Full wwPDB X-ray Structure Validation Report (i)

Oct 17, 2021 – 07:57 AM EDT

PDB ID	:	1KLU
Title	:	Crystal structure of HLA-DR1/TPI(23-37) complexed with staphylococcal enterotoxin C3 variant 3B2 (SEC3-3B2)
Authors	:	Sundberg, E.J.; Sawicki, M.W.; Andersen, P.S.; Sidney, J.; Sette, A.; Mariuzza, R.A.
Deposited on	:	2001-12-12
Resolution	:	1.93 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 following versions of software and data (see references (1)) were used in the production of this report:

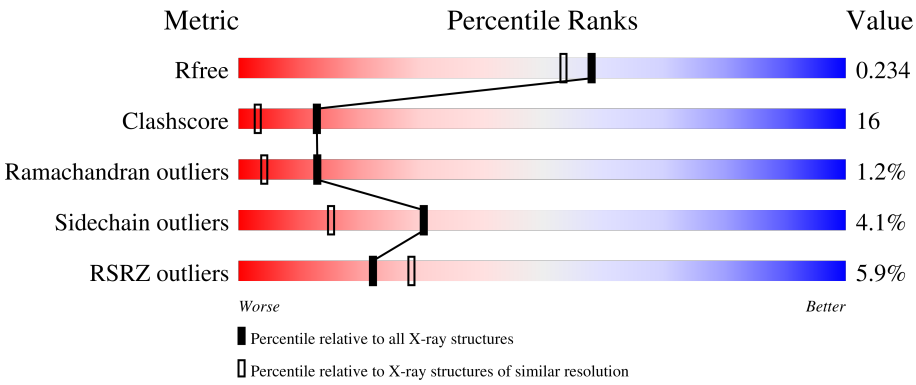
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 1.93 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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% 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	179	4%, 78%, 21%, •
2	B	190	6%, 66%, 27%, 6%
3	C	15	7%, 73%, 27%
4	D	239	6%, 72%, 21%, •, •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5415 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, DR ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	179	1470	952	239	274	5	0	0	0

- Molecule 2 is a protein called HLA CLASS II HISTOCOMPATIBILITY ANTIGEN, DR-1 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	190	1557	979	279	293	6	0	0	0

- Molecule 3 is a protein called Triosephosphate isomerase peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	15	103	64	17	22	0	0	0

- Molecule 4 is a protein called ENTEROTOXIN TYPE C-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	230	1880	1194	306	370	10	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	43	SER	LYS	engineered mutation	UNP P0A0L5
D	45	PHE	LEU	engineered mutation	UNP P0A0L5
D	46	LYS	ALA	engineered mutation	UNP P0A0L5
D	47	TRP	HIS	engineered mutation	UNP P0A0L5

- Molecule 5 is water.

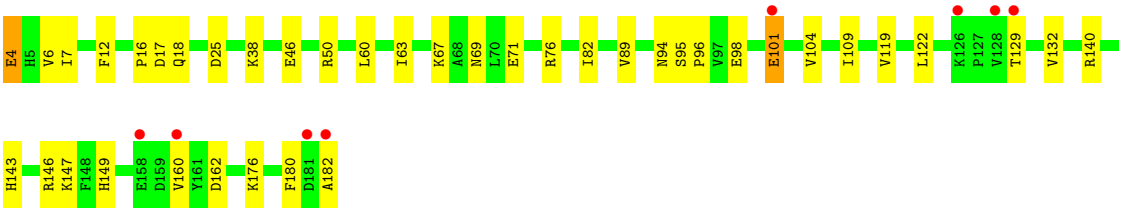
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	123	123	123	0	0
			Total	O		
5	B	106	106	106	0	0
			Total	O		
5	C	25	25	25	0	0
			Total	O		
5	D	151	151	151	0	0

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 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.

