Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:42 PM GMT

PDB ID	:	1UVH
Title	:	X-RAY STRUCTURE OF DPS FROM MYCOBACTERIUM SMEGMATIS
Authors	:	Ilari, A.; Ceci, P.; Falvo, E.; Chiancone, E.
Deposited on	:	2004-01-20
Resolution	:	2.80 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:

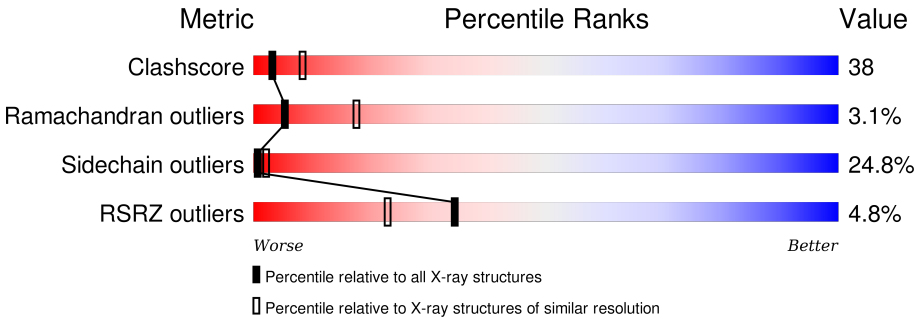
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	183	4% 38% 33% 13% • 14%
1	B	183	5% 38% 35% 10% • 14%
1	C	183	3% 36% 37% 13% • 14%
1	D	183	4% 31% 40% 13% • 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4978 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 STARVATION-INDUCED DNA PROTECTING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	S	0	0	0
			1232	780	212	239	1			
1	B	157	Total	C	N	O	S	0	0	0
			1232	780	212	239	1			
1	C	157	Total	C	N	O	S	0	0	0
			1232	780	212	239	1			
1	D	157	Total	C	N	O	S	0	0	0
			1232	780	212	239	1			

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		

- Molecule 3 is water.

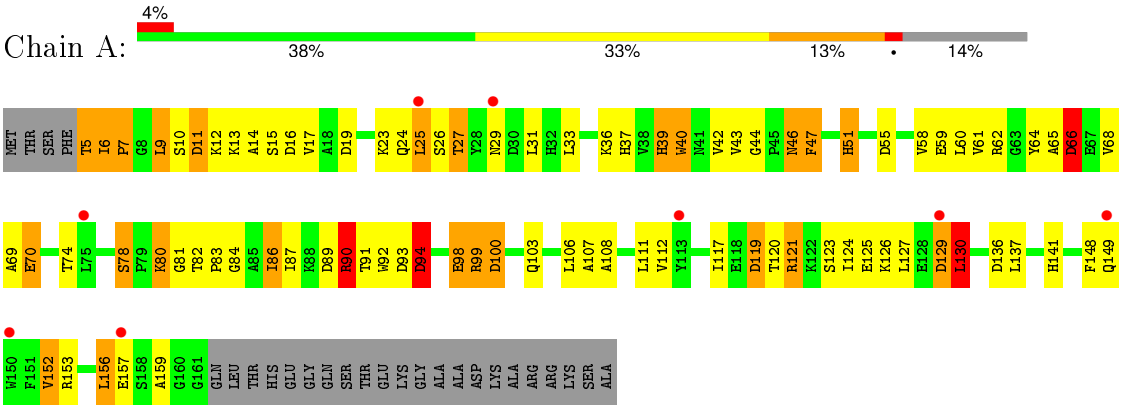
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	9	Total	O	0	0
			9	9		
3	C	5	Total	O	0	0
			5	5		
3	D	22	Total	O	0	0
			22	22		

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.

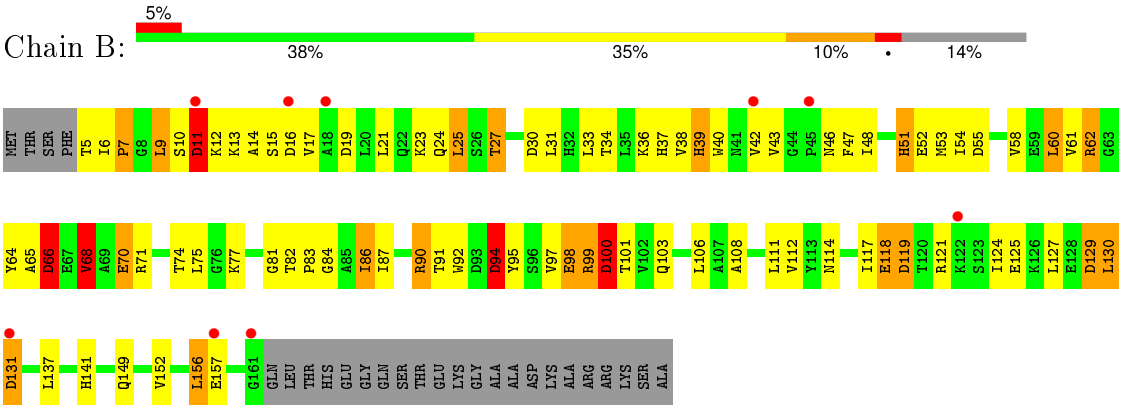
- Molecule 1: STARVATION-INDUCED DNA PROTECTING PROTEIN

Chain A:



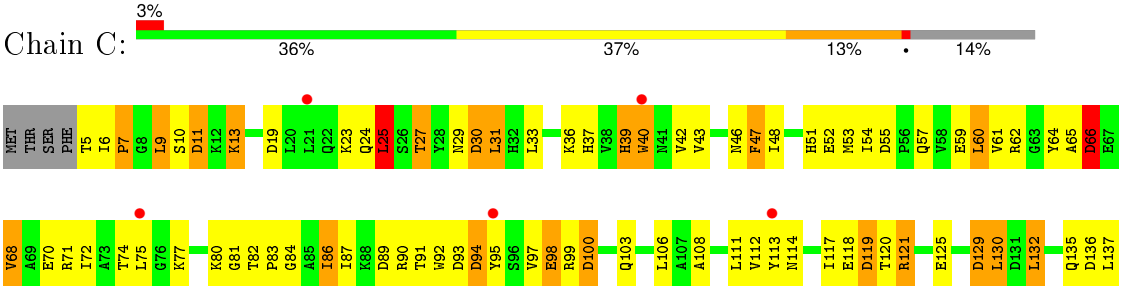
- Molecule 1: STARVATION-INDUCED DNA PROTECTING PROTEIN

