS:HD2	1.77	0.68
3:C:154:LYS:HB2	3:C:154:LYS:NZ	2.09	0.68
2:B:145:THR:CG2	2:B:158:LEU:H	2.07	0.68
3:C:134:VAL:HG22	3:C:230:ILE:HB	1.76	0.67
3:C:237:LYS:HZ3	3:C:237:LYS:HB3	1.62	0.65
1:A:66:ASP:OD1	2:B:11:VAL:HG21	1.96	0.65
2:B:99:VAL:HG21	2:B:184:LEU:HD22	1.79	0.65
3:C:138:GLU:OE1	3:C:234:LEU:HB2	1.96	0.65
3:C:20:LEU:CD2	3:C:20:LEU:H	2.10	0.65
1:A:100:ARG:HB2	1:A:100:ARG:NH1	2.12	0.63
3:C:31:ASN:HD21	3:C:58:LEU:CD2	2.09	0.63
1:A:108:PHE:HE2	1:A:110:ASP:CG	2.01	0.63
2:B:10:GLN:HB2	2:B:31:PHE:HB2	1.81	0.63
2:B:127:ILE:HD11	2:B:175:VAL:HG13	1.80	0.62
3:C:165:ARG:O	3:C:169:VAL:HG13	1.99	0.62
2:B:28:ASP:OD1	2:B:30:TYR:HE1	1.84	0.60
3:C:33:VAL:HG23	3:C:88:ASN:HB3	1.82	0.60
2:B:145:THR:HG22	2:B:158:LEU:O	2.01	0.60
3:C:7:LYS:HD3	3:C:9:ASP:H	1.67	0.60
1:A:70:LEU:O	1:A:74:THR:HB	2.01	0.60
3:C:61:TYR:HB2	3:C:111:LYS:HB3	1.84	0.60
3:C:187:ILE:HB	3:C:200:MET:CE	2.33	0.59
3:C:213:TYR:O	3:C:216:MET:HG2	2.02	0.59
1:A:108:PHE:HD1	1:A:148:PHE:CE2	2.22	0.58
3:C:39:LYS:HE3	3:C:79:ASP:HA	1.85	0.58
3:C:135:ARG:NH2	3:C:231:GLU:OE1	2.37	0.58
3:C:87:ALA:H	3:C:158:GLN:HE21	1.51	0.58
2:B:127:ILE:HD12	2:B:176:GLU:O	2.03	0.57
1:A:123:ARG:HG2	1:A:123:ARG:HH11	1.69	0.57
1:A:11:GLU:HG2	2:B:11:VAL:HB	1.86	0.57
3:C:176:GLU:HG3	3:C:179:ASN:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:TYR:OH	2:B:71:LYS:HE3	2.06	0.56
3:C:24:MET:HG2	3:C:175:TYR:CE2	2.41	0.56
3:C:41:ILE:HD13	3:C:52:SER:HB2	1.87	0.56
1:A:135:THR:O	1:A:147:LYS:HE2	2.05	0.56
2:B:95:VAL:HG23	2:B:122:PHE:HA	1.88	0.56
2:B:97:PRO:CB	2:B:122:PHE:HB3	2.32	0.56
3:C:132:ILE:HD13	3:C:228:VAL:HG13	1.87	0.56
2:B:170:VAL:HG22	2:B:189:ARG:CD	2.36	0.56
2:B:55:ARG:HH11	2:B:55:ARG:HG2	1.71	0.55
3:C:154:LYS:HB2	3:C:154:LYS:HZ3	1.72	0.55
1:A:143:HIS:CE1	2:B:31:PHE:HE2	2.25	0.55
1:A:82:ILE:HB	2:B:33:HIS:CE1	2.42	0.55
3:C:14:SER:HB3	3:C:201:MET:HE2	1.87	0.55
1:A:147:LYS:NZ	1:A:149:HIS:HE1	2.05	0.54
3:C:226:LYS:HG2	3:C:226:LYS:O	2.07	0.54
3:C:38:VAL:HG22	3:C:39:LYS:N	2.22	0.54
2:B:104:ALA:HB2	2:B:116:VAL:HG23	1.90	0.54
3:C:14:SER:CB	3:C:201:MET:HE3	2.34	0.54
1:A:165:VAL:HG13	1:A:174:LEU:HB3	1.89	0.53
1:A:129:THR:HG22	1:A:129:THR:O	2.08	0.53
1:A:14:LEU:HD11	2:B:6:ARG:HB3	1.89	0.53
3:C:154:LYS:HB3	3:C:222:MET:HE3	1.90	0.53
1:A:100:ARG:CZ	1:A:100:ARG:HB2	2.39	0.52
1:A:82:ILE:HB	2:B:33:HIS:ND1	2.23	0.52
3:C:37:ASN:OD1	3:C:121:HIS:ND1	2.41	0.52
