



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:25 PM GMT

PDB ID : 4GW9
Title : Structure of a bacteriophytochrome and light-stimulated protomer swapping
with a gene repressor
Authors : Bellini, D.; Papiz, M.Z.
Deposited on : 2012-09-01
Resolution : 2.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

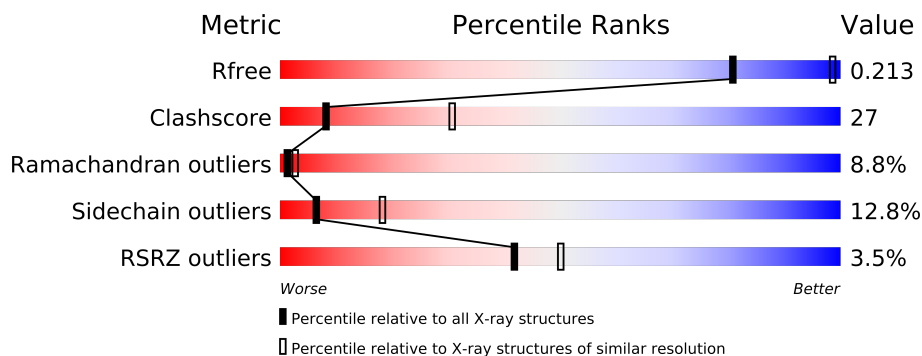
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.90 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}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	655	
1	B	655	
1	C	655	
1	D	655	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19838 atoms, of which 0 are hydrogen and 0 are deuterium.

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 bacteriophytochrome.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	628	Total	C	N	O	S	Se	0	4	0
			4902	3085	883	910	8	16			
1	B	621	Total	C	N	O	S	Se	0	0	0
			4823	3032	870	900	8	13			
1	C	622	Total	C	N	O	S	Se	0	1	0
			4839	3042	875	901	8	13			
1	D	615	Total	C	N	O	S	Se	0	1	0
			4785	3005	865	894	8	13			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	EXPRESSION TAG	UNP B3Q7C0
A	-18	GLY	-	EXPRESSION TAG	UNP B3Q7C0
A	-17	SER	-	EXPRESSION TAG	UNP B3Q7C0
A	-16	SER	-	EXPRESSION TAG	UNP B3Q7C0
A	-15	HIS	-	EXPRESSION TAG	UNP B3Q7C0
A	-14	HIS	-	EXPRESSION TAG	UNP B3Q7C0
A	-13	HIS	-	EXPRESSION TAG	UNP B3Q7C0
A	-12	HIS	-	EXPRESSION TAG	UNP B3Q7C0
A	-11	HIS	-	EXPRESSION TAG	UNP B3Q7C0
A	-10	HIS	-	EXPRESSION TAG	UNP B3Q7C0
A	-9	SER	-	EXPRESSION TAG	UNP B3Q7C0
A	-8	SER	-	EXPRESSION TAG	UNP B3Q7C0
A	-7	GLY	-	EXPRESSION TAG	UNP B3Q7C0
A	-6	LEU	-	EXPRESSION TAG	UNP B3Q7C0
A	-5	VAL	-	EXPRESSION TAG	UNP B3Q7C0
A	-4	PRO	-	EXPRESSION TAG	UNP B3Q7C0
A	-3	ARG	-	EXPRESSION TAG	UNP B3Q7C0
A	-2	GLY	-	EXPRESSION TAG	UNP B3Q7C0
A	-1	SER	-	EXPRESSION TAG	UNP B3Q7C0
A	0	HIS	-	EXPRESSION TAG	UNP B3Q7C0
A	2	VAL	-	SEE REMARK 999	UNP B3Q7C0

Continued on next page...

Continued from previous page...

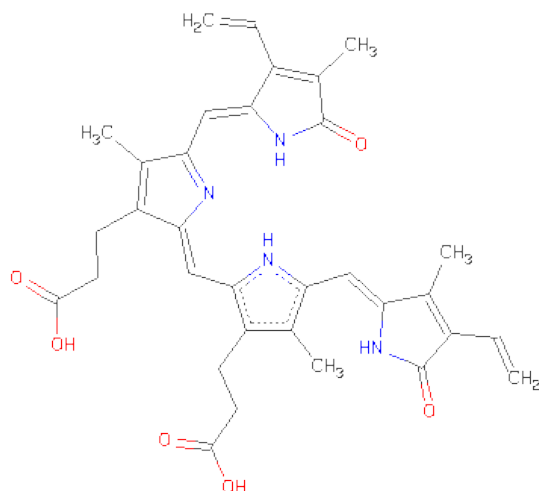
Chain	Residue	Modelled	Actual	Comment	Reference
A	291	ILE	MET	SEE REMARK 999	UNP B3Q7C0
A	360	ASP	ALA	SEE REMARK 999	UNP B3Q7C0
B	-19	MSE	-	EXPRESSION TAG	UNP B3Q7C0
B	-18	GLY	-	EXPRESSION TAG	UNP B3Q7C0
B	-17	SER	-	EXPRESSION TAG	UNP B3Q7C0
B	-16	SER	-	EXPRESSION TAG	UNP B3Q7C0
B	-15	HIS	-	EXPRESSION TAG	UNP B3Q7C0
B	-14	HIS	-	EXPRESSION TAG	UNP B3Q7C0
B	-13	HIS	-	EXPRESSION TAG	UNP B3Q7C0
B	-12	HIS	-	EXPRESSION TAG	UNP B3Q7C0
B	-11	HIS	-	EXPRESSION TAG	UNP B3Q7C0
B	-10	HIS	-	EXPRESSION TAG	UNP B3Q7C0
B	-9	SER	-	EXPRESSION TAG	UNP B3Q7C0
B	-8	SER	-	EXPRESSION TAG	UNP B3Q7C0
B	-7	GLY	-	EXPRESSION TAG	UNP B3Q7C0
B	-6	LEU	-	EXPRESSION TAG	UNP B3Q7C0
B	-5	VAL	-	EXPRESSION TAG	UNP B3Q7C0
B	-4	PRO	-	EXPRESSION TAG	UNP B3Q7C0
B	-3	ARG	-	EXPRESSION TAG	UNP B3Q7C0
B	-2	GLY	-	EXPRESSION TAG	UNP B3Q7C0
B	-1	SER	-	EXPRESSION TAG	UNP B3Q7C0
B	0	HIS	-	EXPRESSION TAG	UNP B3Q7C0
B	2	VAL	-	SEE REMARK 999	UNP B3Q7C0
B	291	ILE	MET	SEE REMARK 999	UNP B3Q7C0
B	360	ASP	ALA	SEE REMARK 999	UNP B3Q7C0
C	-19	MSE	-	EXPRESSION TAG	UNP B3Q7C0
C	-18	GLY	-	EXPRESSION TAG	UNP B3Q7C0
C	-17	SER	-	EXPRESSION TAG	UNP B3Q7C0
C	-16	SER	-	EXPRESSION TAG	UNP B3Q7C0
C	-15	HIS	-	EXPRESSION TAG	UNP B3Q7C0
C	-14	HIS	-	EXPRESSION TAG	UNP B3Q7C0
C	-13	HIS	-	EXPRESSION TAG	UNP B3Q7C0
C	-12	HIS	-	EXPRESSION TAG	UNP B3Q7C0
C	-11	HIS	-	EXPRESSION TAG	UNP B3Q7C0
C	-10	HIS	-	EXPRESSION TAG	UNP B3Q7C0
C	-9	SER	-	EXPRESSION TAG	UNP B3Q7C0
C	-8	SER	-	EXPRESSION TAG	UNP B3Q7C0
C	-7	GLY	-	EXPRESSION TAG	UNP B3Q7C0
C	-6	LEU	-	EXPRESSION TAG	UNP B3Q7C0
C	-5	VAL	-	EXPRESSION TAG	UNP B3Q7C0
C	-4	PRO	-	EXPRESSION TAG	UNP B3Q7C0
C	-3	ARG	-	EXPRESSION TAG	UNP B3Q7C0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	EXPRESSION TAG	UNP B3Q7C0
C	-1	SER	-	EXPRESSION TAG	UNP B3Q7C0
C	0	HIS	-	EXPRESSION TAG	UNP B3Q7C0
C	2	VAL	-	SEE REMARK 999	UNP B3Q7C0
C	291	ILE	MET	SEE REMARK 999	UNP B3Q7C0
C	360	ASP	ALA	SEE REMARK 999	UNP B3Q7C0
D	-19	MSE	-	EXPRESSION TAG	UNP B3Q7C0
D	-18	GLY	-	EXPRESSION TAG	UNP B3Q7C0
D	-17	SER	-	EXPRESSION TAG	UNP B3Q7C0
D	-16	SER	-	EXPRESSION TAG	UNP B3Q7C0
D	-15	HIS	-	EXPRESSION TAG	UNP B3Q7C0
D	-14	HIS	-	EXPRESSION TAG	UNP B3Q7C0
D	-13	HIS	-	EXPRESSION TAG	UNP B3Q7C0
D	-12	HIS	-	EXPRESSION TAG	UNP B3Q7C0
D	-11	HIS	-	EXPRESSION TAG	UNP B3Q7C0
D	-10	HIS	-	EXPRESSION TAG	UNP B3Q7C0
D	-9	SER	-	EXPRESSION TAG	UNP B3Q7C0
D	-8	SER	-	EXPRESSION TAG	UNP B3Q7C0
D	-7	GLY	-	EXPRESSION TAG	UNP B3Q7C0
D	-6	LEU	-	EXPRESSION TAG	UNP B3Q7C0
D	-5	VAL	-	EXPRESSION TAG	UNP B3Q7C0
D	-4	PRO	-	EXPRESSION TAG	UNP B3Q7C0
D	-3	ARG	-	EXPRESSION TAG	UNP B3Q7C0
D	-2	GLY	-	EXPRESSION TAG	UNP B3Q7C0
D	-1	SER	-	EXPRESSION TAG	UNP B3Q7C0
D	0	HIS	-	EXPRESSION TAG	UNP B3Q7C0
D	2	VAL	-	SEE REMARK 999	UNP B3Q7C0
D	291	ILE	MET	SEE REMARK 999	UNP B3Q7C0
D	360	ASP	ALA	SEE REMARK 999	UNP B3Q7C0

^ Molecule 2 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula: C₃₃H₃₄N₄O₆).



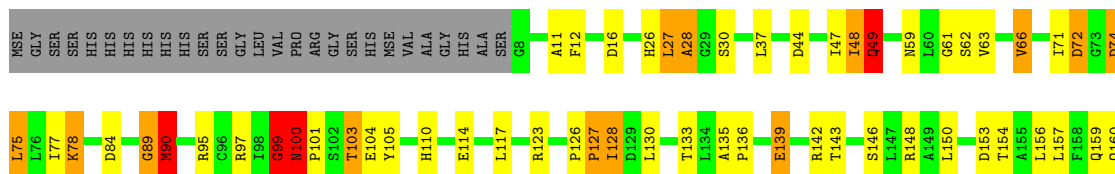
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			43	33	4	6		
2	B	1	Total	C	N	O	0	0
			43	33	4	6		
2	C	1	Total	C	N	O	0	0
			43	33	4	6		
2	D	1	Total	C	N	O	0	0
			43	33	4	6		