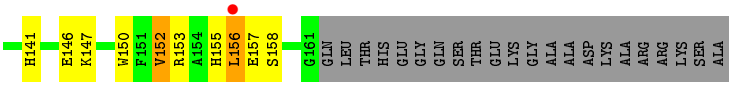
Chain B:



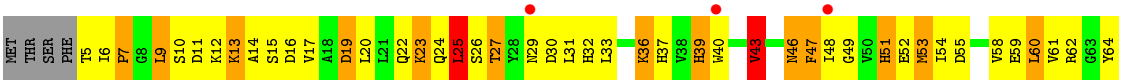
- Molecule 1: STARVATION-INDUCED DNA PROTECTING PROTEIN

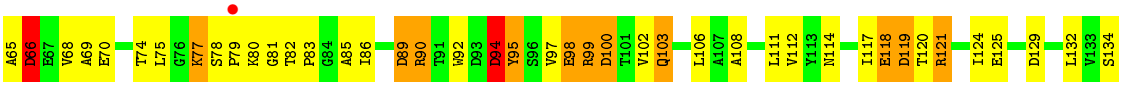
Chain C:

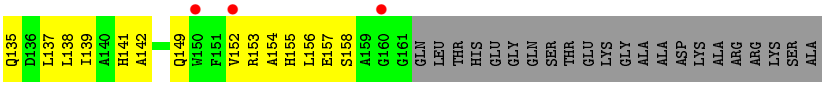




• Molecule 1: STARVATION-INDUCED DNA PROTECTING PROTEIN







4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	124.30Å 124.30Å 304.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.80 39.32 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.0 (40.00-2.80) 99.6 (39.32-2.81)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.91 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.260 , 0.340 0.269 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	67.3	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 27.4	EDS
Estimated twinning fraction	0.477 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.479 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l 0.479 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	1 of 22345 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4978	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: FE

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	0.96	1/1256 (0.1%)	1.15	12/1706 (0.7%)
1	B	1.02	2/1256 (0.2%)	1.21	15/1706 (0.9%)
1	C	1.01	1/1256 (0.1%)	1.17	13/1706 (0.8%)
1	D	0.92	1/1256 (0.1%)	1.14	13/1706 (0.8%)
All	All	0.98	5/5024 (0.1%)	1.17	53/6824 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	D	0	2
All	All	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	68	VAL	CB-CG2	15.45	1.85	1.52
1	B	68	VAL	CB-CG2	13.97	1.82	1.52
1	D	70	GLU	CD-OE1	7.58	1.33	1.25
1	B	70	GLU	CD-OE1	7.46	1.33	1.25
1	A	70	GLU	CD-OE1	6.05	1.32	1.25

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	66	ASP	CB-CG-OD2	12.44	129.50	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	66	ASP	CB-CG-OD2	9.92	127.22	118.30
1	B	55	ASP	CB-CG-OD2	9.22	126.60	118.30
1	D	119	ASP	CB-CG-OD2	9.15	126.53	118.30
1	B	11	ASP	CB-CG-OD2	8.62	126.06	118.30
1	B	66	ASP	CB-CG-OD1	-8.57	110.58	118.30
1	B	94	ASP	CB-CG-OD2	8.46	125.91	118.30
1	C	119	ASP	CB-CG-OD2	8.40	125.86	118.30
1	D	66	ASP	CB-CG-OD1	-8.39	110.75	118.30
1	D	94	ASP	CB-CG-OD2	8.29	125.76	118.30
1	C	94	ASP	CB-CG-OD2	8.25	125.72	118.30
1	A	55	ASP	CB-CG-OD2	7.77	125.29	118.30
1	A	94	ASP	CB-CG-OD2	7.63	125.17	118.30
1	D	66	ASP	CB-CG-OD2	7.46	125.01	118.30
1	A	66	ASP	CB-CG-OD1	-7.45	111.59	118.30
1	C	66	ASP	CB-CG-OD1	-7.29	111.74	118.30
1	B	25	LEU	CB-CG-CD1	-7.22	98.73	111.00
1	A	66	ASP	CB-CG-OD2	7.14	124.73	118.30
1	B	119	ASP	CB-CG-OD2	7.13	124.72	118.30
1	A	11	ASP	CB-CG-OD2	6.96	124.56	118.30
1	C	55	ASP	CB-CG-OD2	6.94	124.55	118.30
1	C	68	VAL	CA-CB-CG2	6.78	121.07	110.90
1	B	25	LEU	CB-CG-CD2	6.53	122.10	111.00
1	A	129	ASP	CB-CG-OD2	6.49	124.14	118.30
1	C	93	ASP	CB-CG-OD2	6.34	124.01	118.30
1	A	89	ASP	CB-CG-OD2	6.29	123.97	118.30
1	A	119	ASP	CB-CG-OD2	6.26	123.94	118.30
1	C	11	ASP	CB-CG-OD2	6.22	123.90	118.30
1	C	129	ASP	CB-CG-OD2	6.05	123.75	118.30
1	D	11	ASP	CB-CG-OD2	6.03	123.73	118.30
1	A	16	ASP	CB-CG-OD2	5.90	123.61	118.30
1	C	136	ASP	CB-CG-OD2	5.80	123.52	118.30
1	D	100	ASP	CB-CG-OD2	5.78	123.50	118.30
1	C	25	LEU	CB-CG-CD2	5.75	120.77	111.00
1	D	19	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	93	ASP	CB-CG-OD2	5.57	123.32	118.30
1	B	16	ASP	CB-CG-OD2	5.55	123.30	118.30
1	C	30	ASP	CB-CG-OD2	5.45	123.20	118.30
1	B	30	ASP	CB-CG-OD2	5.44	123.19	118.30
1	B	131	ASP	CB-CG-OD2	5.42	123.18	118.30
1	D	16	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	62	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	100	ASP	CB-CG-OD2	5.37	123.14	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	30	ASP	CB-CG-OD2	5.34	123.10	118.30
1	B	129	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	100	ASP	CB-CG-OD2	5.30	123.07	118.30
1	D	129	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	136	ASP	CB-CG-OD2	5.16	122.95	118.30
1	B	156	LEU	CA-CB-CG	5.13	127.10	115.30
1	C	89	ASP	CB-CG-OD2	5.12	122.91	118.30
1	D	89	ASP	CB-CG-OD2	5.07	122.87	118.30
1	D	55	ASP	CB-CG-OD2	5.05	122.85	118.30
1	D	25	LEU	CA-CB-CG	-5.00	103.80	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	6	ILE	Peptide
1	A	90	ARG	Sidechain
1	B	6	ILE	Peptide
1	B	90	ARG	Sidechain
1	D	6	ILE	Peptide
1	D	90	ARG	Sidechain

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	1232	0	1219	103	0
1	B	1232	0	1219	101	0
1	C	1232	0	1219	119	0
1	D	1232	0	1219	98	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	1	0
2	D	1	0	0	1	0
3	A	10	0	0	0	0
3	B	9	0	0	1	0
3	C	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	22	0	0	1	0
All	All	4978	0	4876	369	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 38.

