



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 2, 2016 – 12:01 AM GMT

PDB ID : 8ATC
Title : COMPLEX OF N-PHOSPHONACETYL-L-ASPARTATE WITH ASPARTATE CARBAMOYLTRANSFERASE. X-RAY REFINEMENT, ANALYSIS OF CONFORMATIONAL CHANGES AND CATALYTIC AND ALLOSTERIC MECHANISMS
Authors : Ke, H.; Lipscomb, W.N.; Cho, Y.; Honzatko, R.B.
Deposited on : 1989-08-25
Resolution : 2.50 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

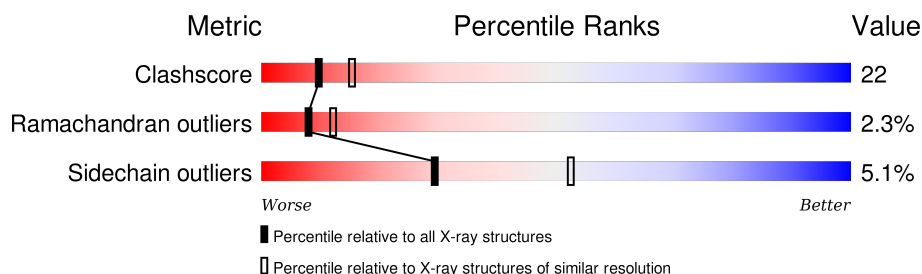
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.




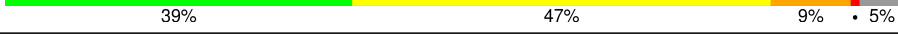
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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 $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	310	 72% 22% 5%
1	C	310	 65% 28% 7%
2	B	153	 41% 46% 8% 5%
2	D	153	 39% 47% 9% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8072 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 ASPARTATE CARBAMOYLTRANSFERASE (R STATE), CATALYTIC CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	C	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	GLN	GLU	CONFLICT	UNP P0A786
A	147	GLN	GLU	CONFLICT	UNP P0A786
A	149	GLU	GLN	CONFLICT	UNP P0A786
A	196	GLU	GLN	CONFLICT	UNP P0A786
C	60	GLN	GLU	CONFLICT	UNP P0A786
C	147	GLN	GLU	CONFLICT	UNP P0A786
C	149	GLU	GLN	CONFLICT	UNP P0A786
C	196	GLU	GLN	CONFLICT	UNP P0A786

- Molecule 2 is a protein called ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1138	714	201	218	5			
2	D	146	Total	C	N	O	S	0	0	0
			1138	714	201	218	5			

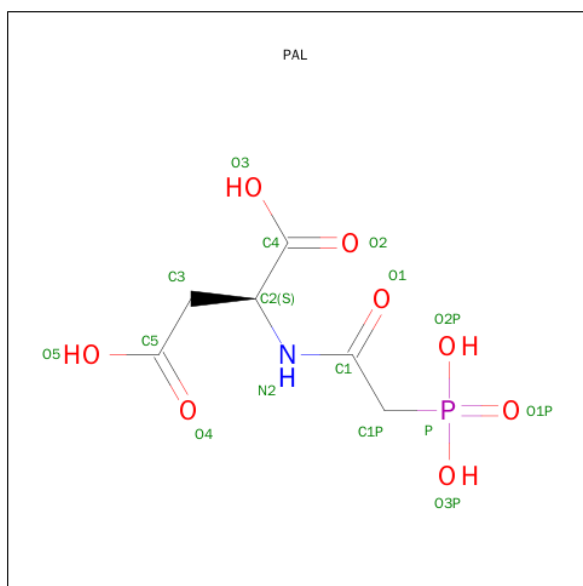
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	8	GLY	GLN	CONFLICT	UNP P0A7F3
D	8	GLY	GLN	CONFLICT	UNP P0A7F3

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is N-(PHOSPHONACETYL)-L-ASPARTIC ACID (three-letter code: PAL) (formula: C₆H₁₀NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			16	6	1	8	1		
4	C	1	Total	C	N	O	P	0	0
			16	6	1	8	1		

- Molecule 5 is water.

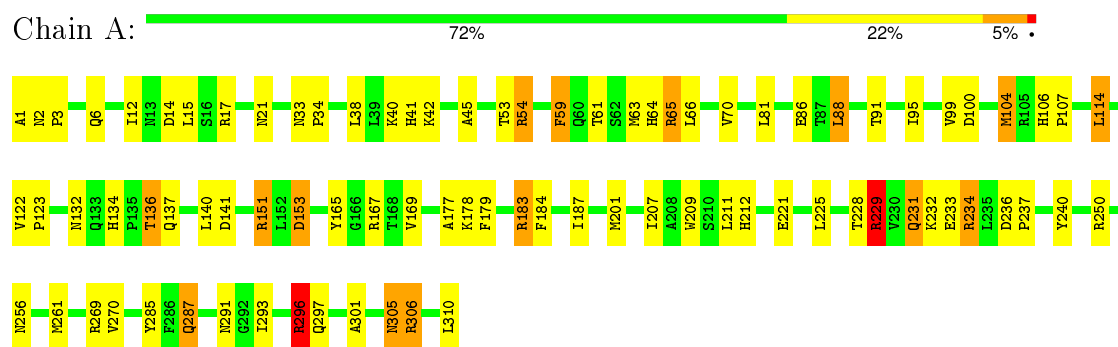
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	365	Total	O	0	0
			365	365		
5	B	128	Total	O	0	0
			128	128		
5	C	313	Total	O	0	0
			313	313		
5	D	126	Total	O	0	0
			126	126		