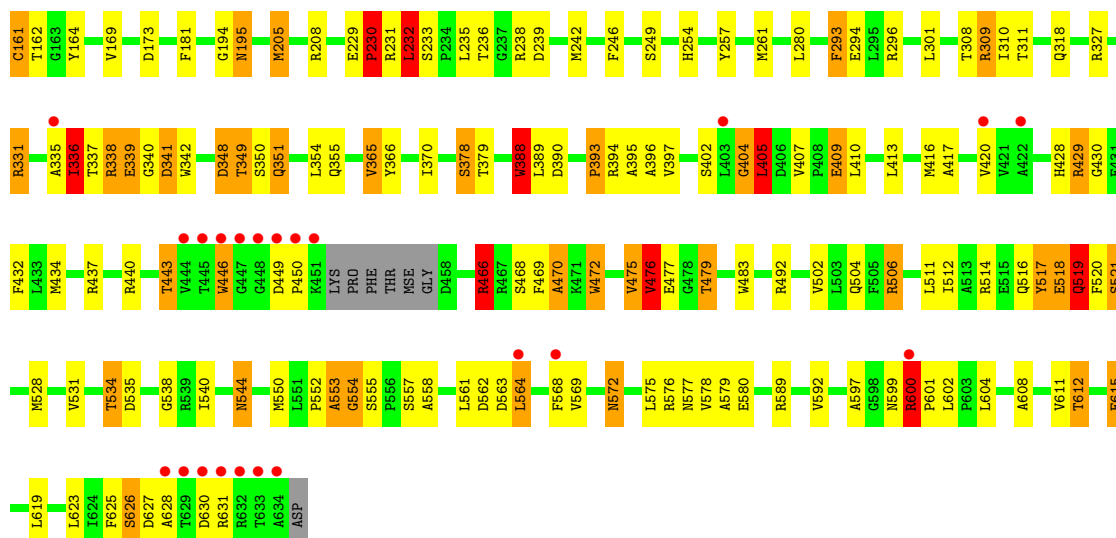
^ Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	79	Total	O	0	0
			79	79		
3	B	69	Total	O	0	0
			69	69		
3	C	92	Total	O	0	0
			92	92		
3	D	77	Total	O	0	0
			77	77		

G

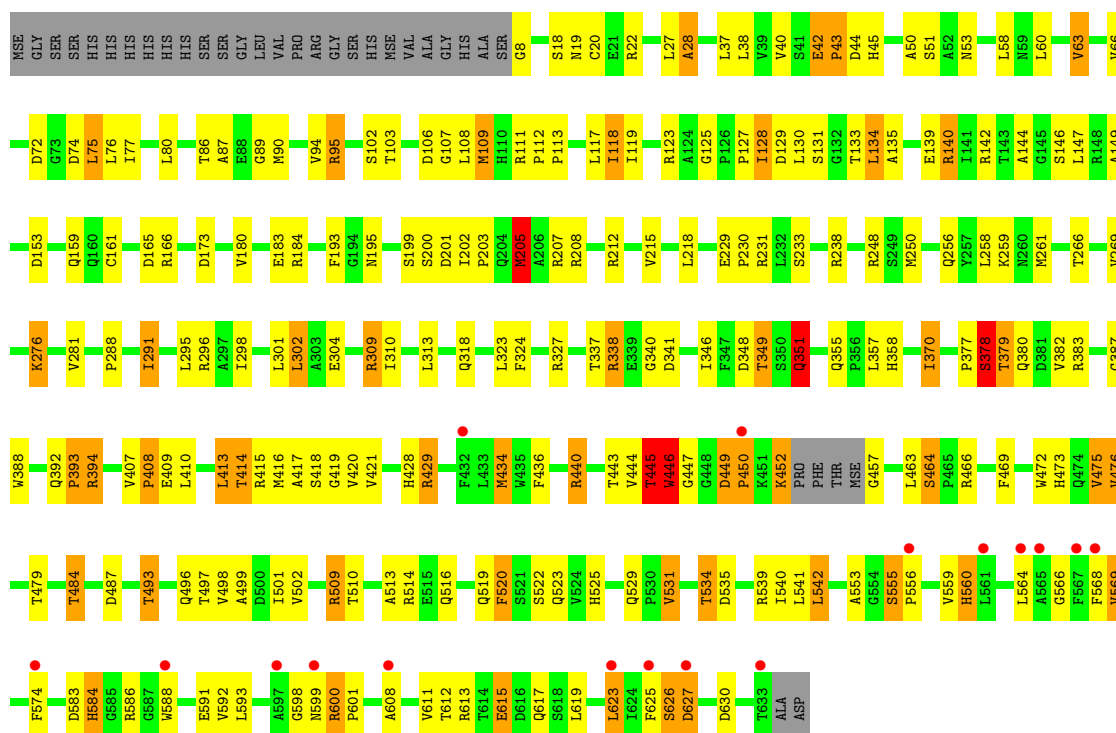
- Molecule 1: bacteriophytochrome





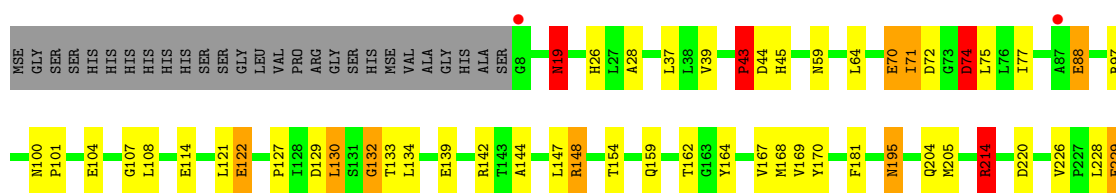
• Molecule 1: bacteriophytochrome

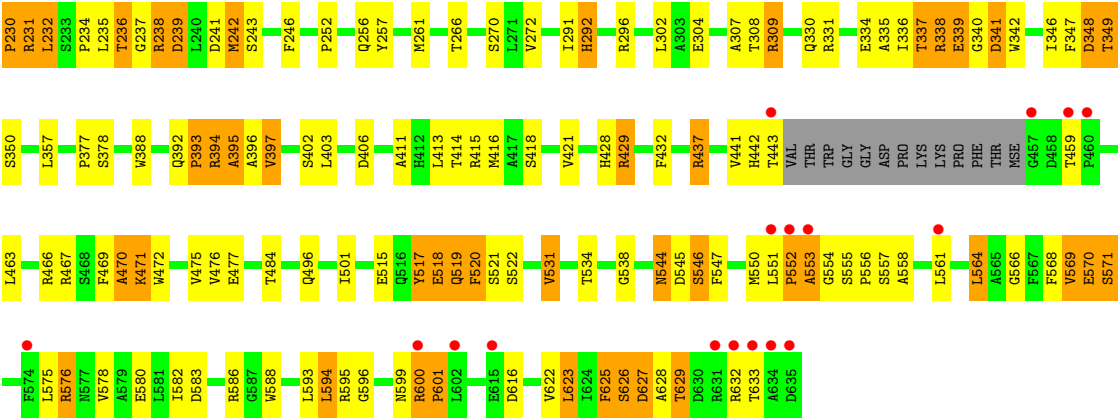
Chain C:



• Molecule 1: bacteriophytochrome

Chain D:





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.94Å 146.87Å 139.55Å 90.00° 101.17° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 73.44 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.7 (15.00-2.90) 97.6 (73.44-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.200 , 0.243 0.209 , 0.213	Depositor DCC
R_{free} test set	4422 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	70.1	Xtriage
Anisotropy	0.739	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 44.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 97750 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19838	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.91	3/5009 (0.1%)	1.19	19/6787 (0.3%)
1	B	0.78	5/4915 (0.1%)	1.15	27/6663 (0.4%)
1	C	0.88	4/4934 (0.1%)	1.16	17/6686 (0.3%)
1	D	0.78	1/4875 (0.0%)	1.08	9/6607 (0.1%)
All	All	0.84	13/19733 (0.1%)	1.15	72/26743 (0.3%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	388	TRP	CD2-CE2	8.14	1.51	1.41
1	C	20	CYS	CB-SG	-6.85	1.70	1.82
1	A	446	TRP	CD2-CE2	6.21	1.48	1.41
1	B	388	TRP	CD2-CE2	6.08	1.48	1.41
1	C	266	THR	CB-CG2	5.99	1.72	1.52
1	B	230	PRO	N-CA	-5.47	1.38	1.47
1	D	388	TRP	CD2-CE2	5.43	1.47	1.41
1	C	446	TRP	CD2-CE2	5.25	1.47	1.41
1	A	588	TRP	CD2-CE2	5.23	1.47	1.41
1	B	472	TRP	CD2-CE2	5.14	1.47	1.41
1	C	588	TRP	CD2-CE2	5.09	1.47	1.41
1	B	90	MSE	CG-SE	-5.07	1.78	1.95
1	B	446	TRP	CD2-CE2	5.02	1.47	1.41

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	229	GLU	C-N-CD	-19.55	77.59	120.60
1	B	229	GLU	C-N-CA	13.09	176.96	122.00
1	B	242	MSE	CG-SE-CE	-7.85	81.63	98.90
1	A	506	ARG	NE-CZ-NH1	7.74	124.17	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	99	GLY	N-CA-C	7.38	131.55	113.10
1	D	437	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	B	230	PRO	CA-N-CD	-7.28	101.31	111.50
1	A	404	GLY	N-CA-C	-7.25	94.96	113.10
1	B	466	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	D	625	PHE	CB-CA-C	7.03	124.46	110.40
1	A	331	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	B	519	GLN	N-CA-C	-6.67	93.00	111.00
1	A	487	ASP	CB-CG-OD1	-6.59	112.37	118.30
1	B	280	LEU	CB-CG-CD1	-6.48	99.99	111.00
1	C	229	GLU	C-N-CD	6.47	142.00	128.40
1	C	338	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	B	232	LEU	CA-CB-CG	6.41	130.04	115.30
1	B	337	THR	N-CA-C	-6.41	93.69	111.00
1	C	118	ILE	CB-CA-C	-6.40	98.80	111.60
1	A	518	GLU	N-CA-C	-6.31	93.96	111.00
1	C	231	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	A	27	LEU	CA-CB-CG	6.22	129.61	115.30
1	C	302	LEU	CA-CB-CG	6.21	129.59	115.30
1	D	214	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	61	GLY	N-CA-C	-6.08	97.90	113.10
1	B	205	MSE	CG-SE-CE	-6.06	85.57	98.90
1	B	389	LEU	CA-CB-CG	5.99	129.07	115.30
1	A	116	GLY	N-CA-C	5.94	127.96	113.10
1	C	123	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	564	LEU	CA-CB-CG	5.90	128.88	115.30
1	C	207	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	A	170	TYR	CA-CB-CG	5.67	124.17	113.40
1	A	309	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	D	43	PRO	CA-N-CD	-5.65	103.59	111.50
1	B	404	GLY	N-CA-C	-5.61	99.07	113.10
1	D	349	THR	N-CA-CB	5.61	120.95	110.30
1	D	142	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	C	117	LEU	CB-CG-CD1	-5.55	101.56	111.00
1	B	506	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	C	125	GLY	N-CA-C	5.54	126.94	113.10
1	C	165	ASP	CB-CG-OD1	-5.53	113.33	118.30
1	B	338	ARG	N-CA-C	-5.50	96.16	111.00
1	A	341	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	B	49	GLN	N-CA-C	5.49	125.82	111.00
1	C	248	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	B	518	GLU	N-CA-C	-5.46	96.25	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	220	ASP	CB-CG-OD1	5.44	123.20	118.30
1	C	338	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	331	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	475	VAL	N-CA-C	-5.38	96.48	111.00
1	B	48	ILE	N-CA-C	-5.34	96.58	111.00
1	B	309	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	C	117	LEU	CA-CB-CG	5.30	127.48	115.30
1	A	340	GLY	N-CA-C	5.28	126.30	113.10
1	A	218	LEU	CB-CG-CD2	-5.26	102.06	111.00
1	C	205	MSE	CG-SE-CE	-5.23	87.40	98.90
1	B	28	ALA	N-CA-C	-5.20	96.95	111.00
1	A	129	ASP	N-CA-C	5.19	125.01	111.00
1	C	230	PRO	N-CA-C	-5.18	98.62	112.10
1	C	509	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	D	470	ALA	N-CA-C	-5.15	97.11	111.00
1	B	432	PHE	CB-CA-C	-5.11	100.18	110.40
1	A	462	ASP	CB-CG-OD1	5.11	122.89	118.30
1	A	583	ASP	CB-CG-OD1	5.09	122.89	118.30
1	B	97	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	B	97	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	378	SER	N-CA-CB	5.07	118.11	110.50
1	D	575	LEU	N-CA-C	-5.06	97.34	111.00
1	B	44	ASP	N-CA-C	5.05	124.64	111.00
1	A	207	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	C	207	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	218	LEU	CB-CG-CD1	5.00	119.50	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4902	0	0	164	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4823	0	0	114	0
1	C	4839	0	0	117	0
1	D	4785	0	0	109	0
2	A	43	0	0	9	0
2	B	43	0	0	6	0
2	C	43	0	0	1	0
2	D	43	0	0	5	0
3	A	79	0	0	12	0
3	B	69	0	0	11	0
3	C	92	0	0	9	0
3	D	77	0	0	5	0
All	All	19838	0	0	518	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 27.