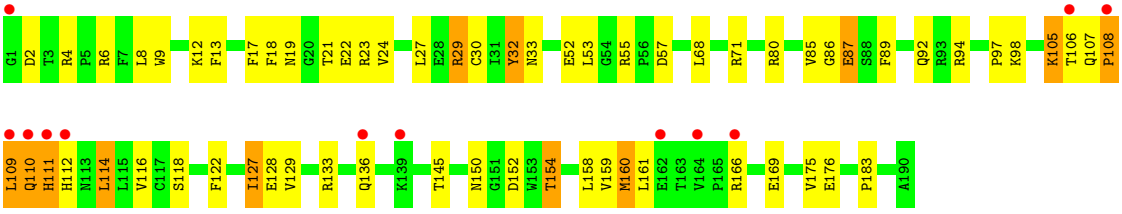
• Molecule 1: HLA CLASS II HISTOCOMPATIBILITY ANTIGEN, DR ALPHA CHAIN

Chain A:



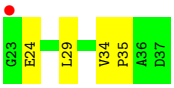
• Molecule 2: HLA CLASS II HISTOCOMPATIBILITY ANTIGEN, DR-1 BETA CHAIN

Chain B:



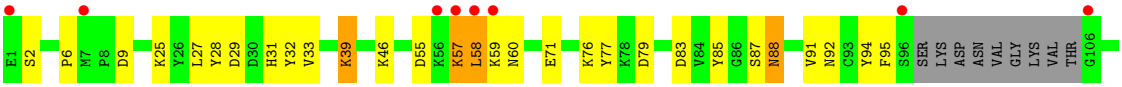
• Molecule 3: Triosephosphate isomerase peptide

Chain C:



• Molecule 4: ENTEROTOXIN TYPE C-3

Chain D:



K117
H118
E119
G120
N121
H122
F123
D124
N125
G126
N127
V131
V135
I143
K152
S153
Q157
I161
F166
K170
K171
N177
S178
T195
F196
W197
K212
Y213
L214
M215
N218
K226
K229
I230
E231
V232
H233
N238
G239

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	171.30Å 171.30Å 121.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.95 – 1.93 36.50 – 1.93	Depositor EDS
% Data completeness (in resolution range)	84.3 (14.95-1.93) 95.7 (36.50-1.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 1.94Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.208 , 0.220 0.223 , 0.234	Depositor DCC
R_{free} test set	5019 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	19.8	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5415	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.37	0/1515	0.65	0/2065
2	B	0.39	0/1597	0.75	4/2168 (0.2%)
3	C	0.49	0/103	0.80	0/138
4	D	0.35	0/1922	0.61	0/2587
All	All	0.37	0/5137	0.67	4/6958 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	109	LEU	N-CA-C	9.62	136.98	111.00
2	B	109	LEU	CB-CG-CD1	-8.77	96.10	111.00
2	B	109	LEU	CA-CB-CG	5.89	128.86	115.30
2	B	109	LEU	CB-CG-CD2	5.15	119.75	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	1470	0	1406	40	0
2	B	1557	0	1488	80	0
3	C	103	0	105	5	0
4	D	1880	0	1807	57	0
5	A	123	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	106	0	0	0	0
5	C	25	0	0	0	0
5	D	151	0	0	1	0
All	All	5415	0	4806	162	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 16.

