Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:55 PM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

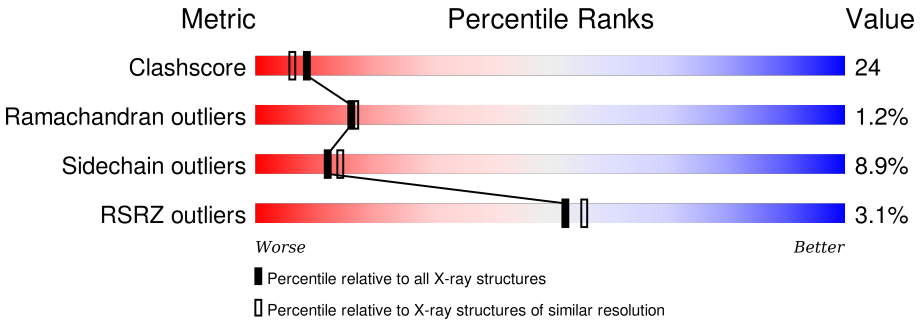
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

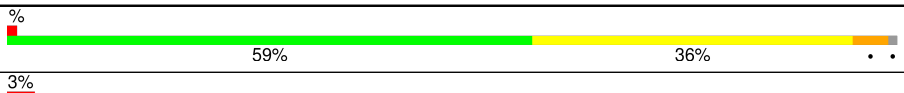
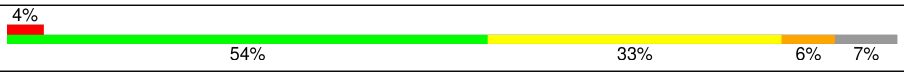
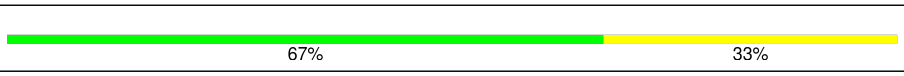
The reported resolution of this entry is 2.45 Å.

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	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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. 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% 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	
2	B	192	
3	C	239	
4	D	6	

2 Entry composition

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.

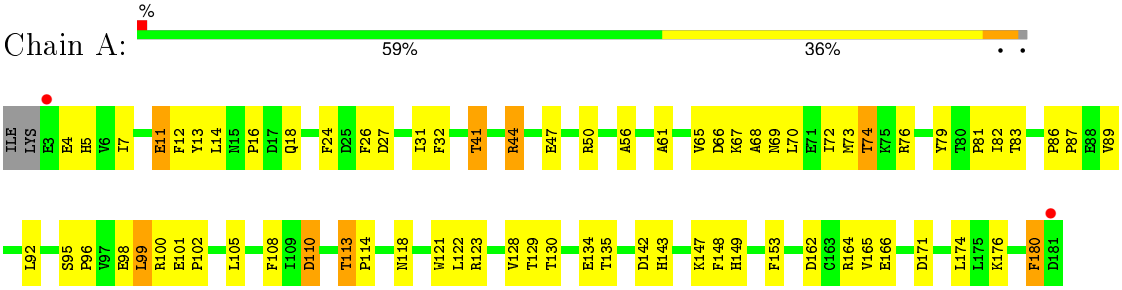
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total	O	0	0
			7	7		
5	C	3	Total	O	0	0
			3	3		

3 Residue-property plots (i)

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.