All (518) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:900:BLA:CMA	2:D:900:BLA:CMB	1.89	1.50
1:D:519:GLN:O	1:D:521:SER:N	1.71	1.20
1:D:551:LEU:O	1:D:553:ALA:N	1.90	1.05
1:A:218:LEU:CD2	1:A:250:MSE:SE	2.55	1.04
1:B:476:VAL:N	3:B:1009:HOH:O	1.92	1.03
2:C:900:BLA:CMA	2:C:900:BLA:CMB	2.37	1.03
2:B:900:BLA:CMA	2:B:900:BLA:CMB	2.40	0.99
1:D:518:GLU:O	1:D:519:GLN:CB	2.16	0.94
1:C:327[A]:ARG:NH1	1:C:351:GLN:OE1	2.03	0.92
1:A:336:ILE:CG2	1:A:342:TRP:CA	2.48	0.90
1:A:518:GLU:OE2	3:A:1038:HOH:O	1.92	0.87
1:B:26:HIS:CD2	1:B:27:LEU:CD1	2.57	0.87
1:A:624:ILE:O	1:A:624:ILE:CD1	2.23	0.86
1:A:339:GLU:O	3:A:1017:HOH:O	1.94	0.84
1:A:334:GLU:O	1:A:336:ILE:N	2.12	0.83
1:A:335:ALA:O	1:A:336:ILE:CB	2.25	0.83
1:B:77:ILE:O	1:B:78:LYS:CB	2.27	0.83
1:A:73:GLY:O	1:A:75:LEU:N	2.11	0.83
2:A:900:BLA:CMB	2:A:900:BLA:CMA	2.57	0.83
1:B:142:ARG:N	3:B:1041:HOH:O	2.11	0.83
1:D:132:GLY:O	1:D:134:LEU:N	2.12	0.83
1:D:144:ALA:O	1:D:309:ARG:NH1	2.11	0.82
1:A:518:GLU:O	1:A:519:GLN:CB	2.28	0.82
1:C:144:ALA:O	1:C:309:ARG:NH1	2.14	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:457:GLY:N	3:C:1089:HOH:O	2.15	0.78
1:B:420:VAL:CG2	1:B:434:MSE:CE	2.61	0.78
1:D:394:ARG:O	1:D:395:ALA:CB	2.31	0.78
1:B:611:VAL:O	1:B:612:THR:CG2	2.31	0.78
1:D:229:GLU:O	1:D:231:ARG:N	2.17	0.78
1:B:553:ALA:C	3:B:1003:HOH:O	2.22	0.77
1:A:71:ILE:O	1:A:72:ASP:CB	2.33	0.77
1:C:42:GLU:O	1:C:43:PRO:C	2.22	0.77
1:C:173:ASP:OD2	1:C:440:ARG:NH2	2.18	0.76
1:C:42:GLU:O	1:C:44:ASP:N	2.18	0.76
1:A:291:ILE:O	1:A:296:ARG:NH1	2.18	0.76
1:A:395:ALA:O	1:A:396:ALA:C	2.24	0.76
1:A:44:ASP:O	1:A:45[A]:HIS:CD2	2.39	0.76
1:D:292[A]:HIS:N	1:D:292[A]:HIS:CD2	2.53	0.76
1:A:337:THR:O	1:A:338:ARG:CG	2.34	0.75
1:A:625:PHE:CB	1:A:626:SER:CA	2.64	0.75
1:A:541:LEU:CD1	1:A:541:LEU:N	2.50	0.75
1:A:591:GLU:CA	3:A:1019:HOH:O	2.35	0.74
2:A:900:BLA:C2B	2:A:900:BLA:CMA	2.66	0.73
1:A:625:PHE:CB	1:A:626:SER:CB	2.67	0.73
1:D:75:LEU:N	3:D:1067:HOH:O	2.22	0.72
1:C:95:ARG:NH1	1:C:106:ASP:OD1	2.23	0.72
1:A:395:ALA:O	1:A:396:ALA:O	2.06	0.71
1:D:519:GLN:O	1:D:520:PHE:C	2.26	0.71
1:D:348:ASP:C	1:D:350:SER:N	2.42	0.71
1:A:336:ILE:CD1	1:A:344:ALA:CB	2.69	0.71
1:C:613:ARG:NH1	1:C:617:GLN:OE1	2.24	0.71
1:C:534:THR:CG2	3:C:1047:HOH:O	2.38	0.71
1:D:336:ILE:CG2	1:D:341:ASP:O	2.39	0.71
1:B:514:ARG:NH1	1:B:518:GLU:OE1	2.24	0.70
1:B:336:ILE:CG2	1:B:342:TRP:CA	2.69	0.70
2:D:900:BLA:NC	3:D:1077:HOH:O	2.24	0.70
1:A:569:VAL:O	1:A:571:SER:N	2.24	0.70
1:A:458:ASP:O	1:A:459:THR:CG2	2.40	0.69
1:B:517:TYR:O	1:B:521:SER:OG	2.10	0.69
1:A:473:HIS:O	1:A:475:VAL:O	2.11	0.69
1:C:218:LEU:CD2	1:C:250:MSE:SE	2.90	0.69
1:D:470:ALA:O	1:D:471:LYS:CB	2.42	0.68
1:D:568:PHE:O	1:D:569:VAL:C	2.31	0.68
1:C:612:THR:CG2	3:C:1084:HOH:O	2.41	0.68
1:D:545:ASP:O	1:D:546:SER:C	2.30	0.68
1:B:475:VAL:CA	3:B:1009:HOH:O	2.41	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:336:ILE:CG1	1:D:341:ASP:O	2.43	0.67
1:C:407:VAL:O	1:C:410:LEU:N	2.27	0.67
1:A:348:ASP:O	1:A:349:THR:CG2	2.43	0.67
1:B:626:SER:OG	1:B:626:SER:O	2.11	0.67
2:A:900:BLA:C1B	2:A:900:BLA:CMA	2.72	0.67
1:D:337:THR:O	1:D:338:ARG:NE	2.28	0.66
1:D:241:ASP:OD2	1:D:243:SER:OG	2.13	0.66
1:D:517:TYR:C	1:D:517:TYR:CD1	2.68	0.66
1:D:625:PHE:CA	1:D:626:SER:OG	2.44	0.66
1:D:336:ILE:CG2	1:D:342:TRP:CA	2.74	0.66
1:D:122:GLU:OE1	1:D:296:ARG:NH2	2.28	0.66
1:A:338:ARG:O	1:A:339:GLU:CG	2.43	0.66
1:A:160:GLN:NE2	3:A:1035:HOH:O	2.28	0.65
2:D:900:BLA:C3A	2:D:900:BLA:CMB	2.73	0.65
1:D:392:GLN:O	1:D:394:ARG:NH2	2.29	0.65
1:D:238:ARG:O	1:D:239:ASP:C	2.34	0.65
1:B:469:PHE:O	1:B:470:ALA:CB	2.45	0.65
1:B:331:ARG:CG	1:B:351:GLN:NE2	2.60	0.65
1:C:180:VAL:O	1:C:193:PHE:O	2.14	0.65
1:B:100:ASN:ND2	1:B:101:PRO:CD	2.60	0.64
1:D:519:GLN:O	1:D:521:SER:CA	2.46	0.64
1:B:579:ALA:N	3:B:1036:HOH:O	2.29	0.64
1:D:393:PRO:O	1:D:394:ARG:CB	2.45	0.64
1:A:233:SER:OG	1:A:236:THR:OG1	2.15	0.64
1:A:332:MSE:CE	1:A:342:TRP:CE3	2.80	0.64
1:A:45[A]:HIS:CE1	1:A:69:ALA:N	2.66	0.64
1:A:453:PRO:CA	1:A:454:PHE:CB	2.76	0.64
1:A:519:GLN:O	1:A:520:PHE:CB	2.45	0.64
2:A:900:BLA:NA	2:A:900:BLA:ND	2.46	0.64
1:B:89:GLY:O	1:B:90:MSE:CG	2.46	0.64
1:B:90:MSE:CE	1:B:110:HIS:CA	2.76	0.63
1:A:171:ARG:NH1	1:A:179:GLU:OE1	2.31	0.63
1:D:334:GLU:O	1:D:336:ILE:O	2.16	0.63
1:A:556:PRO:O	1:A:557:SER:C	2.37	0.63
1:A:128:ILE:CD1	3:A:1072:HOH:O	2.47	0.63
1:B:553:ALA:O	1:B:554:GLY:C	2.38	0.62
1:C:615:GLU:N	3:C:1001:HOH:O	2.33	0.62
1:C:472:TRP:O	1:C:475:VAL:O	2.17	0.62
1:D:545:ASP:O	1:D:547:PHE:N	2.32	0.61
1:B:468:SER:O	1:B:472:TRP:N	2.33	0.61
1:D:600:ARG:O	1:D:601:PRO:O	2.17	0.61
1:C:583:ASP:O	1:C:584:HIS:C	2.39	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:900:BLA:ND	3:D:1077:HOH:O	2.31	0.61
1:A:557:SER:O	1:A:558:ALA:CB	2.48	0.61
1:C:58:LEU:O	1:C:60:LEU:CD2	2.48	0.61
1:B:231:ARG:NH1	1:B:239:ASP:OD2	2.34	0.61
1:D:558:ALA:CB	1:D:564:LEU:CD1	2.78	0.61
1:B:139:GLU:C	3:B:1041:HOH:O	2.38	0.61
1:A:444:VAL:CG2	1:A:445:THR:N	2.64	0.61
1:C:258:LEU:CD2	1:C:261:MSE:CE	2.78	0.61
1:B:99:GLY:O	1:B:100:ASN:ND2	2.33	0.60
1:C:378:SER:O	1:C:382:VAL:N	2.35	0.60
1:C:529:GLN:NE2	1:C:626:SER:O	2.34	0.60
1:B:349:THR:O	1:B:350:SER:OG	2.19	0.60
1:B:143:THR:N	3:B:1041:HOH:O	2.32	0.60
1:B:257:TYR:CE2	1:B:261:MSE:CE	2.84	0.60
1:D:257:TYR:CD2	1:D:261:MSE:CE	2.84	0.60
1:A:100:ASN:OD1	1:A:101:PRO:CD	2.50	0.60
1:D:569:VAL:O	1:D:571:SER:N	2.35	0.59
1:B:293:PHE:O	1:B:294:GLU:C	2.39	0.59
1:D:392:GLN:O	1:D:393:PRO:O	2.20	0.59
1:B:600:ARG:O	1:B:602:LEU:N	2.35	0.59
1:A:357:LEU:O	1:A:358:HIS:C	2.41	0.59
1:D:19:ASN:ND2	1:D:19:ASN:N	2.50	0.59
2:B:900:BLA:NC	3:B:1069:HOH:O	2.31	0.59
1:C:452:LYS:NZ	1:C:452:LYS:O	2.35	0.59
1:C:446:TRP:CG	1:C:447:GLY:N	2.71	0.59
1:A:428:HIS:O	1:A:429:ARG:CB	2.50	0.59
1:A:625:PHE:CB	1:A:626:SER:OG	2.51	0.59
1:C:42:GLU:OE1	1:C:111:ARG:NH1	2.36	0.59
1:B:395:ALA:O	1:B:397:VAL:N	2.35	0.59
1:B:520:PHE:O	1:C:510:THR:CG2	2.50	0.59
1:C:414:THR:O	1:C:418:SER:OG	2.21	0.59
1:C:74:ASP:O	1:C:76:LEU:N	2.36	0.58
1:D:515:GLU:O	1:D:518:GLU:O	2.21	0.58
1:D:168:MSE:CE	1:D:170:TYR:OH	2.51	0.58
1:B:74:ASP:O	1:B:75:LEU:CB	2.50	0.58
1:D:531:VAL:CG1	1:D:544:ASN:OD1	2.51	0.58
1:C:205:MSE:CE	1:C:208:ARG:NE	2.67	0.58
1:C:475:VAL:O	1:C:476:VAL:CG2	2.52	0.58
1:B:27:LEU:C	1:B:28:ALA:O	2.38	0.58
1:A:201:ASP:OD2	1:A:468:SER:OG	2.21	0.58
1:C:259:LYS:NZ	3:C:1026:HOH:O	2.37	0.58
1:C:74:ASP:O	1:C:75:LEU:C	2.41	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:229:GLU:O	1:D:230:PRO:C	2.41	0.57
1:B:59:ASN:CB	1:B:100:ASN:ND2	2.67	0.57
1:B:230:PRO:O	1:B:231:ARG:CB	2.52	0.57
1:C:627:ASP:N	1:C:627:ASP:OD1	2.38	0.57
1:A:134:LEU:O	1:A:135:ALA:CB	2.52	0.57
1:A:472:TRP:O	1:A:476:VAL:CG1	2.53	0.57
1:C:446:TRP:CD2	1:C:447:GLY:N	2.72	0.57
1:D:71:ILE:O	1:D:72:ASP:C	2.42	0.57
1:B:89:GLY:O	1:B:90:MSE:SE	2.72	0.57
1:C:498:VAL:O	1:C:499:ALA:C	2.39	0.57
1:C:51:SER:OG	1:C:53:ASN:OD1	2.22	0.56
1:A:144:ALA:O	1:A:309:ARG:NH1	2.37	0.56
1:A:567:PHE:O	1:A:568:PHE:CB	2.54	0.56
1:A:624:ILE:O	1:A:625:PHE:C	2.43	0.56
1:A:365:VAL:CG2	1:A:430:GLY:O	2.53	0.56
1:A:464:SER:OG	1:A:465:PRO:N	2.37	0.56
1:D:71:ILE:N	1:D:71:ILE:CD1	2.69	0.56
1:B:520:PHE:O	1:C:510:THR:OG1	2.23	0.56
1:B:472:TRP:O	1:B:475:VAL:O	2.24	0.56
1:C:440:ARG:N	1:C:479:THR:O	2.39	0.56