3 Residue-property plots

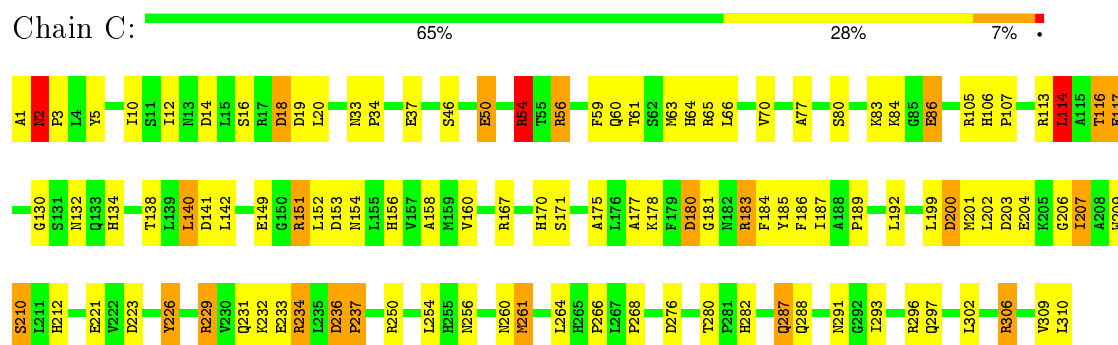
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

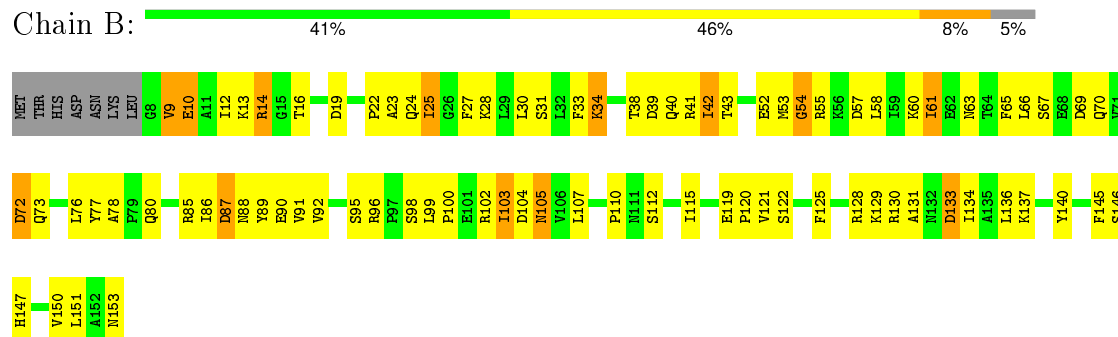
• Molecule 1: ASPARTATE CARBAMOYLTRANSFERASE (R STATE), CATALYTIC CHAIN



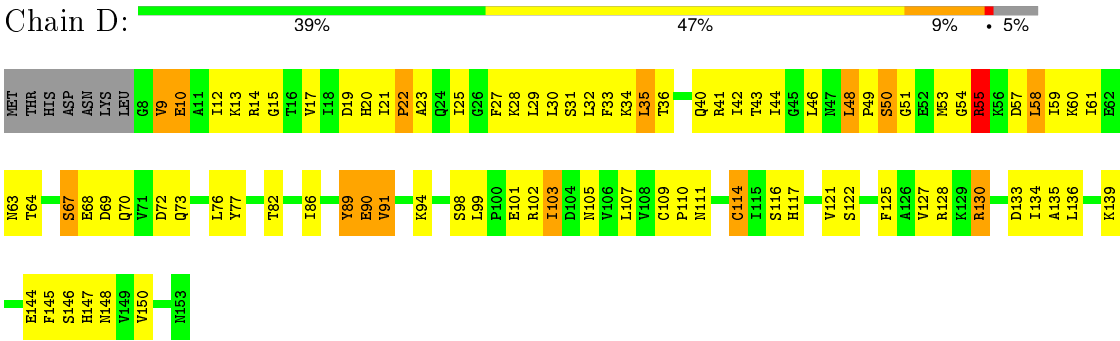
• Molecule 1: ASPARTATE CARBAMOYLTRANSFERASE (R STATE), CATALYTIC CHAIN



• Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN



● Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.11Å 122.11Å 156.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.165 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8072	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PAL

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	0.89	0/2461	1.82	37/3339 (1.1%)
1	C	0.89	0/2461	1.77	40/3339 (1.2%)
2	B	0.84	1/1155 (0.1%)	1.56	13/1561 (0.8%)
2	D	0.83	0/1155	1.54	8/1561 (0.5%)
All	All	0.87	1/7232 (0.0%)	1.72	98/9800 (1.0%)

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	1
1	C	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	54	GLY	N-CA	-5.82	1.37	1.46