All (369) 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)
1:B:68:VAL:CG2	1:B:68:VAL:CB	1.82	1.52
1:C:68:VAL:CG2	1:C:68:VAL:CB	1.85	1.51
1:A:83:PRO:HG2	1:B:90:ARG:NH1	1.39	1.37
1:C:90:ARG:NH1	1:C:94:ASP:HB2	1.37	1.36
1:A:25:LEU:C	1:A:25:LEU:HD12	1.48	1.26
1:C:25:LEU:CB	1:C:68:VAL:HG21	1.65	1.25
1:D:22:GLN:NE2	1:D:25:LEU:HD22	1.54	1.22
1:C:39:HIS:HE1	1:C:51:HIS:CE1	1.58	1.20
1:C:90:ARG:HH22	1:C:94:ASP:CG	1.47	1.15
1:B:25:LEU:HD13	1:B:68:VAL:HG23	1.29	1.14
1:D:22:GLN:NE2	1:D:25:LEU:CD2	2.11	1.13
1:A:90:ARG:NH2	1:B:83:PRO:HG2	1.62	1.13
1:C:25:LEU:HG	1:C:68:VAL:CG2	1.80	1.12
1:D:22:GLN:HE22	1:D:25:LEU:CD2	1.61	1.12
1:A:90:ARG:HH21	1:B:83:PRO:HG2	0.97	1.12
1:C:39:HIS:CE1	1:C:51:HIS:CE1	2.40	1.09
1:D:90:ARG:NH2	1:D:94:ASP:HB2	1.67	1.07
1:A:25:LEU:HD13	1:A:29:ASN:ND2	1.70	1.07
1:C:90:ARG:CZ	1:C:94:ASP:HB2	1.85	1.06
1:C:90:ARG:HH22	1:C:94:ASP:CB	1.69	1.06
1:A:25:LEU:CD1	1:A:25:LEU:C	2.24	1.05
1:C:25:LEU:HD23	1:C:68:VAL:HG22	1.32	1.05
1:A:64:TYR:CD1	1:A:141:HIS:HD2	1.74	1.05
1:B:25:LEU:CD1	1:B:68:VAL:HG23	1.86	1.04
1:B:64:TYR:CD1	1:B:141:HIS:HD2	1.75	1.04
1:D:64:TYR:CG	1:D:141:HIS:HD2	1.75	1.03
1:D:39:HIS:HE1	1:D:51:HIS:CE1	1.76	1.02
1:C:25:LEU:CG	1:C:68:VAL:CG2	2.38	1.02
1:C:25:LEU:HG	1:C:68:VAL:HG23	1.39	1.02
1:D:64:TYR:CD1	1:D:141:HIS:HD2	1.78	1.00
1:C:25:LEU:HD23	1:C:68:VAL:CG2	1.92	0.99
1:A:36:LYS:NZ	1:B:66:ASP:OD1	1.96	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:ARG:NH2	1:C:94:ASP:CB	2.26	0.98
1:A:90:ARG:NH2	1:A:94:ASP:HB2	1.78	0.98
1:A:25:LEU:O	1:A:25:LEU:HD12	1.64	0.98
1:A:90:ARG:CZ	1:A:94:ASP:HB2	1.94	0.97
1:C:25:LEU:CB	1:C:68:VAL:CG2	2.44	0.95
1:C:90:ARG:HH12	1:C:94:ASP:CB	1.79	0.95
1:B:25:LEU:HD13	1:B:68:VAL:CG2	1.94	0.95
1:B:25:LEU:CD1	1:B:68:VAL:CG2	2.44	0.95
1:B:64:TYR:CG	1:B:141:HIS:HD2	1.83	0.95
1:C:25:LEU:CG	1:C:68:VAL:HG21	1.96	0.94
1:C:25:LEU:HB2	1:C:68:VAL:HG21	1.51	0.93
1:C:25:LEU:CA	1:C:68:VAL:HG21	1.99	0.92
1:A:83:PRO:HG2	1:B:90:ARG:HH11	1.09	0.92
1:D:64:TYR:CG	1:D:141:HIS:CD2	2.56	0.92
1:C:83:PRO:HG2	1:D:90:ARG:HH21	1.35	0.91
1:A:64:TYR:CG	1:A:141:HIS:CD2	2.58	0.91
1:C:90:ARG:HH12	1:C:94:ASP:HB2	0.93	0.91
1:A:25:LEU:CD1	1:A:29:ASN:HD22	1.84	0.91
1:A:36:LYS:HZ1	1:B:66:ASP:CG	1.73	0.91
1:B:64:TYR:CG	1:B:141:HIS:CD2	2.59	0.90
1:A:39:HIS:CE1	1:A:51:HIS:NE2	2.38	0.90
1:D:22:GLN:HE22	1:D:25:LEU:HD22	1.17	0.90
1:A:83:PRO:HG2	1:B:90:ARG:HH12	1.35	0.89
1:A:25:LEU:CD1	1:A:29:ASN:ND2	2.34	0.89
1:D:39:HIS:CE1	1:D:51:HIS:CE1	2.60	0.89
1:A:83:PRO:CG	1:B:90:ARG:HH11	1.86	0.89
1:A:64:TYR:CD1	1:A:141:HIS:CD2	2.60	0.89
1:A:25:LEU:HD12	1:A:26:SER:N	1.88	0.88
1:C:25:LEU:CD2	1:C:68:VAL:CG2	2.51	0.87
1:B:39:HIS:CE1	1:B:51:HIS:NE2	2.41	0.87
1:B:64:TYR:CD1	1:B:141:HIS:CD2	2.64	0.86
1:A:39:HIS:HD1	1:A:51:HIS:CD2	1.94	0.85
1:B:39:HIS:HE1	1:B:51:HIS:NE2	1.72	0.85
1:D:90:ARG:CZ	1:D:94:ASP:HB2	2.07	0.85
1:A:90:ARG:HH21	1:B:83:PRO:CG	1.89	0.84
1:C:25:LEU:HB2	1:C:68:VAL:CG2	2.05	0.84
1:A:64:TYR:CG	1:A:141:HIS:HD2	1.93	0.83
1:A:83:PRO:CG	1:B:90:ARG:NH1	2.32	0.83
1:D:66:ASP:OD2	2:D:1162:FE:FE	1.30	0.83
1:C:94:ASP:OD2	1:D:82:THR:HB	1.79	0.83
1:C:94:ASP:OD1	1:D:82:THR:HB	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:ASP:OD2	2:C:1162:FE:FE	1.31	0.83