1:B:550:MSE:CE	1:B:604:LEU:CD1	2.83	0.56
1:A:71:ILE:CG2	1:A:72:ASP:N	2.69	0.55
1:C:60:LEU:N	1:C:60:LEU:CD2	2.69	0.55
1:A:235:LEU:CD1	1:A:235:LEU:O	2.54	0.55
1:A:26:HIS:NE2	1:A:27:LEU:CD2	2.70	0.55
1:B:625:PHE:O	1:B:627:ASP:N	2.39	0.55
1:A:443:THR:O	1:A:445:THR:N	2.39	0.55
1:A:114:GLU:OE1	1:A:236:THR:CG2	2.55	0.55
1:A:568:PHE:CE2	1:A:592:VAL:CG1	2.89	0.55
1:D:599:ASN:O	1:D:600:ARG:C	2.45	0.55
1:D:148:ARG:NH2	1:D:181:PHE:O	2.40	0.55
1:D:519:GLN:O	1:D:522:SER:N	2.39	0.55
1:A:395:ALA:C	1:A:396:ALA:O	2.43	0.55
1:A:458:ASP:OD1	1:A:459:THR:N	2.39	0.55
1:A:362:CYS:SG	1:A:363:ALA:N	2.79	0.55
1:C:27:LEU:C	1:C:28:ALA:O	2.43	0.55
1:A:76:LEU:CD2	1:A:80:LEU:CD1	2.85	0.54
1:A:366:TYR:O	1:A:367:GLU:C	2.44	0.54
1:D:26:HIS:CD2	1:D:205:MSE:CE	2.90	0.54
1:B:428:HIS:O	1:B:429:ARG:CB	2.54	0.54
1:B:127:PRO:O	1:B:128:ILE:CG2	2.55	0.54
1:A:336:ILE:CG2	1:A:341:ASP:O	2.56	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:393:PRO:O	1:D:394:ARG:NE	2.40	0.54
1:A:289:ARG:NH2	3:A:1037:HOH:O	2.40	0.54
1:C:522:SER:O	1:C:525:HIS:N	2.41	0.54
1:D:544:ASN:ND2	1:D:544:ASN:C	2.61	0.54
1:C:309:ARG:O	1:C:310:ILE:C	2.45	0.54
1:A:258:LEU:CB	1:A:263:VAL:CG2	2.86	0.54
1:C:42:GLU:CD	1:C:111:ARG:NH1	2.61	0.54
1:B:580:GLU:N	3:B:1036:HOH:O	2.40	0.54
1:B:162:THR:CG2	1:B:164:TYR:CD2	2.91	0.54
1:D:230:PRO:O	1:D:232:LEU:O	2.26	0.54
1:A:472:TRP:O	1:A:475:VAL:O	2.26	0.54
1:A:74:ASP:OD2	1:A:78:LYS:NZ	2.41	0.54
1:A:42:GLU:OE2	1:A:117:LEU:CD1	2.56	0.53
1:B:126:PRO:O	1:B:128:ILE:N	2.41	0.53
1:A:561:LEU:O	1:A:562:ASP:C	2.46	0.53
1:D:107:GLY:C	1:D:108:LEU:CD1	2.77	0.53
1:B:409:GLU:OE1	1:B:410:LEU:CD1	2.56	0.53
1:D:538:GLY:O	1:D:561:LEU:CD2	2.56	0.53
1:A:347:PHE:O	1:A:348:ASP:C	2.46	0.53
1:A:308:THR:O	1:A:309:ARG:C	2.47	0.53
1:C:591:GLU:O	1:C:592:VAL:CG1	2.56	0.53
1:D:336:ILE:CG2	1:D:337:THR:N	2.72	0.53
1:D:235:LEU:O	1:D:237:GLY:N	2.42	0.53
1:C:388:TRP:CE2	1:C:392:GLN:NE2	2.76	0.53
1:A:515:GLU:O	1:A:518:GLU:O	2.27	0.53
1:A:368:ASP:O	1:A:383:ARG:NH2	2.41	0.53
1:D:580:GLU:O	1:D:583:ASP:O	2.27	0.53
1:A:173:ASP:C	1:A:173:ASP:OD1	2.48	0.53
1:B:534:THR:OG1	1:B:535:ASP:N	2.41	0.52
1:A:223:TYR:CD1	1:A:223:TYR:C	2.82	0.52
1:A:332:MSE:CA	1:A:335:ALA:CB	2.86	0.52
1:B:576:ARG:C	3:B:1036:HOH:O	2.47	0.52
1:B:348:ASP:OD1	1:B:350:SER:N	2.42	0.52
1:A:414:THR:O	1:A:418:SER:OG	2.26	0.52
1:C:516:GLN:O	1:C:519:GLN:O	2.28	0.52
1:C:443:THR:O	1:C:445:THR:N	2.42	0.52
1:B:66:VAL:CG2	1:B:71:ILE:CD1	2.88	0.52
1:C:434:MSE:CE	1:C:436:PHE:CZ	2.93	0.52
1:C:555:SER:CB	1:C:556:PRO:CA	2.87	0.52
1:A:464:SER:OG	1:A:465:PRO:CD	2.58	0.52
1:A:150:LEU:O	1:A:154:THR:CG2	2.58	0.52
1:B:336:ILE:CG2	1:B:341:ASP:O	2.58	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:519:GLN:O	1:C:520:PHE:CB	2.58	0.52
1:D:623:LEU:N	1:D:623:LEU:CD2	2.73	0.52
1:D:568:PHE:O	1:D:570:GLU:N	2.43	0.52
1:D:593:LEU:O	1:D:594:LEU:CB	2.57	0.52
1:B:568:PHE:CD2	1:B:592:VAL:CG2	2.93	0.52
1:D:547:PHE:O	1:D:550:MSE:CG	2.59	0.51
1:A:570:GLU:O	1:A:571:SER:C	2.49	0.51
1:C:139:GLU:OE2	1:C:142:ARG:NH2	2.43	0.51
1:D:74:ASP:C	3:D:1067:HOH:O	2.48	0.51
1:A:222:SER:O	1:A:223:TYR:O	2.29	0.51
1:A:508:VAL:CG1	1:A:512:ILE:CD1	2.88	0.51
1:B:553:ALA:O	1:B:555:SER:OG	2.29	0.51
1:A:475:VAL:O	1:A:476:VAL:CG1	2.58	0.51
1:D:396:ALA:O	1:D:397:VAL:CG2	2.59	0.51
1:D:336:ILE:CD1	1:D:341:ASP:O	2.59	0.51
1:A:348:ASP:OD1	1:A:350:SER:N	2.42	0.51
1:B:437:ARG:NH2	1:B:483:TRP:CE3	2.79	0.51
1:D:97:ARG:NH1	1:D:104:GLU:OE2	2.44	0.51
1:B:443:THR:O	1:B:443:THR:CG2	2.58	0.51
1:A:183:GLU:CG	1:A:184:ARG:N	2.73	0.51
1:C:133:THR:CG2	1:C:161:CYS:SG	2.99	0.51
1:D:88:GLU:OE1	1:D:88:GLU:N	2.43	0.51
1:A:592:VAL:CG1	1:A:593:LEU:N	2.74	0.50
1:C:18:SER:OG	1:C:19:ASN:N	2.43	0.50
1:D:338:ARG:O	1:D:339:GLU:CG	2.60	0.50
1:B:150:LEU:O	1:B:154:THR:N	2.44	0.50
1:B:404:GLY:O	1:B:405:LEU:CB	2.59	0.50
1:C:393:PRO:O	1:C:394:ARG:CZ	2.60	0.50
1:D:100:ASN:CB	1:D:101:PRO:CD	2.90	0.50
1:A:615:GLU:O	1:A:616:ASP:OD1	2.30	0.50
1:B:30:SER:OG	1:B:249:SER:OG	2.29	0.50
1:B:365:VAL:CG2	1:B:430:GLY:O	2.60	0.50
1:D:214:ARG:CG	1:D:214:ARG:NH1	2.75	0.50
1:B:348:ASP:O	1:B:349:THR:CG2	2.60	0.50
1:B:16:ASP:OD1	1:B:16:ASP:C	2.51	0.50
1:D:625:PHE:CB	1:D:626:SER:OG	2.60	0.49
1:B:466:ARG:O	1:B:469:PHE:O	2.30	0.49
1:C:37:LEU:C	1:C:37:LEU:CD2	2.80	0.49
1:D:168:MSE:CE	1:D:170:TYR:CE1	2.95	0.49
1:A:257:TYR:CD2	1:A:261:MSE:CE	2.95	0.49
1:A:446:TRP:O	1:A:448:GLY:N	2.45	0.49
1:A:148:ARG:NH2	1:A:181:PHE:O	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:570:GLU:O	1:A:572:ASN:N	2.44	0.49
1:C:118:ILE:CG2	1:C:119:ILE:N	2.74	0.49
1:B:518:GLU:O	1:B:519:GLN:CG	2.61	0.49
1:B:47:ILE:C	1:B:48:ILE:O	2.46	0.49
1:C:112:PRO:O	1:C:113:PRO:C	2.50	0.49
1:D:348:ASP:OD1	1:D:349:THR:C	2.51	0.49
1:A:163:GLY:O	1:A:164:TYR:O	2.31	0.49
1:B:336:ILE:CG1	1:B:341:ASP:O	2.60	0.49
1:B:572:ASN:O	1:B:575:LEU:N	2.46	0.49
1:A:193:PHE:C	1:A:193:PHE:CD2	2.86	0.49
1:A:403:LEU:C	1:A:404:GLY:O	2.48	0.49
1:C:74:ASP:O	1:C:77:ILE:N	2.45	0.49
1:A:164:TYR:CE2	1:A:289:ARG:CD	2.96	0.49
1:B:516:GLN:O	1:B:517:TYR:CB	2.59	0.49
1:B:336:ILE:CD1	1:B:341:ASP:C	2.81	0.49
1:D:246:PHE:CE1	1:D:296:ARG:NH1	2.80	0.49
1:B:48:ILE:O	1:B:49:GLN:O	2.30	0.49
1:A:109:MSE:O	1:A:118:ILE:O	2.31	0.49
1:D:393:PRO:O	1:D:394:ARG:CG	2.62	0.48
1:B:440:ARG:N	1:B:479:THR:O	2.46	0.48
1:D:534:THR:CG2	1:D:561:LEU:CD2	2.91	0.48
1:B:95:ARG:NH2	1:B:104:GLU:OE1	2.47	0.48
1:B:181:PHE:CG	1:B:181:PHE:O	2.66	0.48
1:A:398:THR:CG2	1:A:399:SER:N	2.76	0.48
1:B:335:ALA:O	1:B:336:ILE:CG2	2.62	0.48
1:A:571:SER:O	1:A:573:ASP:N	2.47	0.48
1:D:70:GLU:O	1:D:71:ILE:C	2.52	0.48
1:D:108:LEU:N	1:D:108:LEU:CD1	2.77	0.48
1:A:615:GLU:O	1:A:616:ASP:CG	2.52	0.48
1:A:186:VAL:O	1:A:187:PRO:C	2.52	0.48
1:C:446:TRP:CE3	1:C:473:HIS:CE1	3.01	0.48
2:A:900:BLA:CBC	2:A:900:BLA:CMC	2.92	0.48
1:D:403:LEU:N	1:D:418:SER:O	2.46	0.48
1:B:173:ASP:C	1:B:173:ASP:OD1	2.51	0.48
1:A:509:ARG:O	1:A:513:ALA:CB	2.62	0.47
1:D:347:PHE:O	1:D:348:ASP:C	2.52	0.47
1:D:348:ASP:O	1:D:350:SER:N	2.47	0.47
1:C:540:ILE:O	1:C:540:ILE:CG2	2.61	0.47
1:A:327:ARG:O	1:A:331:ARG:N	2.46	0.47
1:B:351:GLN:CG	1:B:351:GLN:O	2.62	0.47
1:C:449:ASP:CB	1:C:450:PRO:CD	2.92	0.47
1:A:220:ASP:OD1	1:A:220:ASP:C	2.53	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:155:ALA:O	1:A:167:VAL:CG2	2.62	0.47
1:B:231:ARG:O	1:B:232:LEU:CB	2.62	0.47
2:B:900:BLA:CBC	2:B:900:BLA:CMC	2.93	0.47
1:D:242:MSE:O	1:D:243:SER:C	2.52	0.47
1:B:148:ARG:NH2	1:B:181:PHE:O	2.48	0.47
1:A:559:VAL:O	1:A:560:HIS:O	2.31	0.47
1:C:346:ILE:CG2	1:C:346:ILE:O	2.62	0.47
1:A:555:SER:O	1:A:557:SER:N	2.48	0.47
1:C:569:VAL:CA	1:C:593:LEU:O	2.63	0.47
1:B:553:ALA:O	1:B:555:SER:N	2.49	0.46
1:D:337:THR:O	1:D:338:ARG:CB	2.62	0.46
1:B:535:ASP:OD1	1:B:538:GLY:N	2.48	0.46
1:C:611:VAL:O	1:C:619:LEU:N	2.47	0.46
1:C:166:ARG:NH1	1:C:183:GLU:OE2	2.49	0.46
1:D:552:PRO:O	1:D:553:ALA:O	2.34	0.46
1:B:611:VAL:O	1:B:612:THR:CB	2.64	0.46
1:C:50:ALA:O	1:C:51:SER:C	2.52	0.46
1:B:254:HIS:CE1	2:B:900:BLA:C1A	2.98	0.46
1:A:166:ARG:NH2	1:A:190:GLU:O	2.49	0.46
1:A:95:ARG:NH1	1:A:106:ASP:OD1	2.47	0.46
1:C:337:THR:O	1:C:338:ARG:CB	2.64	0.46
1:D:252:PRO:O	1:D:256:GLN:N	2.49	0.46
1:D:472:TRP:O	1:D:475:VAL:O	2.33	0.46
1:C:309:ARG:O	1:C:313:LEU:N	2.49	0.46
1:B:173:ASP:OD2	1:B:440:ARG:NH2	2.49	0.46