3:C:161:ASP:O	3:C:165:ARG:HG3	2.08	0.52
1:A:108:PHE:CD1	1:A:148:PHE:CE2	2.98	0.52
2:B:163:THR:O	2:B:165:PRO:HD3	2.09	0.52
2:B:102:TYR:O	2:B:103:PRO:O	2.28	0.51
2:B:25:ARG:HD2	2:B:43:ASP:OD2	2.10	0.51
3:C:187:ILE:HB	3:C:200:MET:HE1	1.93	0.51
3:C:38:VAL:O	3:C:81:TYR:HA	2.11	0.51
1:A:61:ALA:HB2	3:C:94:TYR:CE2	2.45	0.50
3:C:189:PHE:O	3:C:195:SER:HA	2.12	0.50
2:B:184:LEU:C	2:B:184:LEU:HD23	2.32	0.50
3:C:7:LYS:HD3	3:C:7:LYS:C	2.32	0.50
1:A:143:HIS:CE1	2:B:31:PHE:CE2	2.99	0.50
2:B:67:LEU:HD11	2:B:71:LYS:HE2	1.94	0.50
2:B:95:VAL:HG22	2:B:123:TYR:N	2.27	0.50
2:B:170:VAL:HG22	2:B:189:ARG:HE	1.74	0.49
2:B:28:ASP:OD1	2:B:30:TYR:CE1	2.64	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:187:ILE:HB	3:C:200:MET:HE3	1.94	0.49
2:B:145:THR:HG21	2:B:158:LEU:HB2	1.95	0.49
3:C:132:ILE:HD13	3:C:228:VAL:CG1	2.42	0.49
3:C:183:GLU:HG3	3:C:184:THR:HG23	1.95	0.48
2:B:102:TYR:C	2:B:103:PRO:O	2.51	0.48
2:B:104:ALA:HB2	2:B:114:LEU:O	2.13	0.48
3:C:12:HIS:N	3:C:12:HIS:CD2	2.82	0.48
3:C:179:ASN:ND2	3:C:180:SER:H	2.11	0.48
3:C:7:LYS:O	3:C:10:GLU:HG3	2.13	0.48
3:C:111:LYS:HD3	3:C:111:LYS:HA	1.63	0.48
1:A:142:ASP:O	1:A:143:HIS:HB2	2.14	0.48
3:C:63:ASN:O	3:C:111:LYS:HB2	2.14	0.48
1:A:108:PHE:CE1	1:A:148:PHE:CZ	3.02	0.48
2:B:18:PHE:HB2	2:B:23:ARG:HB3	1.96	0.48
2:B:55:ARG:NH1	2:B:55:ARG:HG2	2.27	0.48
2:B:97:PRO:HB3	2:B:122:PHE:CB	2.36	0.48
3:C:14:SER:CB	3:C:201:MET:CE	2.79	0.48
2:B:104:ALA:CB	2:B:114:LEU:O	2.62	0.47
2:B:117:CYS:HB2	2:B:131:TRP:CZ2	2.49	0.47
3:C:237:LYS:NZ	3:C:237:LYS:HB3	2.26	0.47
1:A:70:LEU:HD13	2:B:9:GLU:HB2	1.96	0.47
3:C:38:VAL:HG22	3:C:39:LYS:H	1.79	0.47
1:A:5:HIS:HD2	1:A:27:ASP:OD2	1.97	0.47
3:C:42:ASP:CG	3:C:43:GLN:H	2.18	0.47
1:A:12:PHE:C	1:A:12:PHE:CD1	2.88	0.47
1:A:105:LEU:HG	1:A:153:PHE:CE1	2.50	0.47
1:A:7:ILE:HG12	1:A:26:PHE:HD1	1.80	0.47
3:C:61:TYR:HA	3:C:111:LYS:HD2	1.96	0.47
3:C:134:VAL:HG11	3:C:164:THR:HG23	1.97	0.46
3:C:87:ALA:H	3:C:158:GLN:NE2	2.11	0.46
3:C:171:ASN:N	3:C:171:ASN:HD22	2.13	0.46
3:C:232:VAL:HG12	3:C:234:LEU:HD12	1.97	0.46
1:A:147:LYS:HZ2	1:A:149:HIS:HE1	1.62	0.46
3:C:138:GLU:HA	3:C:138:GLU:OE1	2.14	0.46
3:C:25:LYS:HD2	3:C:175:TYR:O	2.15	0.46
2:B:24:VAL:HG21	2:B:80:ARG:HG3	1.97	0.46
2:B:17:PHE:HB3	2:B:20:GLY:O	2.16	0.46
3:C:136:VAL:HG21	3:C:146:PHE:HE1	1.80	0.46
3:C:154:LYS:HB3	3:C:222:MET:CE	2.45	0.46
3:C:180:SER:C	3:C:182:TYR:H	2.18	0.46