All (162) 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:150:ASN:HD22	2:B:154:THR:HG22	1.12	1.14
2:B:127:ILE:HD11	2:B:175:VAL:HG13	1.39	1.04
2:B:116:VAL:HG13	2:B:160:MET:HE1	1.41	1.01
2:B:127:ILE:HD13	2:B:128:GLU:N	1.84	0.91
2:B:52:GLU:HA	2:B:55:ARG:HD2	1.54	0.90
2:B:109:LEU:HD12	2:B:112:HIS:CD2	2.07	0.89
4:D:117:LYS:HE2	4:D:119:GLU:HB3	1.53	0.87
4:D:121:ASN:HD21	4:D:153:SER:H	1.20	0.86
2:B:150:ASN:HD22	2:B:154:THR:CG2	1.91	0.83
1:A:76:ARG:HD3	5:A:305:HOH:O	1.77	0.83
2:B:114:LEU:HD21	2:B:160:MET:HB3	1.62	0.81
1:A:7:ILE:HD13	2:B:17:PHE:CE2	2.18	0.79
2:B:109:LEU:HD12	2:B:112:HIS:CG	2.18	0.78
2:B:150:ASN:ND2	2:B:154:THR:HG22	1.97	0.77
4:D:215:MET:O	4:D:218:ASN:HB2	1.85	0.76
2:B:110:GLN:O	2:B:112:HIS:N	2.18	0.75
4:D:157:GLN:O	4:D:161:ILE:HD13	1.87	0.74
1:A:16:PRO:HD2	2:B:6:ARG:HD3	1.70	0.73
2:B:105:LYS:HE3	2:B:105:LYS:H	1.52	0.73
4:D:39:LYS:NZ	4:D:79:ASP:HA	2.04	0.73
4:D:166:PHE:CZ	4:D:170:LYS:HD2	2.23	0.72
2:B:109:LEU:O	2:B:112:HIS:CD2	2.42	0.72
4:D:39:LYS:HZ1	4:D:79:ASP:C	1.93	0.71
1:A:122:LEU:HB2	1:A:162:ASP:HB2	1.73	0.70
1:A:94:ASN:ND2	1:A:104:VAL:HB	2.07	0.70
2:B:8:LEU:O	2:B:32:TYR:O	2.09	0.69
2:B:21:THR:O	2:B:80:ARG:NH1	2.25	0.69
4:D:88:ASN:H	4:D:88:ASN:HD22	1.40	0.68
4:D:229:LYS:C	4:D:230:ILE:HD12	2.14	0.68
1:A:16:PRO:HD2	2:B:6:ARG:HH11	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LYS:HE3	1:A:149:HIS:HE1	1.59	0.67
4:D:131:VAL:HG12	4:D:230:ILE:HD13	1.78	0.66
2:B:106:THR:HG22	2:B:108:PRO:HD3	1.78	0.65
1:A:7:ILE:HD13	2:B:17:PHE:HE2	1.60	0.65
2:B:116:VAL:HG13	2:B:160:MET:CE	2.23	0.64
2:B:94:ARG:HH11	2:B:94:ARG:HG3	1.61	0.64
4:D:28:TYR:HE2	4:D:161:ILE:HD12	1.62	0.63
2:B:98:LYS:HB2	2:B:98:LYS:NZ	2.13	0.63
2:B:176:GLU:OE2	2:B:183:PRO:HB3	1.99	0.62
4:D:39:LYS:HZ1	4:D:79:ASP:CA	2.12	0.62
2:B:109:LEU:O	2:B:110:GLN:O	2.17	0.62
4:D:230:ILE:HD12	4:D:230:ILE:N	2.15	0.61
2:B:85:VAL:HG13	3:C:24:GLU:HB2	1.82	0.60
2:B:114:LEU:CD2	2:B:160:MET:HB3	2.29	0.60
4:D:143:ILE:HD12	4:D:171:LYS:HE3	1.82	0.60
4:D:2:SER:CB	4:D:195:THR:H	2.16	0.59
4:D:39:LYS:NZ	4:D:79:ASP:C	2.54	0.59
2:B:133:ARG:O	2:B:136:GLN:HG2	2.03	0.58
1:A:94:ASN:HD22	1:A:104:VAL:HB	1.67	0.58
2:B:152:ASP:OD1	2:B:154:THR:HB	2.04	0.58
4:D:121:ASN:ND2	4:D:153:SER:H	1.97	0.58
1:A:6:VAL:C	1:A:7:ILE:HD12	2.24	0.57
2:B:105:LYS:H	2:B:105:LYS:CE	2.16	0.57
2:B:110:GLN:O	2:B:111:HIS:C	2.41	0.57
2:B:97:PRO:HB3	2:B:122:PHE:HB3	1.86	0.57