1:A:385:ILE:CG2	1:A:434:MSE:CE	2.93	0.46
1:A:250:MSE:O	1:A:251:SER:C	2.55	0.46
1:A:605:ALA:CA	3:A:1019:HOH:O	2.64	0.46
1:B:519:GLN:O	1:B:520:PHE:CB	2.60	0.46
1:D:246:PHE:CZ	1:D:296:ARG:NH1	2.84	0.46
1:C:8:GLY:N	3:C:1005:HOH:O	2.48	0.46
2:A:900:BLA:C3A	2:A:900:BLA:CMB	2.94	0.46
1:A:51:SER:OG	1:A:53:ASN:OD1	2.34	0.46
1:B:388:TRP:CZ3	1:B:407:VAL:CG2	2.99	0.46
1:B:26:HIS:CE1	1:B:205:MSE:CE	2.99	0.46
1:D:625:PHE:CB	1:D:626:SER:CA	2.94	0.46
1:A:509:ARG:O	1:A:513:ALA:N	2.49	0.46
1:B:561:LEU:O	1:B:562:ASP:C	2.53	0.46
1:A:336:ILE:CG2	1:A:341:ASP:C	2.84	0.45
1:D:238:ARG:O	1:D:239:ASP:O	2.33	0.45
1:A:173:ASP:OD1	1:A:175:GLN:N	2.49	0.45
1:A:259:LYS:NZ	3:A:1033:HOH:O	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:417:ALA:C	1:C:419:GLY:N	2.68	0.45
1:A:480:SER:O	1:A:481:ASP:C	2.54	0.45
1:B:26:HIS:ND1	1:B:205:MSE:CE	2.80	0.45
1:C:393:PRO:O	1:C:394:ARG:NE	2.48	0.45
1:C:535:ASP:OD1	1:C:539:ARG:N	2.49	0.45
1:B:338:ARG:O	1:B:339:GLU:CB	2.65	0.45
1:A:565:ALA:O	3:A:1040:HOH:O	2.21	0.45
1:B:540:ILE:N	1:B:540:ILE:CD1	2.80	0.45
1:B:544:ASN:ND2	1:B:544:ASN:N	2.64	0.45
1:C:510:THR:O	1:C:514:ARG:N	2.50	0.45
1:D:238:ARG:N	1:D:238:ARG:CD	2.80	0.45
1:A:309:ARG:O	1:A:313:LEU:N	2.50	0.45
1:C:140:ARG:NH1	1:C:153:ASP:OD1	2.50	0.45
1:B:11:ALA:O	1:B:12:PHE:C	2.55	0.45
1:C:40:VAL:CG1	1:C:45:HIS:CA	2.95	0.45
1:D:162:THR:O	1:D:164:TYR:N	2.50	0.45
1:C:519:GLN:O	1:C:520:PHE:CG	2.70	0.45
1:A:366:TYR:C	1:A:368:ASP:N	2.66	0.45
1:B:126:PRO:O	1:B:127:PRO:C	2.55	0.45
1:A:222:SER:OG	1:A:264[B]:ARG:NH1	2.50	0.45
1:C:559:VAL:O	1:C:560:HIS:CB	2.65	0.45
1:A:38:LEU:O	1:A:119:ILE:N	2.50	0.45
1:A:255:LEU:C	1:A:257:TYR:N	2.70	0.44
1:B:146:SER:C	1:B:148:ARG:N	2.70	0.44
1:D:628:ALA:O	1:D:629:THR:CB	2.64	0.44
1:C:338:ARG:O	1:C:340:GLY:N	2.51	0.44
1:D:496:GLN:NE2	1:D:496:GLN:CA	2.80	0.44
1:D:578:VAL:CG1	1:D:582:ILE:CD1	2.95	0.44
1:B:519:GLN:C	1:B:521:SER:N	2.70	0.44
1:C:542:LEU:C	1:C:542:LEU:CD1	2.85	0.44
2:B:900:BLA:C3A	2:B:900:BLA:CMB	2.93	0.44
1:A:308:THR:O	1:A:311:THR:N	2.50	0.44
1:A:613:ARG:O	1:A:617:GLN:O	2.35	0.44
1:D:307:ALA:O	1:D:308:THR:C	2.55	0.44
1:C:599:ASN:O	1:C:601:PRO:N	2.50	0.44
1:A:230:PRO:O	1:A:231:ARG:CB	2.64	0.44
1:B:518:GLU:O	1:B:519:GLN:CB	2.64	0.44
1:A:171:ARG:CG	1:A:278:TRP:CH2	3.01	0.44
1:A:223:TYR:CD1	1:A:223:TYR:O	2.71	0.44
1:A:458:ASP:C	1:A:459:THR:CG2	2.86	0.44
1:D:622:VAL:CG2	1:D:622:VAL:O	2.66	0.44
1:A:336:ILE:CG2	1:A:342:TRP:N	2.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:43:PRO:O	1:D:45:HIS:ND1	2.51	0.44
1:B:233:SER:C	1:B:235:LEU:N	2.70	0.43
1:C:291:ILE:O	1:C:296:ARG:NH1	2.51	0.43
1:C:27:LEU:O	1:C:28:ALA:O	2.34	0.43
1:D:129:ASP:O	1:D:130:LEU:CB	2.65	0.43
1:B:553:ALA:N	3:B:1003:HOH:O	2.51	0.43
1:D:331:ARG:NH1	3:D:1036:HOH:O	2.51	0.43
1:B:71:ILE:O	1:B:72:ASP:CB	2.67	0.43
1:C:133:THR:O	1:C:135:ALA:N	2.52	0.43
1:A:613:ARG:O	1:A:615:GLU:N	2.51	0.43
1:C:413:LEU:O	1:C:413:LEU:CD1	2.67	0.43
1:C:90:MSE:CE	1:C:109:MSE:C	2.86	0.43
1:A:514:ARG:NH1	3:A:1029:HOH:O	2.50	0.43
1:D:392:GLN:O	1:D:394:ARG:NE	2.51	0.43
1:A:434:MSE:CE	1:A:436:PHE:CE1	3.02	0.43
1:A:204:GLN:O	1:A:205:MSE:C	2.57	0.43
1:C:199:SER:O	1:C:201:ASP:N	2.51	0.43
1:A:539:ARG:O	1:A:541:LEU:CD1	2.67	0.43
1:D:626:SER:O	1:D:627:ASP:C	2.56	0.43
1:A:163:GLY:O	1:A:164:TYR:C	2.57	0.43
1:B:103:THR:CG2	1:B:105:TYR:OH	2.66	0.43
1:A:550:MSE:CE	1:A:604:LEU:CD1	2.97	0.43
1:C:484:THR:OG1	1:C:487:ASP:N	2.52	0.43
1:A:336:ILE:O	1:A:340:GLY:N	2.52	0.43
1:D:357:LEU:O	1:D:437:ARG:NH2	2.51	0.43
1:B:37:LEU:C	1:B:37:LEU:CD2	2.87	0.43
1:D:229:GLU:C	1:D:231:ARG:N	2.70	0.43
1:C:446:TRP:CD2	1:C:473:HIS:CE1	3.06	0.43
1:A:26:HIS:CD2	1:A:27:LEU:CD1	3.01	0.43
1:C:37:LEU:CD2	1:C:38:LEU:N	2.82	0.43
1:C:357:LEU:O	1:C:358:HIS:C	2.57	0.43
1:D:246:PHE:CZ	1:D:296:ARG:CZ	3.01	0.43
1:B:63:VAL:O	1:B:66:VAL:CG1	2.67	0.43
1:C:195:ASN:ND2	3:C:1010:HOH:O	2.51	0.43
1:D:428:HIS:O	1:D:429:ARG:CB	2.67	0.43
1:B:393:PRO:O	1:B:394:ARG:CB	2.65	0.43
1:B:84:ASP:OD1	1:B:84:ASP:C	2.57	0.43
1:A:314:GLU:O	1:A:315:SER:C	2.57	0.43
1:D:625:PHE:C	1:D:626:SER:OG	2.56	0.43
1:A:201:ASP:OD2	1:A:468:SER:CB	2.66	0.42
1:B:420:VAL:CG1	1:B:420:VAL:O	2.67	0.42
1:A:92:VAL:CG2	1:A:93:ALA:N	2.81	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:201:ASP:O	2:A:900:BLA:NC	2.52	0.42
1:B:348:ASP:C	1:B:350:SER:N	2.71	0.42
1:D:148:ARG:NH1	1:D:181:PHE:CZ	2.88	0.42
1:C:298:ILE:CG2	1:C:302:LEU:CD2	2.97	0.42
1:D:348:ASP:OD1	1:D:350:SER:N	2.52	0.42
1:C:202:ILE:O	1:C:203:PRO:C	2.55	0.42
1:A:561:LEU:O	1:A:564:LEU:N	2.52	0.42
1:A:368:ASP:OD1	1:A:383:ARG:NH2	2.52	0.42
1:C:370:ILE:CD1	1:C:370:ILE:O	2.67	0.42
1:C:324:PHE:C	1:C:324:PHE:CD2	2.93	0.42
2:B:900:BLA:CMA	2:B:900:BLA:C2B	2.97	0.42
1:C:463:LEU:O	1:C:464:SER:CB	2.67	0.42
1:A:455:THR:OG1	1:A:474:GLN:NE2	2.52	0.42
1:C:146:SER:O	1:C:149:ALA:N	2.53	0.42
1:C:276:LYS:NZ	3:C:1076:HOH:O	2.51	0.42
1:B:246:PHE:CE1	1:B:296:ARG:NH1	2.88	0.42
1:C:496:GLN:O	1:C:497:THR:C	2.58	0.42
1:B:511:LEU:O	1:B:514:ARG:N	2.53	0.42
1:A:449:ASP:O	1:A:450:PRO:C	2.57	0.42
1:D:566:GLY:O	1:D:595:ARG:NH1	2.53	0.42
2:D:900:BLA:CMA	2:D:900:BLA:C2B	2.84	0.42
1:A:216:ARG:NE	2:A:900:BLA:O2D	2.52	0.42
1:C:608:ALA:CB	1:C:623:LEU:CD1	2.98	0.42
1:B:626:SER:O	1:B:628:ALA:N	2.52	0.42
1:C:555:SER:CB	1:C:556:PRO:C	2.89	0.42
1:C:493:THR:O	1:C:497:THR:N	2.53	0.42
1:C:269:VAL:N	1:C:281:VAL:O	2.53	0.42
1:A:131:SER:O	3:A:1008:HOH:O	2.22	0.42
1:D:551:LEU:C	1:D:553:ALA:N	2.69	0.41
1:A:170:TYR:OH	2:A:900:BLA:O2A	2.37	0.41
1:D:28:ALA:O	1:D:242:MSE:SE	2.88	0.41
1:D:402:SER:O	1:D:403:LEU:C	2.58	0.41
1:C:94:VAL:O	1:C:107:GLY:N	2.53	0.41
1:A:153:ASP:O	1:A:154:THR:C	2.58	0.41
1:C:566:GLY:C	1:C:568:PHE:N	2.73	0.41
1:C:63:VAL:O	1:C:66:VAL:CG2	2.68	0.41
1:A:519:GLN:O	1:A:520:PHE:CG	2.72	0.41
1:A:128:ILE:O	1:A:128:ILE:CG2	2.68	0.41
1:A:22:ARG:NH2	3:A:1063:HOH:O	2.52	0.41
1:D:234:PRO:O	1:D:236:THR:N	2.54	0.41
1:A:336:ILE:CG1	1:A:341:ASP:C	2.89	0.41
1:C:58:LEU:C	1:C:60:LEU:CD2	2.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:164:TYR:CD2	1:A:289:ARG:CD	3.04	0.41
1:A:11:ALA:O	1:A:12:PHE:C	2.59	0.41
1:C:541:LEU:CD2	3:C:1082:HOH:O	2.68	0.41
1:C:407:VAL:O	1:C:408:PRO:C	2.59	0.41
1:C:476:VAL:CG2	1:C:476:VAL:O	2.68	0.41
1:B:156:LEU:CD2	1:B:160:GLN:NE2	2.84	0.41
1:B:135:ALA:CB	1:B:136:PRO:CD	2.99	0.41
1:A:336:ILE:CG2	1:A:337:THR:N	2.84	0.41
1:D:204:GLN:O	1:D:205:MSE:C	2.58	0.41
1:C:522:SER:O	1:C:523:GLN:C	2.58	0.41
1:A:223:TYR:CG	1:A:223:TYR:O	2.74	0.41
1:B:608:ALA:CB	1:B:623:LEU:CD2	2.99	0.41
1:B:413:LEU:O	1:B:417:ALA:N	2.54	0.41
1:A:568:PHE:O	1:A:569:VAL:C	2.59	0.41
1:C:387:GLY:O	1:C:388:TRP:C	2.58	0.41
1:C:133:THR:O	1:C:134:LEU:C	2.60	0.41
1:C:509:ARG:O	1:C:513:ALA:N	2.54	0.40
1:D:59:ASN:O	1:D:59:ASN:CG	2.60	0.40
1:C:378:SER:O	1:C:379:THR:C	2.59	0.40
1:A:366:TYR:O	1:A:368:ASP:N	2.55	0.40
1:C:349:THR:C	1:C:351:GLN:N	2.75	0.40
1:B:520:PHE:O	1:C:510:THR:CB	2.69	0.40
1:C:407:VAL:O	1:C:409:GLU:N	2.54	0.40
1:A:529:GLN:O	1:A:544:ASN:ND2	2.54	0.40
1:B:366:TYR:CE1	1:B:506:ARG:NH1	2.90	0.40
1:A:122:GLU:OE2	1:A:296:ARG:NH2	2.54	0.40
1:A:454:PHE:CD1	1:A:455:THR:N	2.89	0.40
1:A:511:LEU:O	1:A:512:ILE:C	2.60	0.40
1:B:194:GLY:O	1:B:195:ASN:O	2.40	0.40
1:C:382:VAL:O	1:C:383:ARG:C	2.59	0.40