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	229	ARG	NE-CZ-NH1	21.80	131.20	120.30
1	C	229	ARG	CD-NE-CZ	19.45	150.83	123.60
1	A	229	ARG	NE-CZ-NH1	19.19	129.90	120.30
1	A	229	ARG	CD-NE-CZ	18.24	149.14	123.60
1	A	54	ARG	NE-CZ-NH1	16.62	128.61	120.30
1	C	229	ARG	NE-CZ-NH2	-16.23	112.18	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	296	ARG	NE-CZ-NH1	14.58	127.59	120.30
1	A	183	ARG	NE-CZ-NH1	-14.37	113.11	120.30
1	A	17	ARG	NE-CZ-NH2	-14.04	113.28	120.30
1	A	54	ARG	NE-CZ-NH2	-13.36	113.62	120.30
2	B	53	MET	C-N-CA	12.64	148.84	122.30
1	A	234	ARG	NE-CZ-NH1	-12.38	114.11	120.30
1	A	229	ARG	NE-CZ-NH2	-11.24	114.68	120.30
1	A	100	ASP	CB-CG-OD1	10.13	127.42	118.30
1	A	183	ARG	CD-NE-CZ	-10.04	109.54	123.60
1	C	306	ARG	NE-CZ-NH1	10.04	125.32	120.30
1	C	54	ARG	NE-CZ-NH2	-9.83	115.39	120.30
1	A	296	ARG	NE-CZ-NH2	9.11	124.85	120.30
1	C	234	ARG	NE-CZ-NH1	-8.92	115.84	120.30
1	A	114	LEU	CA-CB-CG	8.90	135.78	115.30
1	A	153	ASP	CB-CG-OD1	8.50	125.95	118.30
1	C	234	ARG	CD-NE-CZ	-8.49	111.71	123.60
1	A	65	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	A	54	ARG	CD-NE-CZ	8.05	134.88	123.60
1	A	234	ARG	CD-NE-CZ	-7.90	112.53	123.60
1	C	309	VAL	C-N-CA	7.41	140.23	121.70
1	A	296	ARG	NE-CZ-NH1	-7.41	116.60	120.30
1	C	14	ASP	CA-CB-CG	7.30	129.46	113.40
1	C	183	ARG	CD-NE-CZ	-7.27	113.42	123.60
1	A	165	TYR	CB-CG-CD1	-7.16	116.70	121.00
2	B	115	ILE	C-N-CA	7.14	139.55	121.70
1	C	276	ASP	CB-CG-OD1	7.09	124.68	118.30
1	C	14	ASP	CB-CG-OD2	7.05	124.65	118.30
1	C	86	GLU	CA-CB-CG	6.97	128.73	113.40
2	B	54	GLY	N-CA-C	6.69	129.83	113.10
1	A	167	ARG	NE-CZ-NH2	6.68	123.64	120.30
1	A	306	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	C	200	ASP	CB-CG-OD1	6.53	124.18	118.30
2	B	104	ASP	C-N-CA	6.28	137.40	121.70
2	D	53	MET	N-CA-CB	6.28	121.90	110.60
2	D	90	GLU	C-N-CA	6.21	137.22	121.70
1	A	183	ARG	NH1-CZ-NH2	6.10	126.11	119.40
2	D	55	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	53	THR	N-CA-CB	6.03	121.75	110.30
1	C	54	ARG	NE-CZ-NH1	6.02	123.31	120.30
2	B	128	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	C	114	LEU	CA-CB-CG	5.93	128.94	115.30
1	C	156	HIS	O-C-N	5.90	132.15	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	96	ARG	NE-CZ-NH1	5.88	123.24	120.30
2	B	133	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	A	104	MET	N-CA-CB	-5.86	100.06	110.60
1	A	305	ASN	O-C-N	5.85	132.06	122.70
1	C	113	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	A	179	PHE	CB-CA-C	5.80	122.00	110.40
1	C	50	GLU	CG-CD-OE2	-5.78	106.75	118.30
2	B	140	TYR	CB-CG-CD1	-5.74	117.56	121.00
1	A	221	GLU	OE1-CD-OE2	5.68	130.12	123.30
1	C	296	ARG	NH1-CZ-NH2	-5.68	113.15	119.40
2	B	55	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	C	226	TYR	CB-CG-CD2	-5.64	117.62	121.00
1	C	117	GLU	OE1-CD-OE2	5.63	130.05	123.30
2	D	130	ARG	NE-CZ-NH1	-5.59	117.50	120.30
2	D	53	MET	C-N-CA	5.59	134.04	122.30
1	A	6	GLN	CA-CB-CG	-5.54	101.22	113.40
1	C	19	ASP	CB-CG-OD1	5.54	123.28	118.30
1	A	250	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	C	56	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	C	183	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	C	56	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	C	264	LEU	CA-CB-CG	5.46	127.85	115.30
1	C	221	GLU	CG-CD-OE1	5.43	129.16	118.30
2	B	72	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	C	268	PRO	O-C-N	5.39	131.33	122.70
2	D	114	CYS	CA-CB-SG	5.34	123.61	114.00
1	A	153	ASP	CA-CB-CG	5.33	125.11	113.40
1	A	141	ASP	CB-CG-OD2	-5.32	113.51	118.30
2	D	23	ALA	C-N-CA	5.31	134.99	121.70
1	C	2	ASN	CB-CA-C	5.31	121.02	110.40
1	A	269	ARG	CB-CG-CD	5.30	125.39	111.60
1	A	17	ARG	NH1-CZ-NH2	5.29	125.22	119.40
1	A	141	ASP	CB-CG-OD1	5.28	123.05	118.30
1	C	221	GLU	CA-CB-CG	5.27	124.99	113.40
1	C	180	ASP	CB-CG-OD1	5.27	123.04	118.30
1	C	37	GLU	CG-CD-OE2	-5.22	107.86	118.30
1	A	42	LYS	O-C-N	5.18	130.98	122.70
2	B	14	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	C	116	THR	N-CA-CB	5.14	120.07	110.30
2	B	87	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	C	250	ARG	NE-CZ-NH2	-5.13	117.73	120.30
2	D	68	GLU	O-C-N	5.13	130.91	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	GLU	CG-CD-OE2	-5.12	108.06	118.30
1	A	88	LEU	CB-CA-C	5.12	119.92	110.20
1	C	18	ASP	CB-CA-C	5.10	120.61	110.40
1	A	65	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	C	151	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	C	19	ASP	CB-CG-OD2	-5.05	113.76	118.30
1	C	237	PRO	N-CD-CG	-5.01	95.69	103.20
2	B	72	ASP	CB-CA-C	5.00	120.40	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	296	ARG	Sidechain
1	C	54	ARG	Sidechain

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	2415	0	2422	65	0
1	C	2415	0	2422	81	2
2	B	1138	0	1152	73	0
2	D	1138	0	1154	112	1
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	16	0	5	0	0
4	C	16	0	6	0	0
5	A	365	0	0	6	1
5	B	128	0	0	1	0
5	C	313	0	0	3	1
5	D	126	0	0	3	0
All	All	8072	0	7161	319	4

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 22.