2:B:109:LEU:CD1	2:B:112:HIS:CE1	2.88	0.57
2:B:109:LEU:HD11	2:B:112:HIS:CE1	2.39	0.56
2:B:127:ILE:HD13	2:B:128:GLU:H	1.69	0.56
4:D:88:ASN:H	4:D:88:ASN:ND2	2.02	0.56
4:D:2:SER:HB2	4:D:195:THR:H	1.68	0.56
2:B:94:ARG:HG3	2:B:94:ARG:NH1	2.20	0.56
1:A:89:VAL:HG12	1:A:176:LYS:HG3	1.86	0.56
4:D:131:VAL:CG1	4:D:230:ILE:HD13	2.36	0.56
2:B:159:VAL:N	2:B:160:MET:HE3	2.21	0.56
1:A:7:ILE:HD12	1:A:7:ILE:N	2.20	0.56
2:B:145:THR:HG22	2:B:158:LEU:H	1.71	0.55
4:D:57:LYS:HB3	4:D:58:LEU:HD22	1.89	0.55
4:D:135:VAL:HB	4:D:143:ILE:CD1	2.37	0.55
2:B:2:ASP:OD1	2:B:4:ARG:HD3	2.06	0.55
4:D:122:HIS:O	4:D:152:LYS:HE3	2.07	0.54
4:D:58:LEU:HD22	4:D:58:LEU:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LEU:O	1:A:63:ILE:HG22	2.08	0.53
2:B:24:VAL:HG23	2:B:80:ARG:NH1	2.24	0.53
2:B:114:LEU:HD23	2:B:161:LEU:C	2.30	0.53
1:A:38:LYS:O	4:D:212:LYS:HE2	2.09	0.52
2:B:109:LEU:O	2:B:112:HIS:HD2	1.91	0.52
2:B:108:PRO:HG2	2:B:109:LEU:H	1.75	0.52
2:B:109:LEU:CD1	2:B:112:HIS:CG	2.91	0.52
2:B:111:HIS:O	2:B:112:HIS:CD2	2.63	0.52
1:A:143:HIS:HD2	2:B:12:LYS:NZ	2.08	0.51
2:B:57:ASP:OD1	3:C:35:PRO:HD2	2.10	0.51
4:D:39:LYS:HZ2	4:D:79:ASP:HA	1.73	0.51
2:B:114:LEU:HD23	2:B:161:LEU:O	2.11	0.51
2:B:166:ARG:O	2:B:169:GLU:HG3	2.11	0.51
4:D:39:LYS:HZ1	4:D:79:ASP:HA	1.70	0.51
4:D:57:LYS:CB	4:D:58:LEU:HD22	2.41	0.50
4:D:87:SER:H	4:D:157:GLN:NE2	2.10	0.50
4:D:46:LYS:HB2	4:D:71:GLU:HG3	1.94	0.50
2:B:86:GLY:HA2	2:B:89:PHE:CE1	2.47	0.49
1:A:67:LYS:O	1:A:71:GLU:HG2	2.13	0.49
4:D:161:ILE:CD1	4:D:161:ILE:N	2.76	0.49
4:D:83:ASP:OD1	4:D:118:HIS:HD2	1.95	0.49
1:A:16:PRO:HD2	2:B:6:ARG:CD	2.39	0.49
2:B:109:LEU:C	2:B:110:GLN:O	2.51	0.49
2:B:106:THR:HG22	2:B:108:PRO:CD	2.41	0.48
2:B:127:ILE:HD12	2:B:129:VAL:HG23	1.93	0.48
4:D:76:LYS:HD2	4:D:77:TYR:CE1	2.48	0.48
4:D:226:LYS:HG2	5:D:262:HOH:O	2.11	0.48
1:A:160:VAL:O	1:A:160:VAL:HG23	2.13	0.48
2:B:127:ILE:HD12	2:B:129:VAL:CG2	2.43	0.48
1:A:82:ILE:HG13	2:B:33:ASN:HB3	1.96	0.48
2:B:98:LYS:HB2	2:B:98:LYS:HZ2	1.79	0.47
4:D:231:GLU:HB3	4:D:233:HIS:CE1	2.49	0.47
1:A:16:PRO:HD2	2:B:6:ARG:NH1	2.27	0.47
1:A:140:ARG:HG3	1:A:146:ARG:HG3	1.98	0.46
1:A:16:PRO:HG2	2:B:6:ARG:NH1	2.31	0.46
2:B:116:VAL:HA	2:B:160:MET:HE2	1.98	0.46
1:A:89:VAL:CG1	1:A:176:LYS:HG3	2.45	0.46
2:B:107:GLN:O	2:B:108:PRO:C	2.53	0.45
4:D:31:HIS:O	4:D:32:TYR:HB3	2.16	0.45
1:A:7:ILE:N	1:A:7:ILE:CD1	2.79	0.45
4:D:28:TYR:CE2	4:D:161:ILE:HD12	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:GLU:OE2	1:A:50:ARG:NE	2.44	0.45