1:B:25:LEU:HA	1:B:68:VAL:HG21	1.61	0.82
1:A:24:GLN:HA	1:A:27:THR:CG2	2.10	0.82
1:C:90:ARG:NH2	1:C:94:ASP:HA	1.94	0.81
1:B:24:GLN:HA	1:B:27:THR:CG2	2.12	0.80
1:D:25:LEU:HD23	1:D:26:SER:N	1.97	0.79
1:A:64:TYR:CE1	1:A:141:HIS:HD2	2.00	0.79
1:D:24:GLN:HA	1:D:27:THR:CG2	2.13	0.79
1:A:66:ASP:OD1	1:B:36:LYS:CE	2.32	0.78
1:A:25:LEU:HD13	1:A:29:ASN:HD21	1.46	0.78
1:C:9:LEU:HD13	1:C:10:SER:H	1.48	0.77
1:C:90:ARG:NH2	1:C:94:ASP:CG	2.32	0.77
1:C:25:LEU:HA	1:C:68:VAL:HG21	1.67	0.77
1:A:90:ARG:CZ	1:A:94:ASP:CB	2.63	0.77
1:C:24:GLN:HA	1:C:27:THR:HG23	1.65	0.76
1:B:25:LEU:HD12	1:B:68:VAL:CG2	2.14	0.76
1:C:64:TYR:CG	1:C:141:HIS:CD2	2.74	0.76
1:C:36:LYS:CE	1:D:66:ASP:OD1	2.35	0.75
1:B:39:HIS:CE1	1:B:51:HIS:CD2	2.75	0.75
1:A:24:GLN:HA	1:A:27:THR:HG23	1.67	0.75
1:A:61:VAL:O	1:A:64:TYR:HB2	1.86	0.75
1:C:90:ARG:CZ	1:C:94:ASP:CB	2.61	0.74
1:D:64:TYR:CD1	1:D:141:HIS:CD2	2.70	0.74
1:A:39:HIS:ND1	1:A:51:HIS:CD2	2.55	0.74
1:B:25:LEU:HD12	1:B:68:VAL:HG21	1.70	0.74
1:C:94:ASP:CG	1:D:82:THR:HB	2.08	0.73
1:D:61:VAL:O	1:D:64:TYR:HB2	1.89	0.72
1:D:90:ARG:NH2	1:D:94:ASP:CB	2.48	0.72
1:A:39:HIS:HE1	1:A:51:HIS:NE2	1.87	0.72
1:C:64:TYR:CD1	1:C:141:HIS:CD2	2.77	0.72
1:D:90:ARG:CZ	1:D:94:ASP:CB	2.68	0.71
1:C:64:TYR:CE1	1:C:141:HIS:HD2	2.09	0.70
1:C:64:TYR:CD1	1:C:141:HIS:HD2	2.09	0.70
1:C:90:ARG:NH2	1:C:94:ASP:CA	2.55	0.69
1:B:70:GLU:OE2	1:C:147:LYS:NZ	2.21	0.69
1:C:25:LEU:CD2	1:C:68:VAL:HG22	2.15	0.69
1:A:62:ARG:O	1:A:65:ALA:HB3	1.93	0.69
1:D:22:GLN:HE22	1:D:25:LEU:HD21	1.56	0.68
1:A:66:ASP:OD1	1:B:36:LYS:HE3	1.93	0.68
1:B:90:ARG:NH1	1:B:94:ASP:HB2	2.08	0.68
1:C:61:VAL:O	1:C:64:TYR:HB2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:VAL:O	1:B:64:TYR:HB2	1.94	0.67
1:B:25:LEU:CD1	1:B:68:VAL:HG21	2.24	0.67
1:C:24:GLN:HA	1:C:27:THR:CG2	2.24	0.67
1:C:64:TYR:CZ	1:C:141:HIS:HD2	2.13	0.67
1:A:25:LEU:CD1	1:A:25:LEU:O	2.38	0.67
1:D:64:TYR:CD2	1:D:141:HIS:CD2	2.83	0.67
1:A:64:TYR:CD2	1:A:141:HIS:CD2	2.84	0.65
1:C:90:ARG:NH1	1:C:94:ASP:CB	2.34	0.65
1:D:137:LEU:HG	1:D:141:HIS:HE1	1.61	0.65
1:C:64:TYR:CD2	1:C:141:HIS:CD2	2.85	0.65
1:C:94:ASP:OD1	1:D:82:THR:CB	2.45	0.65
1:C:9:LEU:HD13	1:C:10:SER:N	2.12	0.65
1:B:90:ARG:CZ	1:B:94:ASP:HB2	2.27	0.64
1:A:46:ASN:N	1:A:46:ASN:OD1	2.29	0.64
1:B:149:GLN:HA	1:B:152:VAL:HG12	1.80	0.64
1:C:106:LEU:HB3	1:C:152:VAL:HG23	1.78	0.63
1:C:94:ASP:OD2	1:D:82:THR:CB	2.47	0.63
1:A:106:LEU:HB3	1:A:152:VAL:HG23	1.80	0.63
1:A:39:HIS:CE1	1:A:51:HIS:CD2	2.85	0.63
1:D:108:ALA:O	1:D:112:VAL:HG23	1.99	0.63
1:C:25:LEU:CD2	1:C:68:VAL:HG21	2.25	0.63
1:B:98:GLU:O	1:B:99:ARG:C	2.38	0.62
1:C:33:LEU:HD11	1:D:33:LEU:HD11	1.80	0.62
1:A:36:LYS:HZ2	1:A:40:TRP:HZ3	1.48	0.61
1:A:86:ILE:HD11	1:B:83:PRO:HB3	1.82	0.61
1:D:137:LEU:HG	1:D:141:HIS:CE1	2.35	0.61
1:B:68:VAL:HB	1:B:68:VAL:CG2	2.16	0.60
1:D:85:ALA:O	1:D:89:ASP:OD2	2.19	0.60
1:A:121:ARG:HA	1:A:124:ILE:HD12	1.83	0.60
1:C:37:HIS:HE1	1:C:97:VAL:O	1.84	0.60
1:B:43:VAL:HG12	1:B:100:ASP:O	2.00	0.60
1:A:64:TYR:CE1	1:A:141:HIS:CD2	2.88	0.60
1:D:25:LEU:HB2	1:D:68:VAL:CG2	2.32	0.59
1:C:24:GLN:NE2	1:C:120:THR:OG1	2.33	0.59
1:C:64:TYR:CE2	1:C:141:HIS:HD2	2.20	0.59