All (319) 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:D:30:LEU:HD13	2:D:59:ILE:HD13	1.20	1.11
2:D:22:PRO:HB2	2:D:25:ILE:HD12	1.35	1.09
2:B:9:VAL:O	2:B:10:GLU:HG2	1.54	1.04
2:D:10:GLU:HB2	2:D:43:THR:HG21	1.44	1.00
1:A:287:GLN:HE21	1:A:287:GLN:N	1.63	0.96
2:D:22:PRO:HB2	2:D:25:ILE:CD1	1.96	0.95
2:D:82:THR:CG2	2:D:94:LYS:HE3	1.96	0.95
1:A:287:GLN:NE2	1:A:287:GLN:H	1.67	0.93
2:D:82:THR:HG21	2:D:94:LYS:HE3	1.51	0.92
1:C:114:LEU:HD22	2:D:121:VAL:HG11	1.50	0.92
1:C:234:ARG:HH11	1:C:234:ARG:HG3	1.35	0.91
2:D:40:GLN:OE1	2:D:63:ASN:HB2	1.72	0.90
2:D:134:ILE:H	2:D:147:HIS:HD2	1.20	0.89
2:D:46:LEU:HA	2:D:57:ASP:OD2	1.73	0.88
2:D:9:VAL:O	2:D:10:GLU:HG2	1.75	0.85
2:B:58:LEU:HD21	2:B:60:LYS:HE3	1.59	0.85
2:D:30:LEU:HD13	2:D:59:ILE:CD1	2.04	0.84
2:B:105:ASN:HB3	2:B:122:SER:HB3	1.58	0.83
2:D:30:LEU:CD1	2:D:59:ILE:HD13	2.08	0.82
1:A:287:GLN:HE21	1:A:287:GLN:H	0.84	0.82
2:B:42:ILE:HD13	2:B:61:ILE:HG23	1.62	0.82
2:D:134:ILE:H	2:D:147:HIS:CD2	1.98	0.82
1:C:287:GLN:H	1:C:287:GLN:HE21	1.25	0.82
2:B:134:ILE:H	2:B:147:HIS:CD2	1.98	0.81
2:D:30:LEU:HD21	2:D:44:ILE:CD1	2.11	0.81
2:D:30:LEU:HD21	2:D:44:ILE:HD13	1.63	0.81
2:B:134:ILE:H	2:B:147:HIS:HD2	1.28	0.80
1:C:234:ARG:NH1	1:C:234:ARG:HG3	1.97	0.78
1:A:234:ARG:HH11	1:A:234:ARG:HG3	1.48	0.78
2:D:42:ILE:HG12	2:D:61:ILE:HG23	1.66	0.77
2:D:133:ASP:HB2	2:D:147:HIS:CD2	2.20	0.77
2:D:36:THR:HG22	2:D:36:THR:O	1.81	0.77
2:B:72:ASP:HB3	2:B:100:PRO:HG3	1.65	0.77
2:D:9:VAL:HG11	2:D:58:LEU:HD13	1.69	0.75
2:D:58:LEU:HD21	2:D:60:LYS:CE	2.17	0.75
1:C:200:ASP:O	1:C:204:GLU:HG3	1.86	0.74
2:D:32:LEU:CD1	2:D:77:TYR:CZ	2.69	0.74
2:B:13:LYS:HG3	2:B:89:TYR:CE1	2.21	0.74
1:A:114:LEU:CD2	2:B:121:VAL:HG11	2.18	0.74
2:B:103:ILE:HD12	2:B:107:LEU:HD12	1.70	0.74
2:B:10:GLU:HG3	2:B:43:THR:HG21	1.71	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:32:LEU:HD11	2:D:77:TYR:OH	1.89	0.73
2:B:134:ILE:HB	2:B:147:HIS:CD2	2.23	0.73
1:C:184:PHE:O	1:C:209:TRP:HA	1.88	0.73
1:C:66:LEU:HD21	1:C:297:GLN:HE21	1.53	0.72
2:D:9:VAL:HG11	2:D:58:LEU:CD1	2.19	0.72
2:D:10:GLU:CB	2:D:43:THR:HG21	2.19	0.72
1:A:64:HIS:HD2	5:A:325:HOH:O	1.72	0.72
2:B:76:LEU:HD11	2:B:103:ILE:HD13	1.71	0.72
1:C:287:GLN:H	1:C:287:GLN:NE2	1.87	0.71
1:A:106:HIS:ND1	1:A:107:PRO:HD2	2.05	0.70
2:D:99:LEU:HD21	2:D:134:ILE:HD13	1.73	0.70
2:B:67:SER:HB2	2:B:70:GLN:HG3	1.74	0.70
1:C:106:HIS:CG	1:C:107:PRO:HD2	2.26	0.70
1:C:114:LEU:CD2	2:D:121:VAL:HG11	2.19	0.70
2:B:38:THR:CG2	2:B:42:ILE:HD11	2.22	0.70
2:D:76:LEU:HD11	2:D:103:ILE:CD1	2.21	0.69
2:D:76:LEU:HD11	2:D:103:ILE:HD11	1.75	0.69
2:B:86:ILE:HA	2:B:90:GLU:O	1.93	0.69
1:A:65:ARG:HB2	1:A:297:GLN:HE21	1.57	0.69
2:D:58:LEU:C	2:D:58:LEU:HD23	2.15	0.68
1:A:137:GLN:NE2	5:A:378:HOH:O	2.26	0.68
1:A:234:ARG:NH1	1:A:234:ARG:HG3	2.08	0.67
2:D:82:THR:HG23	2:D:94:LYS:HE3	1.76	0.67
2:D:29:LEU:HD21	2:D:77:TYR:CB	2.25	0.67
1:C:106:HIS:ND1	1:C:107:PRO:HD2	2.10	0.67
2:D:48:LEU:O	2:D:55:ARG:HA	1.95	0.66
1:C:114:LEU:HD22	2:D:121:VAL:CG1	2.26	0.66
2:D:58:LEU:HD21	2:D:60:LYS:HE3	1.77	0.65
2:B:38:THR:HG21	2:B:42:ILE:HD11	1.79	0.65
1:A:237:PRO:HA	1:A:240:TYR:CD1	2.31	0.65
1:C:234:ARG:NH1	1:C:234:ARG:CG	2.54	0.65
2:D:58:LEU:HD21	2:D:60:LYS:HG3	1.79	0.65
1:A:236:ASP:OD2	1:A:237:PRO:HD2	1.96	0.65
2:D:67:SER:OG	2:D:70:GLN:HG3	1.98	0.64
1:A:225:LEU:HB3	1:A:261:MET:HE1	1.80	0.64
1:C:141:ASP:OD1	1:C:288:GLN:NE2	2.29	0.64
2:D:14:ARG:HA	2:D:86:ILE:HG22	1.80	0.64
2:B:40:GLN:OE1	2:B:63:ASN:HB2	1.98	0.62
1:C:261:MET:O	1:C:282:HIS:ND1	2.31	0.62