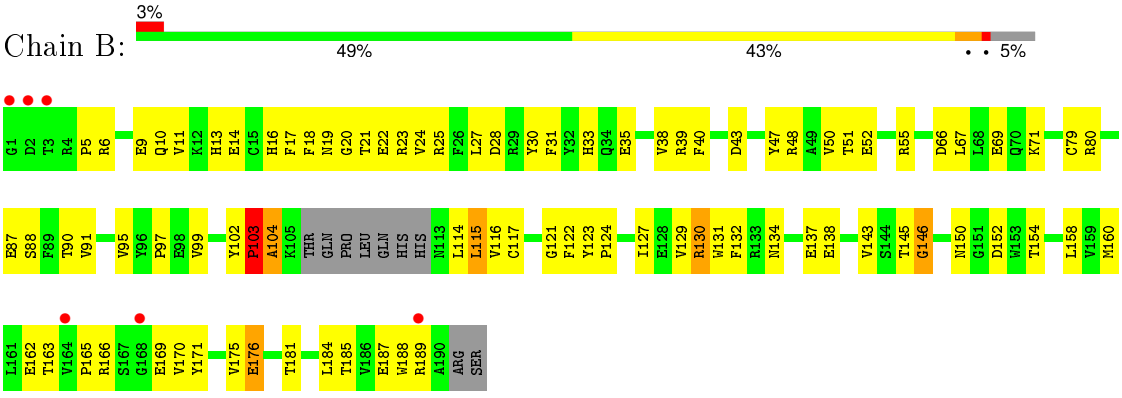
- Molecule 1: HLA CLASS II HISTOCOMPATIBILITY ANTIGEN

Chain A:



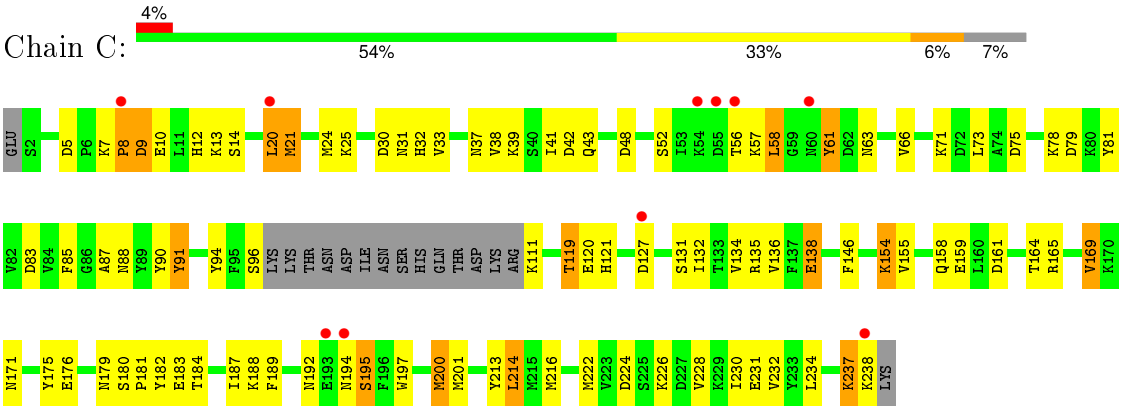
- Molecule 2: HLA CLASS II HISTOCOMPATIBILITY ANTIGEN

Chain B:



- Molecule 3: ENTEROTOXIN TYPE B

Chain C:



- Molecule 4: DIPEPTIDE MIMETIC INHIBITOR

Chain D:

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.38 (at 2.44Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.237 , 0.268 0.255 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	39.9	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 40.5	EDS
Estimated twinning fraction	0.005 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 38325 reflections	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 4.89% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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(^{o})	Ideal(^{o})
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 (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	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
3:C:20:LEU:CD2	3:C:20:LEU:H	2.10	0.65
3:C:138:GLU:OE1	3:C:234:LEU:HB2	1.96	0.65
2:B:99:VAL:HG21	2:B:184:LEU:HD22	1.79	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
3:C:61:TYR:HB2	3:C:111:LYS:HB3	1.84	0.60
1:A:70:LEU:O	1:A:74:THR:HB	2.01	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:HH11	1:A:123:ARG:HG2	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:95:VAL:HG23	2:B:122:PHE:HA	1.88	0.56
1:A:135:THR:O	1:A:147:LYS:HE2	2.05	0.56
2:B:47:TYR:OH	2:B:71:LYS:HE3	2.06	0.56
3:C:41:ILE:HD13	3:C:52:SER:HB2	1.87	0.56
3:C:24:MET:HG2	3:C:175:TYR:CE2	2.41	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
3:C:154:LYS:HB2	3:C:154:LYS:HZ3	1.72	0.55
2:B:55:ARG:HH11	2:B:55:ARG:HG2	1.71	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:O	3:C:226:LYS:HG2	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:104:ALA:HB2	2:B:114:LEU:O	2.13	0.48
2:B:102:TYR:C	2:B:103:PRO:O	2.51	0.48
3:C:12:HIS:CD2	3:C:12:HIS:N	2.82	0.48
3:C:179:ASN:ND2	3:C:180:SER:H	2.11	0.48
3:C:111:LYS:HD3	3:C:111:LYS:HA	1.63	0.48
3:C:7:LYS:O	3:C:10:GLU:HG3	2.13	0.48
3:C:63:ASN:O	3:C:111:LYS:HB2	2.14	0.48
1:A:142:ASP:O	1:A:143:HIS:HB2	2.14	0.48
1:A:108:PHE:CE1	1:A:148:PHE:CZ	3.02	0.48
3:C:14:SER:CB	3:C:201:MET:CE	2.79	0.48
2:B:97:PRO:HB3	2:B:122:PHE:CB	2.36	0.48
2:B:55:ARG:NH1	2:B:55:ARG:HG2	2.27	0.48
2:B:18:PHE:HB2	2:B:23:ARG:HB3	1.96	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
3:C:61:TYR:HA	3:C:111:LYS:HD2	1.96	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:232:VAL:HG12	3:C:234:LEU:HD12	1.97	0.46
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:138:GLU:HA	3:C:138:GLU:OE1	2.14	0.46
1:A:147:LYS:HZ2	1:A:149:HIS:HE1	1.62	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
3:C:136:VAL:HG21	3:C:146:PHE:HE1	1.80	0.46
2:B:17:PHE:HB3	2:B:20:GLY:O	2.16	0.46
3:C:180:SER:C	3:C:182:TYR:H	2.18	0.46
3:C:154:LYS:HB3	3:C:222:MET:CE	2.45	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
3:C:33:VAL:CG2	3:C:88:ASN:HB3	2.46	0.45
2:B:38:VAL:HG22	2:B:39:ARG:N	2.32	0.45
1:A:69:ASN:O	1:A:73:MET:HB2	2.17	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:145:THR:CG2	2:B:158:LEU:HB2	2.48	0.43
2:B:130:ARG:HG3	2:B:130:ARG:HH11	1.82	0.43
2:B:145:THR:HG22	2:B:158:LEU:H	1.83	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
1:A:32:PHE:C	1:A:32:PHE:CD1	2.91	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
3:C:180:SER:O	3:C:237:LYS:HE2	2.19	0.43
2:B:145:THR:O	2:B:146:GLY:C	2.56	0.43
2:B:170:VAL:HG22	2:B:189:ARG:HG2	2.00	0.42
3:C:21:MET:HG3	3:C:179:ASN:CA	2.43	0.42
2:B:31:PHE:CD1	2:B:31:PHE:N	2.87	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
2:B:40:PHE:HB2	2:B:47:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ALA:O	1:A:72:ILE:HD13	2.19	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
3:C:187:ILE:HG23	3:C:187:ILE:O	2.20	0.41
1:A:121:TRP:HB2	1:A:128:VAL:HG23	2.02	0.41
2:B:137:GLU:CG	2:B:138:GLU:N	2.82	0.41
3:C:154:LYS:HB2	3:C:154:LYS:HZ2	1.85	0.41
1:A:24:PHE:HB3	1:A:31:ILE:HD12	2.02	0.41
2:B:95:VAL:O	2:B:95:VAL:HG23	2.20	0.41
2:B:171:TYR:HB2	2:B:188:TRP:O	2.21	0.41
3:C:7:LYS:HA	3:C:8:PRO:HD2	1.84	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:188:LYS:HA	3:C:197:TRP:HA	2.02	0.41
2:B:170:VAL:HG13	2:B:187:GLU:HG3	2.03	0.41
1:A:147:LYS:NZ	1:A:149:HIS:CE1	2.86	0.41
1:A:81:PRO:HB3	2:B:5:PRO:CB	2.51	0.41
2:B:115:LEU:HD12	2:B:171:TYR:CD2	2.56	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
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
1:A:13:TYR:CE2	1:A:67:LYS:HG3	2.55	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:189:PHE:CD2	3:C:230:ILE:HD13	2.56	0.40
3:C:214:LEU:HD12	3:C:214:LEU:HA	1.94	0.40
1:A:123:ARG:HH11	1:A:123:ARG:CG	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
1:A:101:GLU:HA	1:A:102:PRO:HD3	1.92	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%)	11 10
3	C	219/239 (92%)	199 (91%)	16 (7%)	4 (2%)	11 9
4	D	1/6 (17%)	1 (100%)	0	0	100 100
All	All	576/618 (93%)	523 (91%)	46 (8%)	7 (1%)	16 17