2:B:145:THR:HG23	2:B:145:THR:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:GLU:OE2	2:B:13:HIS:HE1	1.99	0.46
1:A:122:LEU:HB2	1:A:162:ASP:HB2	1.98	0.46
3:C:13:LYS:HB3	3:C:183:GLU:OE1	2.16	0.46
1:A:100:ARG:CB	1:A:100:ARG:NH1	2.79	0.45
3:C:138:GLU:HG3	3:C:182:TYR:HE2	1.81	0.45
2:B:170:VAL:CG1	2:B:187:GLU:HG3	2.46	0.45
3:C:85:PHE:CD2	3:C:159:GLU:HG3	2.52	0.45
1:A:69:ASN:O	1:A:73:MET:HB2	2.17	0.45
2:B:38:VAL:HG22	2:B:39:ARG:N	2.32	0.45
3:C:33:VAL:CG2	3:C:88:ASN:HB3	2.46	0.45
1:A:108:PHE:CD2	1:A:110:ASP:HB3	2.51	0.45
2:B:127:ILE:HD11	2:B:175:VAL:CG1	2.46	0.45
1:A:99:LEU:HD12	1:A:180:PHE:CE1	2.51	0.45
3:C:176:GLU:HG2	3:C:181:PRO:HD3	1.98	0.44
3:C:48:ASP:HB2	3:C:66:VAL:O	2.17	0.44
1:A:16:PRO:O	1:A:18:GLN:HG3	2.16	0.44
3:C:85:PHE:CE2	3:C:159:GLU:HG3	2.52	0.44
1:A:118:ASN:HB2	1:A:166:GLU:HB2	2.00	0.44
2:B:28:ASP:HB3	2:B:40:PHE:HB3	1.99	0.44
3:C:90:TYR:O	3:C:91:TYR:C	2.56	0.44
1:A:86:PRO:HA	1:A:87:PRO:HD3	1.84	0.43
2:B:130:ARG:HG3	2:B:130:ARG:HH11	1.82	0.43
2:B:145:THR:CG2	2:B:158:LEU:HB2	2.48	0.43
2:B:145:THR:HG22	2:B:158:LEU:H	1.83	0.43
1:A:32:PHE:C	1:A:32:PHE:CD1	2.91	0.43
2:B:116:VAL:HG12	2:B:117:CYS:N	2.34	0.43
2:B:18:PHE:HD1	2:B:23:ARG:O	2.01	0.43
3:C:194:ASN:OD1	3:C:195:SER:N	2.51	0.43
3:C:238:LYS:O	3:C:238:LYS:HG2	2.18	0.43
2:B:114:LEU:CD2	2:B:162:GLU:HA	2.41	0.43
3:C:176:GLU:CG	3:C:179:ASN:O	2.65	0.43
1:A:165:VAL:CG1	1:A:174:LEU:HB3	2.47	0.43
3:C:30:ASP:O	3:C:32:HIS:HD2	2.02	0.43
2:B:145:THR:O	2:B:146:GLY:C	2.56	0.43
3:C:180:SER:O	3:C:237:LYS:HE2	2.19	0.43
2:B:170:VAL:HG22	2:B:189:ARG:HG2	2.00	0.42
2:B:31:PHE:CD1	2:B:31:PHE:N	2.87	0.42
3:C:21:MET:HG3	3:C:179:ASN:CA	2.43	0.42
1:A:47:GLU:O	1:A:50:ARG:HB2	2.19	0.42
2:B:134:ASN:OD1	2:B:169:GLU:HA	2.19	0.42
1:A:68:ALA:O	1:A:72:ILE:HD13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:PHE:HB2	2:B:47:TYR:CE2	2.54	0.42
2:B:132:PHE:CD1	2:B:137:GLU:HA	2.47	0.42
1:A:11:GLU:CG	2:B:11:VAL:HB	2.49	0.42
1:A:81:PRO:HB3	2:B:5:PRO:HB2	2.02	0.42
4:D:805:ARG:HA	4:D:806:MAA:HM1	1.66	0.42
3:C:85:PHE:CD2	3:C:85:PHE:C	2.92	0.42
1:A:72:ILE:HD12	1:A:72:ILE:H	1.85	0.42
1:A:89:VAL:O	1:A:176:LYS:HE3	2.19	0.42
2:B:50:VAL:HG12	2:B:51:THR:HG23	2.02	0.42
2:B:95:VAL:O	2:B:95:VAL:CG2	2.67	0.41
1:A:121:TRP:HB2	1:A:128:VAL:HG23	2.02	0.41
3:C:187:ILE:HG23	3:C:187:ILE:O	2.20	0.41
2:B:137:GLU:CG	2:B:138:GLU:N	2.82	0.41