1:A:187:ILE:HG12	1:A:212:HIS:HB2	1.82	0.62
1:A:106:HIS:CG	1:A:107:PRO:HD2	2.35	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:GLU:HB2	2:B:60:LYS:HD2	1.82	0.61
2:B:99:LEU:HD12	2:B:129:LYS:HB3	1.81	0.61
2:B:134:ILE:N	2:B:147:HIS:HD2	1.98	0.61
2:B:69:ASP:O	2:B:72:ASP:N	2.34	0.61
2:B:9:VAL:O	2:B:10:GLU:CG	2.40	0.61
2:D:40:GLN:OE1	2:D:63:ASN:CB	2.45	0.61
2:D:25:ILE:O	2:D:29:LEU:HG	2.00	0.60
2:D:32:LEU:HD11	2:D:77:TYR:CZ	2.35	0.60
1:C:310:LEU:HD12	1:C:310:LEU:N	2.16	0.60
2:D:21:ILE:O	2:D:22:PRO:C	2.40	0.60
1:A:114:LEU:HD23	2:B:121:VAL:HG11	1.84	0.59
2:D:32:LEU:CD1	2:D:77:TYR:OH	2.48	0.59
1:C:138:THR:OG1	1:C:171:SER:HB3	2.01	0.59
2:D:145:PHE:HB2	2:D:150:VAL:HG23	1.84	0.59
1:A:225:LEU:HB3	1:A:261:MET:CE	2.33	0.58
2:B:76:LEU:HD11	2:B:103:ILE:CD1	2.33	0.58
2:D:13:LYS:HG3	2:D:89:TYR:CE1	2.39	0.58
2:B:99:LEU:CD1	2:B:129:LYS:HB3	2.33	0.58
1:A:2:ASN:HB2	1:A:3:PRO:HD2	1.86	0.58
2:D:9:VAL:HG13	2:D:60:LYS:HE3	1.85	0.58
1:A:65:ARG:HB2	1:A:297:GLN:NE2	2.19	0.58
2:D:13:LYS:HG2	2:D:13:LYS:O	2.04	0.57
1:A:14:ASP:OD2	5:A:474:HOH:O	2.17	0.57
2:B:91:VAL:O	2:B:91:VAL:HG12	2.03	0.57
2:B:87:ASP:HB3	2:B:92:VAL:HG21	1.86	0.57
1:A:231:GLN:HE21	1:A:234:ARG:HH12	1.53	0.57
2:B:16:THR:OG1	2:B:65:PHE:HA	2.05	0.56
2:D:107:LEU:HD13	2:D:150:VAL:HG11	1.87	0.56
2:B:119:GLU:OE2	2:B:120:PRO:HD2	2.05	0.56
2:D:20:HIS:HE1	5:D:916:HOH:O	1.89	0.56
2:D:12:ILE:HD11	2:D:17:VAL:CG2	2.35	0.56
1:A:88:LEU:HD11	1:A:104:MET:CE	2.36	0.56
1:A:61:THR:HB	1:A:293:ILE:HD11	1.88	0.56
1:A:234:ARG:NH1	1:A:234:ARG:CG	2.60	0.56
1:C:236:ASP:HB2	1:C:237:PRO:HD2	1.87	0.56
1:A:106:HIS:CE1	1:A:107:PRO:HD2	2.41	0.55
1:A:229:ARG:NH2	1:A:233:GLU:OE1	2.32	0.55
1:A:12:ILE:CG2	1:A:12:ILE:O	2.54	0.55
1:C:114:LEU:CD2	2:D:121:VAL:CG1	2.82	0.55
1:C:130:GLY:O	1:C:167:ARG:HD3	2.06	0.55
1:C:201:MET:HG2	1:C:201:MET:O	1.97	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:GLU:CB	2:B:60:LYS:HD2	2.37	0.55
1:C:189:PRO:HG2	1:C:192:LEU:HB2	1.87	0.55
1:A:169:VAL:CG1	1:A:228:THR:HG21	2.37	0.54
2:D:10:GLU:OE1	2:D:41:ARG:NH2	2.41	0.54
2:B:27:PHE:CE2	2:D:27:PHE:CE2	2.96	0.54
1:A:88:LEU:HD21	1:A:104:MET:HE1	1.88	0.54
2:B:133:ASP:OD2	2:B:146:SER:OG	2.24	0.54
2:B:130:ARG:HB2	2:B:133:ASP:O	2.07	0.54
1:C:10:ILE:HD11	1:C:116:THR:CG2	2.38	0.54
1:C:154:ASN:HA	1:C:181:GLY:O	2.08	0.54
2:B:102:ARG:HA	2:B:125:PHE:O	2.08	0.54
1:C:117:GLU:OE1	2:D:139:LYS:NZ	2.33	0.53
2:D:29:LEU:HD22	2:D:33:PHE:HE1	1.73	0.53
2:B:40:GLN:O	2:B:42:ILE:HG12	2.09	0.53
1:A:225:LEU:CB	1:A:261:MET:CE	2.87	0.53
2:D:17:VAL:HG23	2:D:86:ILE:HD12	1.90	0.53
2:B:136:LEU:HD12	2:B:150:VAL:HG21	1.91	0.52
2:B:22:PRO:O	2:B:25:ILE:HB	2.10	0.52
2:B:103:ILE:HD12	2:B:107:LEU:CD1	2.39	0.52
1:A:65:ARG:CB	1:A:297:GLN:NE2	2.73	0.52
2:B:39:ASP:OD1	2:D:55:ARG:NH1	2.43	0.52
1:C:138:THR:HG21	1:C:175:ALA:HB2	1.91	0.52
1:A:287:GLN:NE2	1:A:287:GLN:N	2.40	0.52
1:C:310:LEU:CD1	1:C:310:LEU:N	2.73	0.52
2:D:29:LEU:HD21	2:D:77:TYR:CG	2.45	0.51
2:B:102:ARG:HB2	2:B:125:PHE:O	2.09	0.51
1:A:81:LEU:HA	1:A:86:GLU:HB3	1.92	0.51
1:C:310:LEU:CD1	1:C:310:LEU:H	2.23	0.51
2:D:107:LEU:HD13	2:D:150:VAL:CG1	2.39	0.51
1:A:38:LEU:HD12	1:A:66:LEU:HD22	1.91	0.51
1:A:1:ALA:HA	1:A:306:ARG:CG	2.41	0.51
1:A:1:ALA:HA	1:A:306:ARG:HG2	1.91	0.51
2:D:90:GLU:CG	2:D:91:VAL:N	2.73	0.51
2:D:58:LEU:CD2	2:D:60:LYS:HG3	2.40	0.51
1:C:61:THR:O	1:C:65:ARG:HG2	2.11	0.51
1:C:204:GLU:C	1:C:206:GLY:H	2.15	0.50
2:D:9:VAL:CG1	2:D:60:LYS:HE3	2.42	0.50
1:C:229:ARG:NH2	1:C:233:GLU:OE1	2.42	0.50