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%)	13 16
2	B	163/173 (94%)	149 (91%)	14 (9%)	13 16
3	C	209/225 (93%)	189 (90%)	20 (10%)	10 12

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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%)	12 14

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	ALC	D	804	4	10,11,12	0.46	0	10,13,15	0.48	0
4	MAA	D	806	4	4,5,6	0.59	0	2,5,7	1.63	1 (50%)
4	HAQ	D	807	4	17,19,20	1.60	5 (29%)	18,28,30	1.54	3 (16%)
4	SEL	D	808	4	5,5,5	0.51	0	2,5,5	1.08	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	ALC	D	804	4	-	0/4/14/16	0/1/1/1
4	MAA	D	806	4	-	0/1/4/6	0/0/0/0
4	HAQ	D	807	4	-	0/0/27/29	0/3/3/3
4	SEL	D	808	4	-	0/4/4/4	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	807	HAQ	CB2-CG2	-2.86	1.45	1.50
4	D	807	HAQ	C-N2	-2.43	1.33	1.37
4	D	807	HAQ	CA-C	2.15	1.55	1.52
4	D	807	HAQ	CG-CE1	2.84	1.57	1.51
4	D	807	HAQ	CE2-CZ	3.29	1.45	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	807	HAQ	CB2-CA2-N2	-3.30	100.09	103.63
4	D	806	MAA	O-C-CA	-2.23	117.86	124.64
4	D	807	HAQ	CA2-N2-C	2.59	121.88	118.49
4	D	807	HAQ	CG2-CB2-CA2	2.76	107.50	103.22

There are no chirality outliers.

There are no torsion outliers.

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)

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, 95^{th} 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%)	-0.48	2 (1%) 82 84	20, 34, 59, 89	0
2	B	183/192 (95%)	0.01	6 (3%) 50 53	19, 41, 84, 95	0
3	C	223/239 (93%)	-0.04	10 (4%) 37 40	25, 48, 84, 100	0
4	D	1/6 (16%)	-1.01	0 100 100	37, 37, 37, 37	0
All	All	586/618 (94%)	-0.16	18 (3%) 52 56	19, 41, 81, 100	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	GLY	12.7
3	C	56	THR	5.2
2	B	164	VAL	5.0
3	C	60	ASN	4.6
2	B	3	THR	4.2
2	B	189	ARG	3.9
3	C	54	LYS	3.8
3	C	238	LYS	3.6
3	C	20	LEU	3.3
1	A	181	ASP	3.2
3	C	8	PRO	3.0
2	B	168	GLY	2.8
2	B	2	ASP	2.7
3	C	127	ASP	2.7
1	A	3	GLU	2.7
3	C	193	GLU	2.5
3	C	55	ASP	2.4
3	C	194	ASN	2.3

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. 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, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
4	HAQ	D	807	17/18	0.92	0.13	-	32,35,45,46	0
4	ALC	D	804	11/12	0.95	0.15	-	24,30,36,39	0
4	MAA	D	806	6/7	0.95	0.16	-	27,30,30,32	0
4	SEL	D	808	6/6	0.86	0.20	-	35,38,42,48	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.