1:D:121:ARG:HA	1:D:124:ILE:HD12	1.84	0.59
1:B:65:ALA:O	1:B:68:VAL:HG23	2.02	0.59
1:D:24:GLN:HA	1:D:27:THR:HG22	1.84	0.59
1:D:62:ARG:O	1:D:65:ALA:HB3	2.03	0.59
1:C:64:TYR:CG	1:C:141:HIS:HD2	2.18	0.59
1:A:84:GLY:HA3	1:B:94:ASP:OD1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:HIS:CD2	1:D:81:GLY:H	2.20	0.58
1:A:36:LYS:NZ	1:B:66:ASP:CG	2.52	0.58
1:B:7:PRO:HB3	1:B:75:LEU:O	2.04	0.58
1:A:86:ILE:O	1:A:90:ARG:HB2	2.04	0.58
1:A:83:PRO:HB3	1:B:86:ILE:HD11	1.85	0.58
1:B:64:TYR:CE1	1:B:141:HIS:HD2	2.20	0.58
1:C:68:VAL:CG2	1:C:68:VAL:HB	2.17	0.57
1:C:64:TYR:CD2	1:C:141:HIS:HD2	2.22	0.57
1:A:99:ARG:HD3	1:C:158:SER:O	2.04	0.57
1:A:90:ARG:NH1	1:A:94:ASP:HB3	2.19	0.57
1:B:24:GLN:HA	1:B:27:THR:HG23	1.87	0.57
1:A:149:GLN:HA	1:A:152:VAL:CG1	2.34	0.57
1:B:64:TYR:CD2	1:B:141:HIS:CD2	2.93	0.57
1:D:98:GLU:O	1:D:99:ARG:C	2.40	0.57
1:C:98:GLU:O	1:C:99:ARG:C	2.43	0.57
1:B:58:VAL:O	1:B:62:ARG:HG3	2.04	0.56
1:C:62:ARG:O	1:C:65:ALA:HB3	2.05	0.56
1:A:25:LEU:HD12	1:A:26:SER:CA	2.36	0.56
1:C:64:TYR:CE1	1:C:141:HIS:CD2	2.93	0.56
1:D:58:VAL:O	1:D:62:ARG:HG3	2.06	0.56
1:A:5:THR:O	1:A:6:ILE:HG23	2.06	0.56
1:A:23:LYS:O	1:A:27:THR:HG22	2.05	0.55
1:C:90:ARG:NH2	1:C:94:ASP:HB2	1.98	0.55
1:C:39:HIS:CE1	1:C:51:HIS:NE2	2.74	0.55
1:C:83:PRO:HG2	1:D:90:ARG:NH2	2.15	0.55
1:C:25:LEU:HD22	1:C:29:ASN:ND2	2.21	0.55
1:D:36:LYS:HG3	1:D:40:TRP:CZ3	2.43	0.54
1:D:95:TYR:CE1	1:D:97:VAL:HB	2.43	0.54
1:A:153:ARG:O	1:A:156:LEU:HD22	2.07	0.54
1:C:47:PHE:CD2	1:C:48:ILE:N	2.76	0.54
1:D:46:ASN:N	1:D:46:ASN:OD1	2.41	0.54
1:C:91:THR:HG22	1:C:91:THR:O	2.08	0.54
1:C:36:LYS:HG3	1:C:40:TRP:CZ3	2.43	0.53
1:A:81:GLY:H	1:B:37:HIS:CD2	2.25	0.53
1:B:65:ALA:HA	1:B:68:VAL:HG22	1.89	0.53
1:A:10:SER:O	1:A:12:LYS:N	2.41	0.53
1:A:47:PHE:O	1:A:51:HIS:HB2	2.09	0.53
1:D:17:VAL:HA	1:D:20:LEU:HD12	1.89	0.53
1:D:60:LEU:HD11	1:D:64:TYR:CZ	2.44	0.53
1:B:65:ALA:HA	1:B:68:VAL:CG2	2.39	0.52
1:D:94:ASP:C	1:D:94:ASP:OD2	2.47	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:PRO:HB3	1:D:75:LEU:O	2.09	0.52
1:D:24:GLN:HA	1:D:27:THR:HG23	1.88	0.52
1:B:121:ARG:HA	1:B:124:ILE:HD12	1.91	0.52
1:A:60:LEU:HD11	1:A:64:TYR:CZ	2.45	0.52
1:C:95:TYR:CE1	1:C:97:VAL:HB	2.45	0.52
1:D:25:LEU:HD23	1:D:25:LEU:C	2.30	0.52
1:C:81:GLY:H	1:D:37:HIS:CD2	2.28	0.52
1:D:90:ARG:NH1	1:D:94:ASP:HB3	2.24	0.52
1:B:23:LYS:O	1:B:27:THR:HG22	2.10	0.52
1:B:9:LEU:HD13	1:B:10:SER:N	2.25	0.51
1:A:43:VAL:HG12	1:A:100:ASP:O	2.10	0.51
1:A:94:ASP:C	1:A:94:ASP:OD2	2.48	0.51
1:C:64:TYR:CE2	1:C:141:HIS:CD2	2.99	0.51
1:A:90:ARG:NH1	1:A:94:ASP:CB	2.73	0.51
1:A:9:LEU:CD1	1:A:10:SER:H	2.24	0.51
1:B:24:GLN:HA	1:B:27:THR:HG22	1.90	0.51
1:B:48:ILE:O	1:B:52:GLU:HG3	2.10	0.51
1:C:36:LYS:HE2	1:D:66:ASP:OD1	2.08	0.51
1:B:14:ALA:HA	1:B:17:VAL:CG1	2.41	0.51
1:D:86:ILE:O	1:D:90:ARG:HB2	2.11	0.50
1:B:62:ARG:O	1:B:65:ALA:HB3	2.11	0.50
1:C:83:PRO:HB3	1:D:86:ILE:HD11	1.93	0.50
1:D:23:LYS:O	1:D:27:THR:HG22	2.10	0.50
1:C:80:LYS:HD3	1:D:98:GLU:OE2	2.10	0.50
1:C:137:LEU:HG	1:C:141:HIS:CE1	2.47	0.50
1:C:114:ASN:O	1:C:118:GLU:HB2	2.11	0.50
1:A:33:LEU:HD11	1:B:33:LEU:HD11	1.93	0.50
1:B:65:ALA:O	1:B:68:VAL:CG2	2.60	0.50