2:D:49:PRO:O	2:D:50:SER:HB2	2.11	0.50
2:D:15:GLY:HA2	2:D:64:THR:O	2.11	0.49
2:B:73:GLN:O	2:B:77:TYR:HD2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:LEU:O	1:C:207:ILE:N	2.40	0.49
1:A:45:ALA:HB2	1:A:99:VAL:HG11	1.94	0.49
2:D:130:ARG:HD2	2:D:135:ALA:HB2	1.95	0.49
2:B:23:ALA:O	2:B:24:GLN:HB2	2.11	0.49
1:A:88:LEU:HD11	1:A:104:MET:HE3	1.95	0.49
1:C:151:ARG:O	1:C:152:LEU:HD23	2.13	0.49
1:A:114:LEU:CD2	2:B:121:VAL:CG1	2.89	0.49
1:C:80:SER:OG	1:C:84:LYS:HD2	2.13	0.49
2:B:134:ILE:CB	2:B:147:HIS:CD2	2.95	0.48
2:D:76:LEU:HD23	2:D:134:ILE:HD12	1.94	0.48
1:C:77:ALA:O	1:C:83:LYS:HE3	2.13	0.48
2:D:69:ASP:O	2:D:73:GLN:HG3	2.14	0.48
1:C:5:TYR:CD2	1:C:306:ARG:HA	2.47	0.48
2:D:30:LEU:HD21	2:D:44:ILE:HD11	1.93	0.48
2:B:85:ARG:C	2:B:86:ILE:HG13	2.34	0.48
1:A:177:ALA:HB1	1:A:207:ILE:HD12	1.95	0.48
1:C:64:HIS:HE1	5:C:345:HOH:O	1.96	0.48
2:D:36:THR:CG2	2:D:36:THR:O	2.50	0.48
2:B:87:ASP:O	2:B:88:ASN:HB3	2.14	0.48
1:C:63:MET:SD	1:C:70:VAL:HG22	2.53	0.48
1:C:2:ASN:HA	1:C:3:PRO:HD3	1.79	0.48
1:C:20:LEU:HD13	1:C:142:LEU:CD1	2.44	0.47
2:B:41:ARG:NH1	5:B:224:HOH:O	2.48	0.47
1:C:203:ASP:O	1:C:206:GLY:HA2	2.14	0.47
1:A:106:HIS:CG	1:A:107:PRO:CD	2.97	0.47
2:B:125:PHE:HA	2:B:137:LYS:O	2.15	0.47
1:C:160:VAL:HG22	1:C:187:ILE:HB	1.97	0.47
2:D:102:ARG:HA	2:D:127:VAL:HG23	1.96	0.47
2:D:134:ILE:N	2:D:147:HIS:HD2	1.99	0.47
1:C:151:ARG:NH1	1:C:154:ASN:O	2.47	0.47
1:C:12:ILE:HD13	1:C:12:ILE:HA	1.75	0.47
2:D:28:LYS:HE3	5:D:835:HOH:O	2.14	0.47
1:A:122:VAL:HA	1:A:123:PRO:HD3	1.78	0.47
2:D:133:ASP:OD1	2:D:133:ASP:N	2.34	0.47
1:C:287:GLN:NE2	1:C:287:GLN:N	2.61	0.47
1:C:140:LEU:C	1:C:140:LEU:HD12	2.35	0.47
2:B:33:PHE:HA	2:B:33:PHE:HD2	1.57	0.47
2:D:42:ILE:CG1	2:D:61:ILE:HG23	2.40	0.46
1:C:151:ARG:HD2	1:C:153:ASP:O	2.15	0.46
2:D:32:LEU:HD13	2:D:77:TYR:CZ	2.49	0.46
1:C:231:GLN:HE21	1:C:234:ARG:HH12	1.63	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:LEU:HD13	1:C:114:LEU:O	2.15	0.46
1:C:175:ALA:O	1:C:178:LYS:HB2	2.15	0.46
2:D:99:LEU:HD21	2:D:134:ILE:CD1	2.44	0.46
1:C:61:THR:HB	1:C:293:ILE:HD11	1.98	0.46
1:A:209:TRP:HZ3	1:A:211:LEU:HD21	1.81	0.46
2:B:110:PRO:HG2	2:B:145:PHE:CG	2.50	0.46
2:D:58:LEU:HD21	2:D:60:LYS:HE2	1.97	0.46
2:D:14:ARG:CA	2:D:86:ILE:HG22	2.45	0.46
2:D:130:ARG:CD	2:D:135:ALA:HB2	2.46	0.46
1:C:149:GLU:OE2	1:C:260:ASN:ND2	2.40	0.46
2:B:25:ILE:O	2:B:25:ILE:CG2	2.64	0.46
2:D:20:HIS:O	2:D:22:PRO:HD3	2.15	0.46
1:A:61:THR:HB	1:A:293:ILE:CD1	2.45	0.46
1:C:201:MET:O	1:C:201:MET:CG	2.59	0.46
2:D:12:ILE:HD11	2:D:17:VAL:HG23	1.97	0.46
2:D:9:VAL:HG11	2:D:58:LEU:HD11	1.96	0.45
1:C:223:ASP:O	1:C:261:MET:HA	2.16	0.45
2:D:46:LEU:CA	2:D:57:ASP:OD2	2.57	0.45
2:D:10:GLU:O	2:D:60:LYS:NZ	2.45	0.45
1:A:261:MET:HG3	5:A:639:HOH:O	2.16	0.45
2:B:130:ARG:HB3	2:B:131:ALA:H	1.45	0.45
2:B:78:ALA:C	2:B:80:GLN:H	2.19	0.45
1:C:199:LEU:HD13	1:C:209:TRP:CH2	2.52	0.45
2:D:9:VAL:HG13	2:D:60:LYS:CE	2.46	0.45
1:C:186:PHE:CE1	1:C:199:LEU:HD21	2.51	0.45
1:A:237:PRO:HA	1:A:240:TYR:CE1	2.52	0.45
1:A:88:LEU:HD11	1:A:104:MET:HE1	1.98	0.45
1:A:151:ARG:HG3	1:A:153:ASP:O	2.17	0.45
2:D:19:ASP:O	2:D:20:HIS:HB2	2.16	0.45
1:A:12:ILE:HG22	1:A:12:ILE:O	2.15	0.45
1:C:204:GLU:OE1	2:D:128:ARG:NH2	2.50	0.45
1:C:170:HIS:CD2	1:C:170:HIS:N	2.82	0.45
1:C:226:TYR:CZ	1:C:266:PRO:HD3	2.52	0.45
1:C:50:GLU:HB3	1:C:105:ARG:HG2	1.99	0.44
1:A:59:PHE:HZ	1:A:136:THR:HG21	1.82	0.44
2:D:136:LEU:O	2:D:144:GLU:HA	2.18	0.44
2:B:10:GLU:HB2	2:B:60:LYS:HZ2	1.83	0.44
2:B:30:LEU:HD23	2:D:27:PHE:HE2	1.83	0.44