There are no symmetry-related clashes.

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	630/655 (96%)	479 (76%)	89 (14%)	62 (10%)	1	2
1	B	617/655 (94%)	473 (77%)	88 (14%)	56 (9%)	1	2
1	C	619/655 (94%)	482 (78%)	94 (15%)	43 (7%)	2	4
1	D	612/655 (93%)	480 (78%)	76 (12%)	56 (9%)	1	2
All	All	2478/2620 (95%)	1914 (77%)	347 (14%)	217 (9%)	1	3

All (217) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	PHE
1	A	55	ALA
1	A	72	ASP
1	A	74	ASP
1	A	110	HIS
1	A	128	ILE
1	A	129	ASP
1	A	135	ALA
1	A	164	TYR
1	A	193	PHE
1	A	223	TYR
1	A	335	ALA
1	A	336	ILE
1	A	338	ARG
1	A	339	GLU
1	A	348	ASP
1	A	396	ALA
1	A	450	PRO
1	A	454	PHE
1	A	526	ALA
1	A	553	ALA
1	A	557	SER
1	A	558	ALA
1	A	560	HIS
1	A	568	PHE
1	A	570	GLU
1	A	571	SER
1	A	615	GLU
1	A	616	ASP
1	A	625	PHE
1	A	633	THR
1	B	49	GLN
1	B	75	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	89	GLY
1	B	90	MSE
1	B	100	ASN
1	B	127	PRO
1	B	130	LEU
1	B	195	ASN
1	B	230	PRO
1	B	232	LEU
1	B	340	GLY
1	B	348	ASP
1	B	396	ALA
1	B	405	LEU
1	B	519	GLN
1	B	564	LEU
1	B	569	VAL
1	B	601	PRO
1	B	626	SER
1	C	42	GLU
1	C	43	PRO
1	C	72	ASP
1	C	75	LEU
1	C	87	ALA
1	C	127	PRO
1	C	134	LEU
1	C	341	ASP
1	C	348	ASP
1	C	351	GLN
1	C	378	SER
1	C	444	VAL
1	C	520	PHE
1	C	555	SER
1	C	560	HIS
1	C	630	ASP
1	D	43	PRO
1	D	71	ILE
1	D	114	GLU
1	D	130	LEU
1	D	229	GLU
1	D	230	PRO
1	D	236	THR
1	D	338	ARG
1	D	339	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	340	GLY
1	D	348	ASP
1	D	393	PRO
1	D	394	ARG
1	D	395	ALA
1	D	397	VAL
1	D	471	LYS
1	D	519	GLN
1	D	520	PHE
1	D	552	PRO
1	D	553	ALA
1	D	556	PRO
1	D	557	SER
1	D	570	GLU
1	D	571	SER
1	D	601	PRO
1	D	627	ASP
1	D	629	THR
1	A	71	ILE
1	A	100	ASN
1	A	116	GLY
1	A	126	PRO
1	A	256	GLN
1	A	429	ARG
1	A	445	THR
1	A	447	GLY
1	A	451	LYS
1	A	519	GLN
1	A	520	PHE
1	A	562	ASP
1	A	572	ASN
1	A	628	ALA
1	B	62	SER
1	B	74	ASP
1	B	78	LYS
1	B	99	GLY
1	B	336	ILE
1	B	339	GLU
1	B	341	ASP
1	B	378	SER
1	B	429	ARG
1	B	470	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	517	TYR
1	B	552	PRO
1	B	553	ALA
1	B	554	GLY
1	B	557	SER
1	B	597	ALA
1	B	599	ASN
1	B	612	THR
1	B	631	ARG
1	C	28	ALA
1	C	89	GLY
1	C	200	SER
1	C	393	PRO
1	C	394	ARG
1	C	445	THR
1	C	449	ASP
1	C	553	ALA
1	C	569	VAL
1	C	584	HIS
1	C	598	GLY
1	C	626	SER
1	D	127	PRO
1	D	132	GLY
1	D	133	THR
1	D	239	ASP
1	D	411	ALA
1	D	429	ARG
1	D	441	VAL
1	D	477	GLU
1	D	546	SER
1	D	576	ARG
1	D	596	GLY
1	D	616	ASP
1	D	633	THR
1	A	342	TRP
1	A	614	THR
1	B	128	ILE
1	B	349	THR
1	B	450	PRO
1	B	477	GLU
1	B	563	ASP
1	B	615	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	630	ASP
1	C	147	LEU
1	C	377	PRO
1	C	429	ARG
1	C	484	THR
1	D	378	SER
1	D	476	VAL
1	D	554	GLY
1	D	594	LEU
1	D	626	SER
1	A	114	GLU
1	A	309	ARG
1	A	455	THR
1	A	459	THR
1	A	561	LEU
1	A	634	ALA
1	B	72	ASP
1	B	133	THR
1	B	161	CYS
1	B	402	SER
1	B	443	THR
1	B	449	ASP
1	B	521	SER
1	B	558	ALA
1	B	600	ARG
1	C	131	SER
1	C	380	GLN
1	C	531	VAL
1	C	600	ARG
1	D	70	GLU
1	D	231	ARG
1	D	335	ALA
1	D	341	ASP
1	D	600	ARG
1	A	308	THR
1	A	415	ARG
1	A	476	VAL
1	C	128	ILE
1	C	615	GLU
1	D	19	ASN
1	D	74	ASP
1	D	195	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	377	PRO
1	A	144	ALA
1	A	449	ASP
1	A	465	PRO
1	A	632	ARG
1	C	428	HIS
1	C	450	PRO
1	D	555	SER
1	A	569	VAL
1	C	408	PRO
1	C	464	SER
1	C	476	VAL
1	D	569	VAL
1	A	333	ILE
1	B	355	GLN
1	B	476	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	525/526 (100%)	443 (84%)	82 (16%)	4	11
1	B	515/526 (98%)	457 (89%)	58 (11%)	9	25
1	C	517/526 (98%)	453 (88%)	64 (12%)	7	19
1	D	511/526 (97%)	448 (88%)	63 (12%)	7	20
All	All	2068/2104 (98%)	1801 (87%)	267 (13%)	6	17