1:A:24:PHE:HB3	1:A:31:ILE:HD12	2.02	0.41
3:C:154:LYS:HB2	3:C:154:LYS:HZ2	1.85	0.41
2:B:171:TYR:HB2	2:B:188:TRP:O	2.21	0.41
2:B:95:VAL:O	2:B:95:VAL:HG23	2.20	0.41
1:A:72:ILE:N	1:A:72:ILE:HD12	2.35	0.41
1:A:79:TYR:N	1:A:79:TYR:CD1	2.89	0.41
3:C:7:LYS:HA	3:C:8:PRO:HD2	1.84	0.41
3:C:188:LYS:HA	3:C:197:TRP:HA	2.02	0.41
1:A:147:LYS:NZ	1:A:149:HIS:CE1	2.86	0.41
2:B:115:LEU:HD12	2:B:171:TYR:CD2	2.56	0.41
2:B:170:VAL:HG13	2:B:187:GLU:HG3	2.03	0.41
1:A:81:PRO:HB3	2:B:5:PRO:CB	2.51	0.41
1:A:100:ARG:CB	1:A:100:ARG:HH11	2.34	0.41
1:A:121:TRP:O	1:A:128:VAL:HG22	2.20	0.41
1:A:13:TYR:CE2	1:A:67:LYS:HG3	2.55	0.40
2:B:14:GLU:OE1	2:B:16:HIS:HE1	2.04	0.40
3:C:71:LYS:HG2	3:C:75:ASP:OD2	2.22	0.40
2:B:184:LEU:HD23	2:B:185:THR:N	2.36	0.40
2:B:24:VAL:HG11	2:B:79:CYS:CB	2.52	0.40
1:A:164:ARG:HA	1:A:174:LEU:O	2.21	0.40
3:C:214:LEU:HD12	3:C:214:LEU:HA	1.94	0.40
3:C:189:PHE:CD2	3:C:230:ILE:HD13	2.56	0.40
1:A:101:GLU:HA	1:A:102:PRO:HD3	1.92	0.40
1:A:123:ARG:CG	1:A:123:ARG:HH11	2.33	0.40
1:A:95:SER:HB2	1:A:96:PRO:CD	2.51	0.40
2:B:90:THR:OG1	2:B:91:VAL:N	2.53	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	177/181 (98%)	165 (93%)	12 (7%)	0	100	100
2	B	179/192 (93%)	158 (88%)	18 (10%)	3 (2%)	9	7
3	C	219/239 (92%)	199 (91%)	16 (7%)	4 (2%)	8	6
4	D	1/6 (17%)	1 (100%)	0	0	100	100
All	All	576/618 (93%)	523 (91%)	46 (8%)	7 (1%)	13	12

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	78	LYS
3	C	91	TYR
3	C	192	ASN
2	B	103	PRO
3	C	8	PRO
2	B	146	GLY
2	B	124	PRO

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	164/166 (99%)	150 (92%)	14 (8%)	10	12
2	B	163/173 (94%)	149 (91%)	14 (9%)	10	11
3	C	209/225 (93%)	189 (90%)	20 (10%)	8	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	1/1 (100%)	1 (100%)	0	100	100
All	All	537/565 (95%)	489 (91%)	48 (9%)	9	10

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	44	ARG
1	A	65	VAL
1	A	74	THR
1	A	76	ARG
1	A	83	THR
1	A	92	LEU
1	A	98	GLU
1	A	99	LEU
1	A	110	ASP
1	A	113	THR
1	A	130	THR
1	A	171	ASP
1	A	180	PHE
2	B	21	THR
2	B	35	GLU
2	B	48	ARG
2	B	52	GLU
2	B	66	ASP
2	B	69	GLU
2	B	87	GLU
2	B	88	SER
2	B	115	LEU
2	B	130	ARG
2	B	143	VAL
2	B	160	MET
2	B	176	GLU
2	B	181	THR
3	C	5	ASP
3	C	9	ASP
3	C	20	LEU
3	C	21	MET
3	C	56	THR
3	C	58	LEU
3	C	73	LEU
3	C	96	SER

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Mol	Chain	Res	Type
3	C	119	THR