1:C:94:ASP:OD2	1:C:95:TYR:N	2.44	0.50
1:C:84:GLY:O	1:C:87:ILE:HG12	2.12	0.50
1:A:24:GLN:NE2	1:A:120:THR:OG1	2.43	0.50
1:C:54:ILE:O	1:C:57:GLN:N	2.44	0.50
1:A:94:ASP:OD1	1:B:84:GLY:HA3	2.12	0.50
1:C:82:THR:HG21	1:D:95:TYR:HB3	1.94	0.49
1:B:137:LEU:HG	1:B:141:HIS:CE1	2.47	0.49
1:B:94:ASP:C	1:B:94:ASP:OD2	2.51	0.49
1:D:10:SER:OG	1:D:13:LYS:HB2	2.12	0.49
1:D:25:LEU:HG	1:D:25:LEU:O	2.09	0.49
1:A:80:LYS:HD3	1:B:98:GLU:OE2	2.13	0.49
1:B:39:HIS:ND1	1:B:51:HIS:CD2	2.81	0.48
1:D:49:GLY:O	1:D:53:MET:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:GLY:O	1:A:87:ILE:HG12	2.14	0.48
1:B:95:TYR:CE1	1:B:97:VAL:HB	2.49	0.48
1:B:82:THR:O	1:B:86:ILE:HG23	2.14	0.48
1:D:24:GLN:NE2	1:D:120:THR:OG1	2.46	0.48
1:A:9:LEU:HD13	1:A:10:SER:H	1.78	0.48
1:C:108:ALA:O	1:C:112:VAL:HG23	2.14	0.47
1:A:37:HIS:CD2	1:B:81:GLY:H	2.32	0.47
1:B:94:ASP:OD2	1:B:95:TYR:O	2.33	0.47
1:A:62:ARG:CZ	1:B:62:ARG:HD3	2.44	0.47
1:A:9:LEU:HD13	1:A:10:SER:N	2.29	0.47
1:D:10:SER:OG	1:D:10:SER:O	2.29	0.47
1:B:14:ALA:HA	1:B:17:VAL:HG12	1.97	0.47
1:B:131:ASP:OD1	1:C:121:ARG:NH2	2.48	0.47
1:B:108:ALA:O	1:B:112:VAL:HG23	2.15	0.47
1:D:153:ARG:O	1:D:155:HIS:N	2.48	0.47
1:A:130:LEU:HD23	1:A:130:LEU:H	1.81	0.46
1:A:39:HIS:ND1	1:A:51:HIS:NE2	2.63	0.46
1:A:25:LEU:HD12	1:A:26:SER:HA	1.97	0.46
1:D:17:VAL:O	1:D:20:LEU:HB2	2.15	0.46
1:A:14:ALA:HA	1:A:17:VAL:CG1	2.46	0.46
1:D:25:LEU:CD2	1:D:25:LEU:C	2.83	0.46
1:D:37:HIS:HE1	1:D:97:VAL:O	1.99	0.46
1:A:123:SER:O	1:A:127:LEU:HG	2.16	0.46
1:A:98:GLU:O	1:A:99:ARG:C	2.53	0.46
1:A:108:ALA:O	1:A:112:VAL:HG23	2.15	0.46
1:A:82:THR:HG21	1:B:95:TYR:HB3	1.98	0.46
1:C:94:ASP:OD2	1:D:82:THR:CG2	2.64	0.46
1:D:68:VAL:CG2	1:D:69:ALA:N	2.79	0.46
1:C:152:VAL:O	1:C:155:HIS:HB2	2.15	0.45
1:B:21:LEU:O	1:B:25:LEU:N	2.40	0.45
1:C:86:ILE:HD11	1:D:83:PRO:HB3	1.96	0.45
1:D:132:LEU:O	1:D:135:GLN:HB3	2.16	0.45
1:A:78:SER:HB2	1:B:99:ARG:HB2	1.98	0.45
1:C:111:LEU:O	1:C:114:ASN:HB2	2.17	0.45
1:B:17:VAL:HG23	1:B:127:LEU:HD21	1.99	0.45
1:C:72:ILE:HA	1:C:75:LEU:HD12	1.99	0.45
1:A:148:PHE:O	1:A:152:VAL:HG12	2.17	0.45
1:C:77:LYS:NZ	3:C:2001:HOH:O	2.22	0.45
1:B:106:LEU:HD13	1:B:152:VAL:HG23	1.99	0.45
1:C:24:GLN:O	1:C:25:LEU:C	2.53	0.45
1:A:36:LYS:HZ3	1:A:39:HIS:CD2	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:TYR:CZ	1:A:141:HIS:HD2	2.34	0.44
1:C:84:GLY:HA3	1:D:94:ASP:OD1	2.16	0.44
1:C:61:VAL:HA	1:C:64:TYR:HB2	1.99	0.44
1:D:114:ASN:O	1:D:118:GLU:HB2	2.17	0.44
1:D:52:GLU:O	1:D:53:MET:C	2.54	0.44
1:D:32:HIS:CG	1:D:62:ARG:HG2	2.53	0.44
1:A:44:GLY:O	1:C:155:HIS:HA	2.16	0.44
1:B:34:THR:O	1:B:38:VAL:HG23	2.17	0.44
1:A:84:GLY:O	1:A:87:ILE:CG1	2.66	0.44
1:D:149:GLN:HA	1:D:152:VAL:HG12	1.99	0.44
1:A:107:ALA:O	1:A:111:LEU:HG	2.17	0.44
1:B:74:THR:HG23	1:C:150:TRP:HB2	2.00	0.44
1:D:134:SER:O	1:D:138:LEU:HD12	2.17	0.44
1:A:36:LYS:HG3	1:A:40:TRP:CZ3	2.53	0.44
1:C:40:TRP:CD1	1:D:79:PRO:HG2	2.53	0.44
1:D:111:LEU:O	1:D:114:ASN:HB2	2.18	0.44
1:B:98:GLU:O	1:B:100:ASP:N	2.51	0.43
1:C:36:LYS:NZ	1:D:66:ASP:OD1	2.50	0.43
1:B:10:SER:O	1:B:12:LYS:N	2.50	0.43
1:B:64:TYR:CD2	1:B:141:HIS:HD2	2.29	0.43
1:C:25:LEU:HD13	1:C:80:LYS:O	2.18	0.43
1:D:25:LEU:HD21	1:D:80:LYS:O	2.18	0.43