2:D:58:LEU:C	2:D:58:LEU:CD2	2.85	0.44
2:B:99:LEU:HD21	2:B:134:ILE:HD13	1.98	0.44
1:C:212:HIS:CD2	1:C:212:HIS:N	2.86	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LEU:HD12	1:A:140:LEU:C	2.37	0.44
2:B:19:ASP:OD2	2:B:58:LEU:HD12	2.18	0.44
1:C:56:ARG:O	1:C:60:GLN:HG3	2.18	0.43
2:B:119:GLU:HB3	2:B:120:PRO:HD2	2.00	0.43
1:C:177:ALA:HB1	1:C:207:ILE:HD12	2.00	0.43
1:C:232:LYS:NZ	5:C:454:HOH:O	2.50	0.43
1:A:33:ASN:HA	1:A:34:PRO:HD2	1.84	0.43
1:A:291:ASN:HD22	1:A:291:ASN:HA	1.49	0.43
1:A:40:LYS:O	1:A:41:HIS:HB2	2.18	0.43
1:C:186:PHE:HE1	1:C:199:LEU:CD2	2.31	0.43
2:D:12:ILE:HD11	2:D:17:VAL:HG22	2.01	0.43
2:B:105:ASN:HB3	2:B:122:SER:CB	2.41	0.43
2:B:23:ALA:HA	2:B:57:ASP:OD1	2.19	0.43
2:B:10:GLU:HB2	2:B:60:LYS:NZ	2.33	0.43
2:D:35:LEU:O	2:D:42:ILE:HD11	2.19	0.43
2:B:33:PHE:O	2:B:34:LYS:CB	2.66	0.43
1:A:184:PHE:O	1:A:209:TRP:HA	2.19	0.43
1:C:210:SER:HB2	1:C:212:HIS:NE2	2.34	0.43
1:C:254:LEU:HD12	1:C:280:THR:HG21	2.01	0.43
2:D:76:LEU:HD11	2:D:103:ILE:HD13	1.99	0.43
1:C:106:HIS:CE1	1:C:107:PRO:HD2	2.54	0.43
2:B:85:ARG:C	2:B:86:ILE:CG1	2.87	0.43
2:D:70:GLN:HA	2:D:73:GLN:OE1	2.19	0.43
2:B:28:LYS:O	2:B:31:SER:HB3	2.18	0.43
2:D:21:ILE:O	2:D:22:PRO:O	2.37	0.42
2:B:103:ILE:CD1	2:B:107:LEU:CD1	2.97	0.42
2:D:91:VAL:O	2:D:91:VAL:HG12	2.19	0.42
2:D:28:LYS:CE	5:D:835:HOH:O	2.67	0.42
1:C:186:PHE:CE1	1:C:199:LEU:CD2	3.02	0.42
1:C:16:SER:C	1:C:18:ASP:N	2.72	0.42
1:A:64:HIS:HE1	5:A:388:HOH:O	2.02	0.42
2:D:110:PRO:HD2	2:D:145:PHE:CZ	2.54	0.42
2:D:103:ILE:HG13	2:D:127:VAL:CG2	2.50	0.42
1:C:33:ASN:HA	1:C:34:PRO:HD2	1.74	0.42
2:D:133:ASP:CB	2:D:147:HIS:CD2	2.99	0.42
1:A:169:VAL:HG13	1:A:228:THR:HG21	2.00	0.42
2:D:90:GLU:HG2	2:D:91:VAL:N	2.34	0.42
1:C:158:ALA:HA	1:C:185:TYR:O	2.20	0.42
2:B:76:LEU:HD13	2:B:151:LEU:HD21	2.01	0.42
2:D:82:THR:HG21	2:D:94:LYS:CE	2.36	0.42
2:D:102:ARG:HB2	2:D:125:PHE:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:GLN:O	2:B:77:TYR:CD2	2.73	0.42
2:D:109:CYS:O	2:D:117:HIS:HE1	2.03	0.42
2:D:146:SER:O	2:D:147:HIS:C	2.59	0.41
1:C:229:ARG:HH22	1:C:233:GLU:CD	2.22	0.41
2:B:14:ARG:HA	2:B:86:ILE:O	2.20	0.41
1:C:66:LEU:HD23	1:C:66:LEU:HA	1.82	0.41
1:C:178:LYS:NZ	5:C:316:HOH:O	2.52	0.41
1:C:66:LEU:CD2	1:C:297:GLN:HE21	2.28	0.41
2:D:114:CYS:HB3	2:D:116:SER:HB3	2.03	0.41
1:A:21:ASN:HD22	1:A:21:ASN:HA	1.73	0.41
2:D:111:ASN:O	2:D:117:HIS:NE2	2.47	0.41
2:B:9:VAL:HG13	2:B:60:LYS:HZ2	1.86	0.41
1:C:61:THR:HB	1:C:293:ILE:CD1	2.50	0.41
1:A:232:LYS:NZ	5:A:427:HOH:O	2.53	0.41
2:D:9:VAL:HG13	2:D:60:LYS:NZ	2.36	0.41
2:D:99:LEU:HD23	2:D:99:LEU:HA	1.87	0.41
1:A:15:LEU:O	1:A:178:LYS:HE3	2.21	0.41
1:A:137:GLN:O	1:A:140:LEU:HG	2.22	0.40
1:C:160:VAL:HG22	1:C:187:ILE:HD12	2.03	0.40
2:D:105:ASN:HD22	2:D:122:SER:HB3	1.85	0.40
2:B:134:ILE:HB	2:B:147:HIS:CG	2.56	0.40
2:B:16:THR:HG1	2:B:65:PHE:HA	1.85	0.40
1:A:296:ARG:HH11	1:A:296:ARG:HD2	1.56	0.40
1:A:91:THR:HG22	1:A:95:ILE:HD12	2.01	0.40
1:C:2:ASN:HD21	1:C:302:LEU:HA	1.86	0.40
1:C:291:ASN:HD22	1:C:291:ASN:HA	1.60	0.40
1:A:301:ALA:O	1:A:305:ASN:HB2	2.21	0.40
1:A:63:MET:SD	1:A:70:VAL:HG22	2.62	0.40
2:D:72:ASP:OD2	2:D:98:SER:O	2.40	0.40
2:B:110:PRO:HG2	2:B:145:PHE:CD2	2.57	0.40
1:C:46:SER:OG	1:C:60:GLN:NE2	2.52	0.40
2:D:148:ASN:HA	2:D:148:ASN:HD22	1.65	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:602:HOH:O	5:C:602:HOH:O[2_655]	1.34	0.86
5:A:332:HOH:O	5:A:398:HOH:O[2_655]	1.98	0.22
1:C:54:ARG:NH2	1:C:86:GLU:OE2[2_655]	2.02	0.18
1:C:1:ALA:N	2:D:101:GLU:OE1[4_555]	2.03	0.17