All (267) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	30	SER
1	A	31	ILE
1	A	37	LEU
1	A	45[A]	HIS
1	A	45[B]	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	60	LEU
1	A	64	LEU
1	A	70	GLU
1	A	71	ILE
1	A	75	LEU
1	A	76	LEU
1	A	80	LEU
1	A	90	MSE
1	A	95	ARG
1	A	103	THR
1	A	109	MSE
1	A	110	HIS
1	A	133	THR
1	A	138	LEU
1	A	139	GLU
1	A	147	LEU
1	A	148	ARG
1	A	156	LEU
1	A	157	LEU
1	A	159	GLN
1	A	171	ARG
1	A	184	ARG
1	A	186	VAL
1	A	189	LEU
1	A	193	PHE
1	A	195	ASN
1	A	199	SER
1	A	202	ILE
1	A	209	LEU
1	A	218	LEU
1	A	223	TYR
1	A	231	ARG
1	A	239	ASP
1	A	242	MSE
1	A	256	GLN
1	A	257	TYR
1	A	269	VAL
1	A	294	GLU
1	A	309	ARG
1	A	321	SER
1	A	365	VAL
1	A	371	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	378	SER
1	A	388	TRP
1	A	389	LEU
1	A	392	GLN
1	A	405	LEU
1	A	421	VAL
1	A	433	LEU
1	A	456[A]	MSE
1	A	456[B]	MSE
1	A	459	THR
1	A	469	PHE
1	A	476	VAL
1	A	492	ARG
1	A	493	THR
1	A	512	ILE
1	A	528	MSE
1	A	531	VAL
1	A	532	LEU
1	A	541	LEU
1	A	550	MSE
1	A	567	PHE
1	A	573	ASP
1	A	586	ARG
1	A	588	TRP
1	A	592	VAL
1	A	593	LEU
1	A	602	LEU
1	A	607	ARG
1	A	617	GLN
1	A	623	LEU
1	A	624	ILE
1	A	626	SER
1	A	629	THR
1	A	633	THR
1	B	27	LEU
1	B	66	VAL
1	B	100	ASN
1	B	103	THR
1	B	114	GLU
1	B	117	LEU
1	B	123	ARG
1	B	139	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	153	ASP
1	B	157	LEU
1	B	159	GLN
1	B	161	CYS
1	B	169	VAL
1	B	208	ARG
1	B	230	PRO
1	B	236	THR
1	B	238	ARG
1	B	293	PHE
1	B	301	LEU
1	B	308	THR
1	B	309	ARG
1	B	310	ILE
1	B	311	THR
1	B	318	GLN
1	B	327	ARG
1	B	331	ARG
1	B	336	ILE
1	B	351	GLN
1	B	354	LEU
1	B	365	VAL
1	B	370	ILE
1	B	379	THR
1	B	388	TRP
1	B	390	ASP
1	B	393	PRO
1	B	405	LEU
1	B	409	GLU
1	B	416	MSE
1	B	446	TRP
1	B	466	ARG
1	B	476	VAL
1	B	479	THR
1	B	492	ARG
1	B	502	VAL
1	B	504	GLN
1	B	512	ILE
1	B	528	MSE
1	B	531	VAL
1	B	534	THR
1	B	544	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	564	LEU
1	B	572	ASN
1	B	577	ASN
1	B	578	VAL
1	B	589	ARG
1	B	600	ARG
1	B	615	GLU
1	B	619	LEU
1	C	22	ARG
1	C	63	VAL
1	C	80	LEU
1	C	86	THR
1	C	95	ARG
1	C	102	SER
1	C	103	THR
1	C	108	LEU
1	C	109	MSE
1	C	128	ILE
1	C	129	ASP
1	C	130	LEU
1	C	140	ARG
1	C	159	GLN
1	C	184	ARG
1	C	205	MSE
1	C	212	ARG
1	C	215	VAL
1	C	233	SER
1	C	238	ARG
1	C	256	GLN
1	C	276	LYS
1	C	288	PRO
1	C	291	ILE
1	C	295	LEU
1	C	301	LEU
1	C	304	GLU
1	C	309	ARG
1	C	318	GLN
1	C	323	LEU
1	C	349	THR
1	C	351	GLN
1	C	355	GLN
1	C	370	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	378	SER
1	C	379	THR
1	C	413	LEU
1	C	414	THR
1	C	415	ARG
1	C	416	MSE
1	C	420	VAL
1	C	421	VAL
1	C	429	ARG
1	C	434	MSE
1	C	440	ARG
1	C	445	THR
1	C	446	TRP
1	C	452	LYS
1	C	466	ARG
1	C	469	PHE
1	C	475	VAL
1	C	493	THR
1	C	501	ILE
1	C	502	VAL
1	C	531	VAL
1	C	534	THR
1	C	542	LEU
1	C	564	LEU
1	C	574	PHE
1	C	586	ARG
1	C	600	ARG
1	C	623	LEU
1	C	625	PHE
1	C	627	ASP
1	D	19	ASN
1	D	37	LEU
1	D	39	VAL
1	D	43	PRO
1	D	44	ASP
1	D	64	LEU
1	D	74	ASP
1	D	77	ILE
1	D	88	GLU
1	D	121	LEU
1	D	122	GLU
1	D	139	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	147	LEU
1	D	148	ARG
1	D	154	THR
1	D	159	GLN
1	D	167	VAL
1	D	169	VAL
1	D	195	ASN
1	D	214	ARG
1	D	226	VAL
1	D	228	LEU
1	D	232	LEU
1	D	238	ARG
1	D	242	MSE
1	D	266	THR
1	D	270	SER
1	D	272	VAL
1	D	291	ILE
1	D	292[A]	HIS
1	D	292[B]	HIS
1	D	302	LEU
1	D	304	GLU
1	D	309	ARG
1	D	330	GLN
1	D	337	THR
1	D	346	ILE
1	D	406	ASP
1	D	413	LEU
1	D	414	THR
1	D	415	ARG
1	D	416	MSE
1	D	421	VAL
1	D	432	PHE
1	D	442	HIS
1	D	443	THR
1	D	459	THR
1	D	463	LEU
1	D	466	ARG
1	D	467	ARG
1	D	469	PHE
1	D	484	THR
1	D	501	ILE
1	D	517	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	518	GLU
1	D	531	VAL
1	D	544	ASN
1	D	564	LEU
1	D	576	ARG
1	D	586	ARG
1	D	588	TRP
1	D	623	LEU
1	D	632	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA chains 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

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	BLA	A	900	1	46,46,46	3.61	14 (30%)	65,67,67	3.20	32 (49%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BLA	B	900	1	46,46,46	3.35	15 (32%)	65,67,67	2.65	23 (35%)
2	BLA	C	900	1	46,46,46	3.73	14 (30%)	65,67,67	2.66	30 (46%)
2	BLA	D	900	1	46,46,46	3.25	12 (26%)	65,67,67	2.41	33 (50%)

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
2	BLA	A	900	1	-	2/26/74/74	0/4/4/4
2	BLA	B	900	1	-	2/26/74/74	0/4/4/4
2	BLA	C	900	1	-	2/26/74/74	0/4/4/4
2	BLA	D	900	1	-	2/26/74/74	0/4/4/4

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	900	BLA	CHA-C4D	20.32	1.49	1.35
2	A	900	BLA	CHA-C4D	18.20	1.47	1.35
2	B	900	BLA	CHA-C4D	16.14	1.46	1.35
2	D	900	BLA	CHA-C4D	16.10	1.46	1.35
2	A	900	BLA	C3B-C2B	7.18	1.50	1.36
2	A	900	BLA	CHB-C1B	6.99	1.50	1.34
2	B	900	BLA	CHB-C1B	6.89	1.50	1.34
2	D	900	BLA	CHB-C1B	6.74	1.50	1.34
2	B	900	BLA	C3B-C2B	6.54	1.49	1.36
2	C	900	BLA	C3D-C2D	5.79	1.49	1.36
2	D	900	BLA	C3B-C2B	5.74	1.48	1.36
2	D	900	BLA	C3C-C2C	5.54	1.47	1.36
2	C	900	BLA	CHB-C1B	5.49	1.47	1.34
2	B	900	BLA	C3D-C2D	5.44	1.48	1.36
2	C	900	BLA	C3C-C2C	5.36	1.47	1.36
2	D	900	BLA	C3D-C2D	5.08	1.47	1.36
2	C	900	BLA	C3B-C2B	5.03	1.46	1.36
2	B	900	BLA	C3C-C2C	4.80	1.46	1.36
2	A	900	BLA	CHD-C4C	4.54	1.48	1.37
2	D	900	BLA	CHD-C4C	4.34	1.48	1.37
2	A	900	BLA	C3D-C2D	4.30	1.45	1.36
2	B	900	BLA	CHD-C4C	4.11	1.47	1.37
2	A	900	BLA	C3C-C2C	3.99	1.44	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	BLA	C4B-NB	-3.90	1.29	1.37
2	A	900	BLA	C4A-NA	-3.79	1.32	1.36
2	C	900	BLA	CHD-C4C	3.77	1.47	1.37
2	B	900	BLA	CHD-C1D	3.68	1.49	1.40
2	C	900	BLA	C1A-C2A	3.42	1.50	1.42
2	C	900	BLA	CHD-C1D	3.41	1.48	1.40
2	A	900	BLA	C1A-C2A	3.39	1.50	1.42
2	D	900	BLA	CHD-C1D	3.36	1.48	1.40
2	C	900	BLA	OB-C4B	3.32	1.30	1.23
2	D	900	BLA	C4A-C3A	3.30	1.50	1.42
2	C	900	BLA	C2A-C3A	3.30	1.47	1.37
2	B	900	BLA	C4A-C3A	3.30	1.50	1.42
2	A	900	BLA	CHD-C1D	3.26	1.48	1.40
2	A	900	BLA	OB-C4B	3.24	1.29	1.23
2	B	900	BLA	OC-C1C	3.08	1.29	1.23
2	C	900	BLA	C4A-C3A	3.04	1.49	1.42
2	B	900	BLA	C2A-C3A	3.03	1.46	1.37
2	B	900	BLA	OB-C4B	3.01	1.29	1.23
2	D	900	BLA	C2A-C3A	2.92	1.46	1.37
2	B	900	BLA	C1A-C2A	2.83	1.49	1.42
2	C	900	BLA	OC-C1C	2.78	1.29	1.23
2	A	900	BLA	O1A-CGA	2.77	1.32	1.22
2	D	900	BLA	C1A-C2A	2.76	1.48	1.42
2	A	900	BLA	C2A-C3A	2.58	1.45	1.37
2	A	900	BLA	C4C-NC	-2.46	1.33	1.37
2	D	900	BLA	OC-C1C	2.42	1.28	1.23
2	B	900	BLA	C1B-C2B	2.41	1.49	1.45
2	B	900	BLA	C4C-NC	-2.38	1.33	1.37
2	C	900	BLA	C4D-C3D	2.32	1.49	1.45
2	D	900	BLA	OB-C4B	2.24	1.28	1.23
2	C	900	BLA	C4A-NA	-2.23	1.34	1.36
2	B	900	BLA	C4B-NB	-2.10	1.33	1.37