1:C:39:HIS:CE1	1:C:51:HIS:ND1	2.85	0.43
1:D:14:ALA:HA	1:D:17:VAL:CG1	2.49	0.43
1:A:137:LEU:HG	1:A:141:HIS:CE1	2.53	0.43
1:C:132:LEU:O	1:C:135:GLN:HB3	2.18	0.43
1:D:43:VAL:HG12	1:D:100:ASP:O	2.19	0.43
1:C:25:LEU:CD1	1:C:80:LYS:O	2.67	0.43
1:B:137:LEU:HG	1:B:141:HIS:HE1	1.84	0.43
1:D:64:TYR:CE1	1:D:141:HIS:HD2	2.29	0.43
1:D:60:LEU:CD1	1:D:64:TYR:CZ	3.01	0.43
1:D:106:LEU:HD13	1:D:152:VAL:HG23	2.00	0.43
1:B:114:ASN:O	1:B:118:GLU:HB2	2.19	0.43
1:B:91:THR:O	1:B:91:THR:HG22	2.19	0.43
1:B:68:VAL:CG1	1:B:68:VAL:CG2	2.83	0.43
1:C:68:VAL:CG2	1:C:68:VAL:CG1	2.83	0.43
1:D:12:LYS:O	1:D:13:LYS:C	2.57	0.43
1:C:99:ARG:HG2	1:C:100:ASP:N	2.30	0.43
1:D:47:PHE:CD1	1:D:48:ILE:N	2.87	0.43
1:C:31:LEU:HD21	1:C:113:TYR:CE1	2.54	0.43
1:D:77:LYS:HG2	3:D:2007:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:THR:CG2	1:B:91:THR:O	2.66	0.42
1:B:106:LEU:HB3	1:B:152:VAL:HG23	2.00	0.42
1:B:71:ARG:NH1	1:C:146:GLU:OE2	2.44	0.42
1:D:139:ILE:O	1:D:142:ALA:HB3	2.19	0.42
1:B:90:ARG:CZ	1:B:94:ASP:CB	2.97	0.42
1:A:24:GLN:HA	1:A:27:THR:HG22	1.99	0.42
1:A:149:GLN:HA	1:A:152:VAL:HG12	2.01	0.42
1:B:37:HIS:HE1	1:B:97:VAL:O	2.03	0.42
1:A:70:GLU:O	1:A:74:THR:OG1	2.28	0.42
1:C:71:ARG:O	1:C:74:THR:HB	2.20	0.42
1:D:68:VAL:HG23	1:D:69:ALA:N	2.34	0.42
1:C:24:GLN:CA	1:C:27:THR:HG23	2.44	0.42
1:A:36:LYS:NZ	1:A:40:TRP:CZ3	2.86	0.42
1:C:66:ASP:OD2	1:C:70:GLU:OE1	2.38	0.42
1:D:36:LYS:HD3	1:D:58:VAL:HG11	2.01	0.42
1:B:98:GLU:O	1:B:100:ASP:HB2	2.20	0.42
1:C:23:LYS:O	1:C:27:THR:HG22	2.19	0.41
1:C:47:PHE:HD2	1:C:48:ILE:N	2.18	0.41
1:B:60:LEU:HD11	1:B:64:TYR:CZ	2.55	0.41
1:A:12:LYS:O	1:A:15:SER:N	2.53	0.41
1:C:24:GLN:O	1:C:27:THR:HG23	2.20	0.41
1:C:90:ARG:NH2	1:C:94:ASP:OD2	2.47	0.41
1:C:52:GLU:O	1:C:53:MET:C	2.56	0.41
1:C:13:LYS:HG3	1:C:130:LEU:HD22	2.03	0.41
1:A:90:ARG:NH2	1:A:94:ASP:CB	2.66	0.41
1:C:60:LEU:HD23	1:C:60:LEU:HA	1.95	0.41
1:D:29:ASN:HA	1:D:32:HIS:CD2	2.55	0.41
1:D:12:LYS:O	1:D:15:SER:N	2.53	0.41
1:D:52:GLU:O	1:D:54:ILE:N	2.53	0.41
1:A:66:ASP:OD1	1:B:36:LYS:NZ	2.53	0.41
1:A:68:VAL:CG2	1:A:69:ALA:N	2.82	0.41
1:B:64:TYR:CE1	1:B:141:HIS:CD2	3.04	0.41
1:B:52:GLU:C	1:B:54:ILE:N	2.73	0.41
1:B:84:GLY:O	1:B:87:ILE:HG12	2.21	0.41
1:A:60:LEU:CD1	1:A:64:TYR:CZ	3.04	0.41
1:A:149:GLN:O	1:A:152:VAL:HG13	2.20	0.41
1:D:46:ASN:HD21	1:D:103:GLN:HE22	1.69	0.41
1:B:52:GLU:O	1:B:54:ILE:N	2.54	0.41
1:B:12:LYS:O	1:B:15:SER:N	2.54	0.40
1:D:90:ARG:CZ	1:D:94:ASP:HB3	2.51	0.40
1:A:58:VAL:O	1:A:62:ARG:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:TYR:HA	3:B:2008:HOH:O	2.20	0.40
1:A:9:LEU:CD1	1:A:10:SER:N	2.85	0.40
1:D:9:LEU:HA	1:D:9:LEU:HD13	2.00	0.40
1:A:64:TYR:CE2	1:A:141:HIS:CD2	3.09	0.40
1:C:66:ASP:HA	1:D:40:TRP:CZ3	2.57	0.40
1:C:47:PHE:C	1:C:47:PHE:CD2	2.94	0.40
1:B:111:LEU:O	1:B:114:ASN:HB2	2.22	0.40
1:C:30:ASP:OD1	1:C:90:ARG:NH2	2.54	0.40
1:C:153:ARG:O	1:C:156:LEU:HD22	2.21	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	155/183 (85%)	128 (83%)	22 (14%)	5 (3%)	5 17
1	B	155/183 (85%)	130 (84%)	20 (13%)	5 (3%)	5 17
1	C	155/183 (85%)	128 (83%)	25 (16%)	2 (1%)	15 44
1	D	155/183 (85%)	127 (82%)	21 (14%)	7 (4%)	3 10
All	All	620/732 (85%)	513 (83%)	88 (14%)	19 (3%)	5 17