3	C	120	GLU
3	C	127	ASP
3	C	131	SER
3	C	138	GLU
3	C	154	LYS
3	C	155	VAL
3	C	169	VAL
3	C	195	SER
3	C	214	LEU
3	C	224	ASP
3	C	237	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	143	HIS
1	A	149	HIS
2	B	16	HIS
2	B	149	GLN
2	B	150	ASN
2	B	156	GLN
3	C	3	GLN
3	C	23	ASN
3	C	31	ASN
3	C	32	HIS
3	C	92	GLN
3	C	158	GLN
3	C	171	ASN
3	C	179	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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$
4	HAQ	D	807	4	16,19,20	1.56	4 (25%)	18,28,30	1.42	2 (11%)
4	ALC	D	804	4	9,11,12	0.52	0	10,13,15	0.89	1 (10%)
4	MAA	D	806	4	4,5,6	0.83	0	1,5,7	0.64	0
4	SEL	D	808	4	5,5,5	0.37	0	3,5,5	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
4	HAQ	D	807	4	-	0/0/27/29	0/3/3/3
4	ALC	D	804	4	-	0/5/14/16	0/1/1/1
4	MAA	D	806	4	-	1/1/4/6	-
4	SEL	D	808	4	-	0/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	807	HAQ	CE2-CZ	3.21	1.45	1.38
4	D	807	HAQ	CB2-CG2	-3.00	1.45	1.50
4	D	807	HAQ	CG-CE1	2.58	1.57	1.51
4	D	807	HAQ	C-N2	-2.43	1.33	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	807	HAQ	CG2-CB2-CA2	2.94	107.50	103.34
4	D	804	ALC	CG-CB-CA	2.64	118.07	114.52
4	D	807	HAQ	CA2-N2-C	2.44	121.88	118.70

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	806	MAA	CB-CA-N-CM

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	806	MAA	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	807:HAQ	C	808:SEL	N	4.67

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	179/181 (98%)	-0.51	2 (1%) 80 80	20, 34, 59, 89	0
2	B	183/192 (95%)	-0.05	6 (3%) 46 43	19, 41, 84, 95	0
3	C	223/239 (93%)	-0.09	10 (4%) 33 30	25, 48, 84, 100	0
4	D	1/6 (16%)	-1.04	0 100 100	37, 37, 37, 37	0
All	All	586/618 (94%)	-0.21	18 (3%) 49 45	19, 41, 81, 100	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	GLY	12.2
3	C	56	THR	5.0
2	B	164	VAL	4.8
3	C	60	ASN	4.4
2	B	3	THR	4.0
2	B	189	ARG	3.8
3	C	54	LYS	3.7
3	C	238	LYS	3.5
3	C	20	LEU	3.2
1	A	181	ASP	3.1
3	C	8	PRO	2.9
2	B	168	GLY	2.6
2	B	2	ASP	2.6
3	C	127	ASP	2.6
1	A	3	GLU	2.6
3	C	193	GLU	2.4
3	C	55	ASP	2.2
3	C	194	ASN	2.2

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(\AA^2)	Q<0.9
4	SEL	D	808	6/6	0.86	0.20	35,38,42,48	0
4	HAQ	D	807	17/18	0.92	0.13	32,35,45,46	0
4	MAA	D	806	6/7	0.95	0.16	27,30,30,32	0
4	ALC	D	804	11/12	0.95	0.15	24,30,36,39	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.