1:A:69:ASN:OD1	3:C:34:VAL:HG22	2.17	0.45
1:A:129:THR:O	1:A:132:VAL:HG22	2.17	0.45
2:B:27:LEU:HG	2:B:29:ARG:HD2	1.99	0.45
4:D:55:ASP:O	4:D:59:LYS:HE3	2.17	0.44
4:D:39:LYS:NZ	4:D:79:ASP:CA	2.70	0.44
1:A:17:ASP:O	1:A:18:GLN:HB2	2.17	0.44
1:A:16:PRO:CD	2:B:6:ARG:HH11	2.29	0.44
4:D:33:VAL:O	4:D:85:TYR:HA	2.17	0.44
4:D:121:ASN:HD21	4:D:153:SER:N	2.00	0.43
4:D:55:ASP:HB3	4:D:60:ASN:H	1.83	0.43
4:D:230:ILE:N	4:D:230:ILE:CD1	2.80	0.43
4:D:25:LYS:HE2	4:D:29:ASP:OD1	2.19	0.43
1:A:95:SER:HB2	1:A:96:PRO:HD2	2.00	0.43
4:D:87:SER:H	4:D:157:GLN:HE21	1.65	0.43
4:D:125:ASN:HD22	4:D:125:ASN:HA	1.53	0.43
2:B:13:PHE:CD2	3:C:29:LEU:HD23	2.54	0.43
1:A:4:GLU:OE1	2:B:19:ASN:HA	2.20	0.42
1:A:109:ILE:CD1	1:A:119:VAL:HG21	2.48	0.42
2:B:2:ASP:OD1	2:B:4:ARG:CD	2.67	0.42
1:A:180:PHE:CE1	1:A:182:ALA:HB3	2.54	0.42
2:B:19:ASN:HB3	2:B:22:GLU:HB3	2.02	0.42
2:B:158:LEU:HB3	2:B:160:MET:CE	2.49	0.42
4:D:58:LEU:HD22	4:D:58:LEU:H	1.84	0.42
4:D:166:PHE:CE1	4:D:170:LYS:HD2	2.55	0.42
1:A:7:ILE:HD13	2:B:17:PHE:CD2	2.54	0.42
4:D:27:LEU:HD22	4:D:214:LEU:HD11	2.02	0.42
2:B:24:VAL:CG2	2:B:80:ARG:NH1	2.83	0.42
1:A:76:ARG:NH2	2:B:57:ASP:OD2	2.43	0.42
1:A:101:GLU:OE1	1:A:101:GLU:O	2.36	0.42
4:D:212:LYS:HD3	4:D:212:LYS:HA	1.64	0.42
4:D:91:VAL:O	4:D:92:ASN:HB2	2.20	0.42
4:D:161:ILE:HD13	4:D:161:ILE:H	1.85	0.42
4:D:231:GLU:OE1	4:D:233:HIS:HE1	2.03	0.42
2:B:118:SER:HA	2:B:158:LEU:HD23	2.02	0.42
4:D:94:TYR:O	4:D:95:PHE:HB3	2.20	0.42
2:B:9:TRP:CH2	2:B:30:CYS:HB3	2.54	0.41
2:B:109:LEU:CD1	2:B:112:HIS:CD2	2.92	0.41
4:D:177:ASN:O	4:D:178:SER:HB2	2.19	0.41
4:D:6:PRO:HB3	4:D:197:TRP:CZ2	2.56	0.41
2:B:87:GLU:HG3	2:B:92:GLN:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:135:VAL:HB	4:D:143:ILE:HD13	2.02	0.41
1:A:143:HIS:HD2	2:B:12:LYS:HZ1	1.68	0.41
2:B:176:GLU:CD	2:B:183:PRO:HB3	2.41	0.41
1:A:17:ASP:OD1	2:B:6:ARG:HD2	2.21	0.41
1:A:60:LEU:N	1:A:60:LEU:HD22	2.36	0.40
1:A:12:PHE:CD1	1:A:12:PHE:C	2.94	0.40
2:B:18:PHE:CG	2:B:23:ARG:NH2	2.89	0.40
2:B:109:LEU:HD11	2:B:112:HIS:ND1	2.36	0.40
3:C:29:LEU:HD12	3:C:29:LEU:HA	1.89	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	177/179 (99%)	175 (99%)	2 (1%)	0	100 100
2	B	188/190 (99%)	174 (93%)	10 (5%)	4 (2%)	7 1
3	C	13/15 (87%)	13 (100%)	0	0	100 100
4	D	226/239 (95%)	216 (96%)	7 (3%)	3 (1%)	12 4
All	All	604/623 (97%)	578 (96%)	19 (3%)	7 (1%)	13 4