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	PRO
1	A	11	ASP
1	B	7	PRO
1	B	11	ASP
1	C	7	PRO
1	C	130	LEU

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Mol	Chain	Res	Type
1	D	7	PRO
1	A	130	LEU
1	A	159	ALA
1	B	53	MET
1	B	130	LEU
1	D	53	MET
1	A	51	HIS
1	D	51	HIS
1	D	154	ALA
1	B	51	HIS
1	D	95	TYR
1	D	102	VAL
1	D	43	VAL

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	133/153 (87%)	98 (74%)	35 (26%)	0 1
1	B	133/153 (87%)	101 (76%)	32 (24%)	1 2
1	C	133/153 (87%)	100 (75%)	33 (25%)	1 2
1	D	133/153 (87%)	101 (76%)	32 (24%)	1 2
All	All	532/612 (87%)	400 (75%)	132 (25%)	1 2

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	7	PRO
1	A	9	LEU
1	A	13	LYS
1	A	19	ASP
1	A	25	LEU
1	A	27	THR
1	A	31	LEU

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Mol	Chain	Res	Type
1	A	39	HIS
1	A	40	TRP
1	A	42	VAL
1	A	46	ASN
1	A	47	PHE
1	A	59	GLU
1	A	66	ASP
1	A	78	SER
1	A	80	LYS
1	A	86	ILE
1	A	90	ARG
1	A	91	THR
1	A	92	TRP
1	A	94	ASP
1	A	98	GLU
1	A	99	ARG
1	A	103	GLN
1	A	117	ILE
1	A	119	ASP
1	A	121	ARG
1	A	125	GLU
1	A	126	LYS
1	A	129	ASP
1	A	130	LEU
1	A	152	VAL
1	A	156	LEU
1	A	157	GLU
1	B	5	THR
1	B	9	LEU
1	B	11	ASP
1	B	13	LYS
1	B	19	ASP
1	B	27	THR
1	B	31	LEU
1	B	39	HIS
1	B	40	TRP
1	B	42	VAL
1	B	46	ASN
1	B	47	PHE
1	B	60	LEU
1	B	66	ASP
1	B	68	VAL

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Mol	Chain	Res	Type
1	B	77	LYS
1	B	86	ILE
1	B	92	TRP
1	B	94	ASP
1	B	98	GLU
1	B	99	ARG
1	B	100	ASP
1	B	101	THR
1	B	103	GLN
1	B	117	ILE
1	B	118	GLU
1	B	119	ASP
1	B	125	GLU
1	B	129	ASP
1	B	130	LEU
1	B	156	LEU
1	B	157	GLU
1	C	5	THR
1	C	6	ILE
1	C	7	PRO
1	C	9	LEU
1	C	11	ASP
1	C	13	LYS
1	C	19	ASP
1	C	25	LEU
1	C	27	THR
1	C	31	LEU
1	C	39	HIS
1	C	40	TRP
1	C	42	VAL
1	C	43	VAL
1	C	46	ASN
1	C	47	PHE
1	C	59	GLU
1	C	60	LEU
1	C	66	ASP
1	C	86	ILE
1	C	92	TRP
1	C	98	GLU
1	C	100	ASP
1	C	103	GLN
1	C	117	ILE

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Mol	Chain	Res	Type
1	C	119	ASP
1	C	121	ARG
1	C	125	GLU
1	C	129	ASP
1	C	132	LEU
1	C	152	VAL
1	C	156	LEU
1	C	157	GLU
1	D	5	THR
1	D	9	LEU
1	D	13	LYS
1	D	19	ASP
1	D	23	LYS
1	D	25	LEU
1	D	27	THR
1	D	31	LEU
1	D	36	LYS
1	D	39	HIS
1	D	43	VAL
1	D	46	ASN
1	D	47	PHE
1	D	59	GLU
1	D	60	LEU
1	D	66	ASP
1	D	74	THR
1	D	77	LYS
1	D	78	SER
1	D	92	TRP
1	D	94	ASP
1	D	98	GLU
1	D	99	ARG
1	D	103	GLN
1	D	117	ILE
1	D	118	GLU
1	D	119	ASP
1	D	121	ARG
1	D	125	GLU
1	D	156	LEU
1	D	157	GLU
1	D	158	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	29	ASN
1	A	37	HIS
1	A	41	ASN
1	A	141	HIS
1	B	24	GLN
1	B	37	HIS
1	B	39	HIS
1	B	41	ASN
1	B	141	HIS
1	C	29	ASN
1	C	37	HIS
1	C	39	HIS
1	C	41	ASN
1	C	51	HIS
1	C	141	HIS
1	C	155	HIS
1	D	24	GLN
1	D	29	ASN
1	D	37	HIS
1	D	39	HIS
1	D	41	ASN
1	D	51	HIS
1	D	103	GLN
1	D	141	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	157/183 (85%)	0.58	8 (5%)	32	21	32, 58, 78, 88	0
1	B	157/183 (85%)	0.76	9 (5%)	27	17	31, 59, 78, 87	0
1	C	157/183 (85%)	0.63	6 (3%)	44	32	30, 59, 79, 85	0
1	D	157/183 (85%)	0.66	7 (4%)	37	26	31, 58, 81, 87	0
All	All	628/732 (85%)	0.66	30 (4%)	34	23	30, 58, 79, 88	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	11	ASP	4.7
1	A	157	GLU	4.7
1	A	129	ASP	4.7
1	B	157	GLU	4.0
1	D	160	GLY	3.4
1	A	75	LEU	3.3
1	C	75	LEU	2.9
1	B	131	ASP	2.7
1	B	161	GLY	2.6
1	A	113	TYR	2.6
1	A	150	TRP	2.5
1	D	152	VAL	2.5
1	C	40	TRP	2.5
1	B	16	ASP	2.4
1	C	156	LEU	2.4
1	A	29	ASN	2.4
1	D	150	TRP	2.4
1	D	40	TRP	2.3
1	D	29	ASN	2.3
1	B	45	PRO	2.3
1	D	79	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	48	ILE	2.2
1	B	18	ALA	2.2
1	C	21	LEU	2.1
1	A	25	LEU	2.1
1	C	113	TYR	2.1
1	C	95	TYR	2.1
1	A	149	GLN	2.1
1	B	42	VAL	2.0
1	B	122	LYS	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 carbohydrates in this entry.

6.4 Ligands (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
2	FE	B	1162	1/1	0.08	0.31	0.91	56,56,56,56	1
2	FE	D	1162	1/1	0.70	0.20	-0.66	55,55,55,55	1
2	FE	A	1162	1/1	0.62	0.20	-1.00	56,56,56,56	1
2	FE	C	1162	1/1	0.52	0.44	-	55,55,55,55	1

6.5 Other polymers (i)

There are no such residues in this entry.