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	900	BLA	C3B-C4B-NB	7.19	113.16	106.66
2	A	900	BLA	C1A-CHA-C4D	-6.92	116.41	129.92
2	B	900	BLA	C3B-C4B-NB	6.84	112.84	106.66
2	D	900	BLA	C3B-C4B-NB	6.81	112.82	106.66
2	A	900	BLA	C3A-C4A-CHB	-6.77	106.51	125.72
2	A	900	BLA	CHB-C1B-NB	-6.59	106.85	130.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	BLA	CAA-C2A-C1A	6.53	138.70	124.73
2	A	900	BLA	CHB-C1B-C2B	5.88	139.53	126.83
2	C	900	BLA	C1A-C2A-C3A	-5.85	100.86	106.92
2	C	900	BLA	CHB-C1B-NB	-5.65	110.17	130.23
2	A	900	BLA	C2A-C1A-NA	5.63	116.08	106.79
2	A	900	BLA	C1A-C2A-C3A	-5.59	101.13	106.92
2	B	900	BLA	CHB-C1B-NB	-5.59	110.40	130.23
2	A	900	BLA	C3B-C2B-C1B	-5.43	100.18	107.14
2	A	900	BLA	C4A-C3A-C2A	-5.39	103.37	107.04
2	B	900	BLA	C1A-C2A-C3A	-5.29	101.44	106.92
2	B	900	BLA	C2A-C1A-NA	5.18	115.34	106.79
2	A	900	BLA	CAD-CBD-CGD	-5.17	103.94	113.53
2	A	900	BLA	C3B-C4B-NB	5.13	111.29	106.66
2	B	900	BLA	C4D-C3D-C2D	-4.97	101.09	106.86
2	C	900	BLA	C2A-C1A-NA	4.94	114.94	106.79
2	B	900	BLA	C3B-C2B-C1B	-4.93	100.82	107.14
2	C	900	BLA	C4C-NC-C1C	-4.89	103.83	110.74
2	B	900	BLA	CMC-C2C-C1C	4.74	133.87	121.59
2	C	900	BLA	CMB-C2B-C1B	4.69	130.63	124.23
2	A	900	BLA	C3A-C4A-NA	4.62	117.14	108.16
2	D	900	BLA	C2A-C1A-NA	4.57	114.33	106.79
2	C	900	BLA	CHB-C1B-C2B	4.52	136.58	126.83
2	A	900	BLA	CMB-C2B-C1B	4.51	130.38	124.23
2	B	900	BLA	C3D-C4D-ND	4.49	116.90	109.79
2	A	900	BLA	CMC-C2C-C1C	4.33	132.81	121.59
2	B	900	BLA	C2B-C1B-NB	4.25	113.86	107.14
2	A	900	BLA	C4C-NC-C1C	-4.16	104.86	110.74
2	D	900	BLA	C4C-NC-C1C	-4.14	104.89	110.74
2	D	900	BLA	C1A-C2A-C3A	-4.12	102.66	106.92
2	B	900	BLA	CHB-C1B-C2B	4.10	135.68	126.83
2	C	900	BLA	CHD-C1D-ND	-4.07	117.24	124.99
2	A	900	BLA	C2B-C1B-NB	4.05	113.54	107.14
2	D	900	BLA	CMB-C2B-C1B	4.03	129.73	124.23
2	A	900	BLA	CAD-C3D-C4D	4.01	132.27	124.85
2	A	900	BLA	OB-C4B-NB	-3.97	114.75	125.12
2	C	900	BLA	C3B-C2B-C1B	-3.95	102.08	107.14
2	A	900	BLA	C2C-C1C-NC	3.92	117.55	106.27
2	D	900	BLA	C4D-C3D-C2D	-3.90	102.33	106.86
2	B	900	BLA	CAD-CBD-CGD	-3.87	106.35	113.53
2	C	900	BLA	CBA-CAA-C2A	3.86	119.48	112.69
2	C	900	BLA	C2B-C1B-NB	3.81	113.17	107.14
2	D	900	BLA	CHB-C1B-NB	-3.74	116.95	130.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	BLA	CMB-C2B-C1B	3.73	129.31	124.23
2	D	900	BLA	C2C-C1C-NC	3.70	116.93	106.27
2	D	900	BLA	C4A-C3A-C2A	-3.68	104.53	107.04
2	D	900	BLA	C3D-C4D-ND	3.67	115.60	109.79
2	B	900	BLA	CHA-C4D-ND	-3.65	121.84	128.59
2	C	900	BLA	OB-C4B-C3B	-3.60	120.60	130.22
2	C	900	BLA	C2C-C1C-NC	3.54	116.47	106.27
2	D	900	BLA	OB-C4B-C3B	-3.52	120.81	130.22
2	B	900	BLA	C2C-C1C-NC	3.48	116.30	106.27
2	B	900	BLA	C4C-NC-C1C	-3.47	105.84	110.74
2	B	900	BLA	C1A-CHA-C4D	-3.46	123.16	129.92
2	A	900	BLA	O2A-CGA-O1A	3.37	131.86	123.30
2	D	900	BLA	CHA-C4D-ND	-3.27	122.55	128.59
2	C	900	BLA	C3C-C4C-NC	3.27	113.17	106.59
2	C	900	BLA	C1B-NB-C4B	-3.19	106.23	110.74
2	C	900	BLA	CHA-C4D-ND	-3.18	122.72	128.59
2	C	900	BLA	C4D-C3D-C2D	-3.16	103.18	106.86
2	A	900	BLA	CAA-C2A-C3A	-3.10	120.16	129.00
2	C	900	BLA	C1D-C2D-C3D	-3.09	102.81	106.64
2	D	900	BLA	CAD-CBD-CGD	-3.03	107.90	113.53
2	D	900	BLA	CMA-C3A-C4A	2.99	133.19	128.65
2	B	900	BLA	CAA-C2A-C1A	2.98	131.11	124.73
2	C	900	BLA	OC-C1C-C2C	-2.94	114.07	129.00
2	B	900	BLA	O1A-CGA-CBA	-2.93	112.96	123.03
2	B	900	BLA	C1B-NB-C4B	-2.87	106.69	110.74
2	C	900	BLA	O1A-CGA-CBA	-2.84	113.25	123.03
2	A	900	BLA	C4A-NA-C1A	-2.83	102.23	108.72
2	A	900	BLA	O1A-CGA-CBA	-2.76	113.55	123.03
2	D	900	BLA	CHD-C1D-ND	-2.70	119.84	124.99
2	C	900	BLA	C3D-C4D-ND	2.69	114.05	109.79
2	D	900	BLA	C3B-C2B-C1B	-2.67	103.72	107.14
2	C	900	BLA	C2A-C1A-CHA	-2.67	118.14	125.72
2	A	900	BLA	CBD-CAD-C3D	2.64	120.51	112.71
2	D	900	BLA	CBA-CAA-C2A	2.60	117.27	112.69
2	A	900	BLA	CAD-C3D-C2D	-2.59	123.34	128.00
2	D	900	BLA	C3C-C4C-NC	2.58	111.78	106.59
2	D	900	BLA	C1A-CHA-C4D	-2.51	125.02	129.92
2	D	900	BLA	CMD-C2D-C1D	2.51	129.17	125.02
2	D	900	BLA	C2B-C1B-NB	2.51	111.10	107.14
2	D	900	BLA	O1A-CGA-CBA	-2.49	114.45	123.03
2	A	900	BLA	CHA-C4D-ND	-2.46	124.05	128.59
2	C	900	BLA	O2A-CGA-CBA	2.46	122.90	114.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	900	BLA	C4B-C3B-C2B	-2.44	104.84	107.97
2	A	900	BLA	CBC-CAC-C3C	-2.44	114.95	127.09
2	A	900	BLA	CHD-C1D-C2D	-2.41	119.10	125.10
2	C	900	BLA	CAD-C3D-C2D	2.38	132.28	128.00
2	C	900	BLA	C3A-C4A-NA	2.34	112.71	108.16
2	D	900	BLA	CHB-C1B-C2B	2.34	131.87	126.83
2	D	900	BLA	CMC-C2C-C1C	2.33	127.62	121.59
2	D	900	BLA	C2A-C1A-CHA	-2.33	119.12	125.72
2	B	900	BLA	OB-C4B-C3B	-2.33	124.02	130.22
2	D	900	BLA	CAA-C2A-C1A	2.31	129.68	124.73
2	C	900	BLA	C4A-C3A-C2A	-2.31	105.47	107.04
2	D	900	BLA	C1D-C2D-C3D	-2.30	103.79	106.64
2	C	900	BLA	CAA-C2A-C1A	2.29	129.63	124.73
2	D	900	BLA	C1B-NB-C4B	-2.27	107.53	110.74
2	C	900	BLA	CHD-C4C-C3C	-2.26	119.94	127.48
2	B	900	BLA	C3C-C4C-NC	2.25	111.11	106.59
2	A	900	BLA	C3C-C4C-NC	2.22	111.06	106.59
2	B	900	BLA	C4A-C3A-C2A	-2.17	105.56	107.04
2	D	900	BLA	O1D-CGD-CBD	-2.15	115.64	123.03
2	D	900	BLA	C3A-C4A-NA	2.14	112.32	108.16
2	A	900	BLA	C4D-C3D-C2D	-2.13	104.38	106.86
2	B	900	BLA	O2A-CGA-CBA	2.13	121.76	114.22
2	C	900	BLA	CMD-C2D-C3D	2.07	131.95	126.05
2	D	900	BLA	CAD-C3D-C4D	2.06	128.66	124.85
2	A	900	BLA	C4B-C3B-C2B	-2.05	105.35	107.97
2	A	900	BLA	O2D-CGD-O1D	2.04	128.49	123.30
2	D	900	BLA	OC-C1C-C2C	-2.03	118.68	129.00
2	C	900	BLA	C4B-C3B-C2B	-2.03	105.37	107.97

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	BLA	C4A-CHB-C1B-NB
2	C	900	BLA	C4A-CHB-C1B-NB
2	D	900	BLA	C4A-CHB-C1B-NB
2	B	900	BLA	C4A-CHB-C1B-NB
2	D	900	BLA	C1B-CHB-C4A-NA
2	C	900	BLA	C1B-CHB-C4A-NA
2	B	900	BLA	C1B-CHB-C4A-NA
2	A	900	BLA	C1B-CHB-C4A-NA

There are no ring outliers.

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, 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	628/655 (95%)	0.01	28 (4%)	32 39	39, 65, 128, 180	0
1	B	621/655 (94%)	0.05	22 (3%)	42 50	43, 72, 145, 176	0
1	C	622/655 (94%)	-0.07	17 (2%)	52 61	35, 64, 146, 168	0
1	D	615/655 (93%)	0.02	19 (3%)	47 55	47, 70, 124, 175	0
All	All	2486/2620 (94%)	0.00	86 (3%)	42 50	35, 68, 138, 180	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	633	THR	15.1
1	B	446	TRP	8.3
1	A	453	PRO	7.5
1	D	459	THR	7.4
1	B	445	THR	7.4
1	D	634	ALA	7.2
1	B	450	PRO	6.4
1	B	633	THR	6.4
1	A	456[A]	MSE	6.2
1	D	635	ASP	6.0
1	B	444	VAL	6.0
1	D	457	GLY	6.0
1	B	634	ALA	5.7
1	D	633	THR	5.7
1	D	632	ARG	5.6
1	B	449	ASP	5.4
1	B	448	GLY	4.7
1	B	451	LYS	4.5
1	C	564	LEU	4.4
1	D	602	LEU	4.4
1	A	450	PRO	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	600	ARG	4.1
1	A	561	LEU	4.0
1	C	561	LEU	3.9
1	A	554	GLY	3.8
1	A	553	ALA	3.8
1	A	452	LYS	3.7
1	A	597	ALA	3.7
1	A	635	ASP	3.6
1	B	630	ASP	3.5
1	A	445	THR	3.4
1	D	8	GLY	3.4
1	B	447	GLY	3.3
1	B	632	ARG	3.2
1	C	556	PRO	3.2
1	B	568	PHE	3.1
1	A	602	LEU	3.1
1	C	608	ALA	3.1
1	D	561	LEU	3.0
1	C	625	PHE	3.0
1	C	623	LEU	2.9
1	D	460	PRO	2.9
1	D	631	ARG	2.9
1	B	631	ARG	2.9
1	D	553	ALA	2.9
1	A	449	ASP	2.8
1	A	130	LEU	2.8
1	B	420	VAL	2.8
1	D	551	LEU	2.7
1	C	597	ALA	2.6
1	C	565	ALA	2.6
1	C	627	ASP	2.6
1	A	600	ARG	2.5
1	B	422	ALA	2.5
1	C	574	PHE	2.5
1	D	600	ARG	2.4
1	A	599	ASN	2.4
1	A	127	PRO	2.4
1	A	454	PHE	2.4
1	A	564	LEU	2.3
1	A	625	PHE	2.3
1	D	615	GLU	2.3
1	D	552	PRO	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	594	LEU	2.3
1	A	604	LEU	2.3
1	B	628	ALA	2.3
1	D	87	ALA	2.3
1	C	588	TRP	2.3
1	A	631	ARG	2.3
1	B	564	LEU	2.2
1	B	335	ALA	2.2
1	C	432	PHE	2.2
1	D	443	THR	2.2
1	D	574	PHE	2.2
1	B	403	LEU	2.2
1	C	568	PHE	2.2
1	A	634	ALA	2.1
1	A	451	LYS	2.1
1	C	567	PHE	2.1
1	A	425	ILE	2.1
1	C	599	ASN	2.1
1	A	630	ASP	2.1
1	B	629	THR	2.1
1	A	128	ILE	2.0
1	A	624	ILE	2.0
1	C	450	PRO	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	BLA	B	900	43/43	0.25	1.92	54,63,71,75	0
2	BLA	C	900	43/43	0.21	1.09	44,51,58,61	0
2	BLA	A	900	43/43	0.20	0.91	37,41,55,57	0
2	BLA	D	900	43/43	0.22	0.74	59,64,71,73	0

6.5 Other polymers

There are no such residues in this entry.