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	110	GLN
2	B	111	HIS
4	D	57	LYS
4	D	125	ASN
2	B	32	TYR
4	D	124	ASP

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Mol	Chain	Res	Type
2	B	108	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	163/163 (100%)	159 (98%)	4 (2%)	47 35
2	B	171/171 (100%)	161 (94%)	10 (6%)	20 7
3	C	10/10 (100%)	10 (100%)	0	100 100
4	D	211/220 (96%)	202 (96%)	9 (4%)	29 14
All	All	555/564 (98%)	532 (96%)	23 (4%)	30 15

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	25	ASP
1	A	98	GLU
1	A	101	GLU
2	B	29	ARG
2	B	53	LEU
2	B	68	LEU
2	B	71	ARG
2	B	87	GLU
2	B	105	LYS
2	B	114	LEU
2	B	127	ILE
2	B	154	THR
2	B	160	MET
4	D	9	ASP
4	D	39	LYS
4	D	58	LEU
4	D	88	ASN
4	D	124	ASP
4	D	143	ILE

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Mol	Chain	Res	Type
4	D	161	ILE
4	D	212	LYS
4	D	218	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	HIS
1	A	149	HIS
2	B	64	GLN
2	B	70	GLN
2	B	92	GLN
2	B	112	HIS
2	B	150	ASN
2	B	156	GLN
4	D	60	ASN
4	D	88	ASN
4	D	92	ASN
4	D	118	HIS
4	D	121	ASN
4	D	125	ASN
4	D	157	GLN
4	D	218	ASN
4	D	233	HIS

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)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	179/179 (100%)	0.04	8 (4%)	33	40	11, 20, 48, 65	0
2	B	190/190 (100%)	0.18	12 (6%)	20	26	11, 25, 57, 76	0
3	C	15/15 (100%)	0.39	1 (6%)	17	24	14, 19, 43, 46	0
4	D	230/239 (96%)	0.09	15 (6%)	18	25	13, 23, 50, 67	0
All	All	614/623 (98%)	0.11	36 (5%)	22	28	11, 23, 53, 76	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	109	LEU	7.0
2	B	110	GLN	5.9
2	B	106	THR	5.4
2	B	111	HIS	5.2
4	D	126	GLY	4.9
1	A	182	ALA	4.9
4	D	56	LYS	4.9
4	D	239	GLY	4.7
2	B	108	PRO	4.5
4	D	238	ASN	4.3
4	D	58	LEU	4.2
2	B	112	HIS	4.1
4	D	124	ASP	4.0
4	D	57	LYS	4.0
3	C	23	GLY	3.9
2	B	1	GLY	3.8
4	D	125	ASN	3.3
4	D	106	GLY	3.3
4	D	177	ASN	3.3
1	A	101	GLU	3.2
1	A	181	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
4	D	96	SER	3.0
2	B	136	GLN	3.0
1	A	158	GLU	2.9
2	B	166	ARG	2.9
1	A	128	VAL	2.9
2	B	139	LYS	2.8
4	D	7	MET	2.8
2	B	164	VAL	2.6
1	A	160	VAL	2.5
1	A	126	LYS	2.5
1	A	129	THR	2.3
4	D	1	GLU	2.3
4	D	127	ASN	2.2
4	D	59	LYS	2.0
2	B	162	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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.