5.3 Torsion angles

5.3.1 Protein backbone

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	308/310 (99%)	292 (95%)	13 (4%)	3 (1%)	19	34
1	C	308/310 (99%)	290 (94%)	17 (6%)	1 (0%)	46	68
2	B	144/153 (94%)	121 (84%)	17 (12%)	6 (4%)	3	4
2	D	144/153 (94%)	111 (77%)	22 (15%)	11 (8%)	1	1
All	All	904/926 (98%)	814 (90%)	69 (8%)	21 (2%)	8	12

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	10	GLU
2	B	52	GLU
2	B	54	GLY
2	B	105	ASN
2	D	34	LYS
2	D	50	SER
2	D	51	GLY
2	D	54	GLY
2	D	89	TYR
2	D	91	VAL
2	B	9	VAL
2	D	9	VAL
2	D	10	GLU
1	C	132	ASN
2	D	22	PRO
2	B	34	LYS
2	D	35	LEU
1	A	132	ASN
1	A	231	GLN
2	D	67	SER
1	A	270	VAL

5.3.2 Protein sidechains ⓘ

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	261/261 (100%)	249 (95%)	12 (5%)	33	57
1	C	261/261 (100%)	248 (95%)	13 (5%)	30	53
2	B	129/136 (95%)	119 (92%)	10 (8%)	16	29
2	D	129/136 (95%)	124 (96%)	5 (4%)	39	66
All	All	780/794 (98%)	740 (95%)	40 (5%)	29	52

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ARG
1	A	59	PHE
1	A	134	HIS
1	A	136	THR
1	A	151	ARG
1	A	183	ARG
1	A	201	MET
1	A	229	ARG
1	A	256	ASN
1	A	285	TYR
1	A	287	GLN
1	A	310	LEU
2	B	12	ILE
2	B	25	ILE
2	B	42	ILE
2	B	61	ILE
2	B	66	LEU
2	B	95	SER
2	B	98	SER
2	B	103	ILE
2	B	112	SER
2	B	153	ASN
1	C	2	ASN
1	C	59	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	114	LEU
1	C	134	HIS
1	C	140	LEU
1	C	180	ASP
1	C	183	ARG
1	C	207	ILE
1	C	210	SER
1	C	236	ASP
1	C	256	ASN
1	C	261	MET
1	C	287	GLN
2	D	31	SER
2	D	48	LEU
2	D	55	ARG
2	D	58	LEU
2	D	103	ILE

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	21	ASN
1	A	78	ASN
1	A	132	ASN
1	A	147	GLN
1	A	231	GLN
1	A	242	ASN
1	A	256	ASN
1	A	287	GLN
1	A	291	ASN
1	A	297	GLN
2	B	147	HIS
1	C	132	ASN
1	C	137	GLN
1	C	147	GLN
1	C	154	ASN
1	C	231	GLN
1	C	287	GLN
1	C	291	ASN
1	C	297	GLN
2	D	24	GLN
2	D	47	ASN
2	D	84	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	105	ASN
2	D	147	HIS
2	D	148	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	PAL	A	311	-	9,15,15	2.30	5 (55%)	12,21,21	1.40	2 (16%)
4	PAL	C	311	-	9,15,15	2.02	3 (33%)	12,21,21	1.94	7 (58%)

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	PAL	A	311	-	-	0/11/17/17	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PAL	C	311	-	-	0/11/17/17	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	311	PAL	C2-N2	-3.90	1.41	1.46
4	A	311	PAL	P-O2P	-3.51	1.46	1.54
4	C	311	PAL	C2-N2	-3.34	1.41	1.46
4	C	311	PAL	P-O2P	-2.39	1.49	1.54
4	C	311	PAL	C3-C2	2.08	1.56	1.53
4	A	311	PAL	C3-C2	2.08	1.56	1.53
4	A	311	PAL	O1-C1	2.10	1.27	1.23
4	A	311	PAL	P-O3P	2.15	1.60	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	311	PAL	C3-C2-C4	-2.72	105.72	111.55
4	C	311	PAL	C3-C2-C4	-2.53	106.11	111.55
4	C	311	PAL	O3P-P-O1P	-2.49	106.03	112.40
4	C	311	PAL	O1-C1-C1P	-2.34	114.74	120.92
4	C	311	PAL	O1-C1-N2	-2.13	119.39	123.01
4	C	311	PAL	C3-C2-N2	2.02	114.21	108.23
4	A	311	PAL	C1P-C1-N2	2.32	119.38	114.52
4	C	311	PAL	O2P-P-O1P	2.70	119.32	112.40
4	C	311	PAL	C1P-C1-N2	2.76	120.29	114.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.