



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:19 PM UTC

PDB ID : 1PYT / pdb_00001pyt
Title : TERNARY COMPLEX OF PROCARBOXYPEPTIDASE A, PROPRO-
TEINASE E, AND CHYMOTRYPSINOGEN C
Authors : Gomis-Ruth, F.X.; Gomez, M.; Bode, W.; Huber, R.; Aviles, F.X.
Deposited on : 1995-06-21
Resolution : 2.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

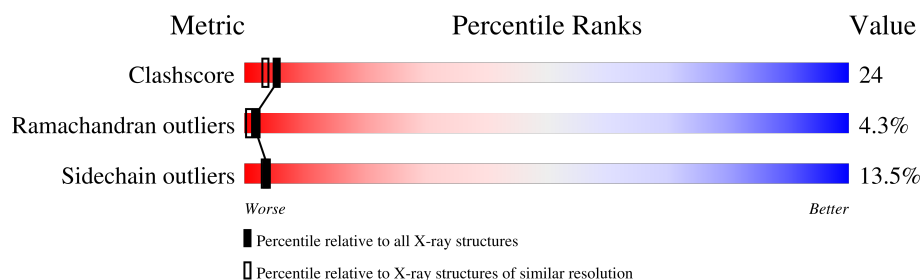
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	94	
2	B	309	
3	C	253	
4	D	251	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7411 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 PROCARBOXYPEPTIDASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	94	Total	C	N	O	S	0	0	0
			760	480	131	147	2			

- Molecule 2 is a protein called PROCARBOXYPEPTIDASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	309	Total	C	N	O	S	0	0	0
			2462	1579	405	473	5			

- Molecule 3 is a protein called PROPROTEINASE E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	248	Total	C	N	O	S	0	0	0
			1880	1185	322	362	11			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	477	GLN	GLU	conflict	UNP P05805
C	557	GLU	GLN	conflict	UNP P05805
C	570A	TYR	TRP	conflict	UNP P05805
C	592	ASP	ASN	conflict	UNP P05805
C	639	ASN	ASP	conflict	UNP P05805

- Molecule 4 is a protein called CHYMOTRYPSINOGEN C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	251	Total	C	N	O	S	0	0	0
			1926	1218	330	367	11			

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Zn	0	0
			1	1		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Ca	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	47	Total	O	0	0
			47	47		
7	B	161	Total	O	0	0
			161	161		
7	C	99	Total	O	0	0
			99	99		
7	D	74	Total	O	0	0
			74	74		

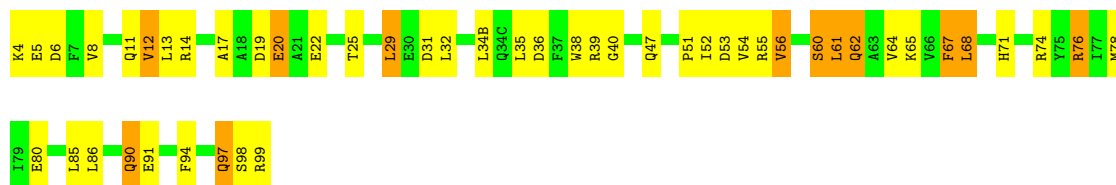
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

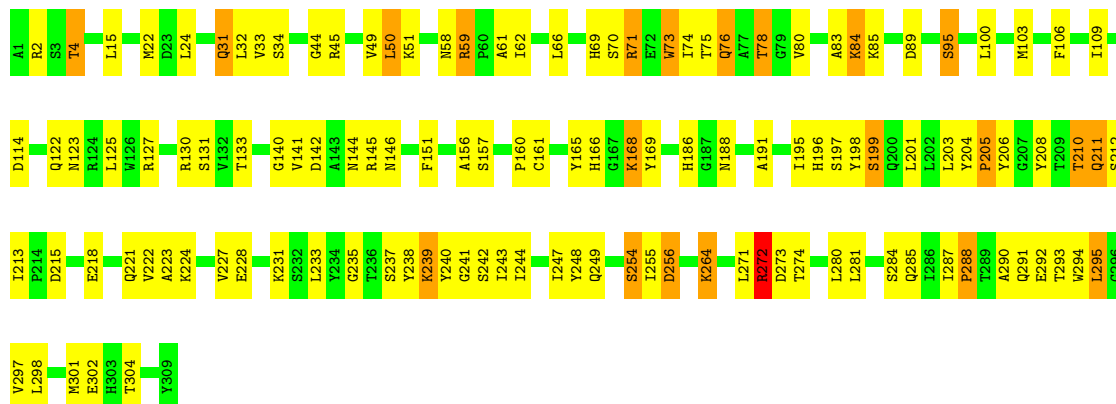
• Molecule 1: PROCARBOXYPEPTIDASE A

Chain A: 



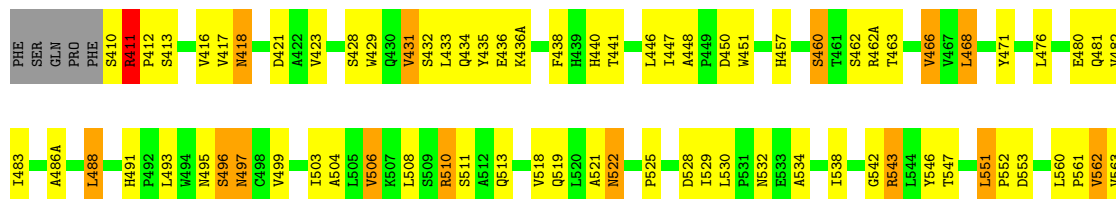
• Molecule 2: PROCARBOXYPEPTIDASE A

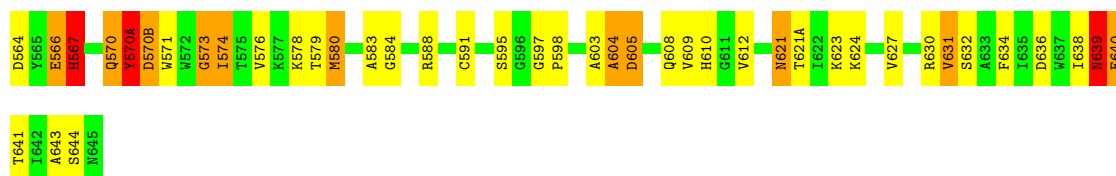
Chain B: 



• Molecule 3: PROPROTEINASE E

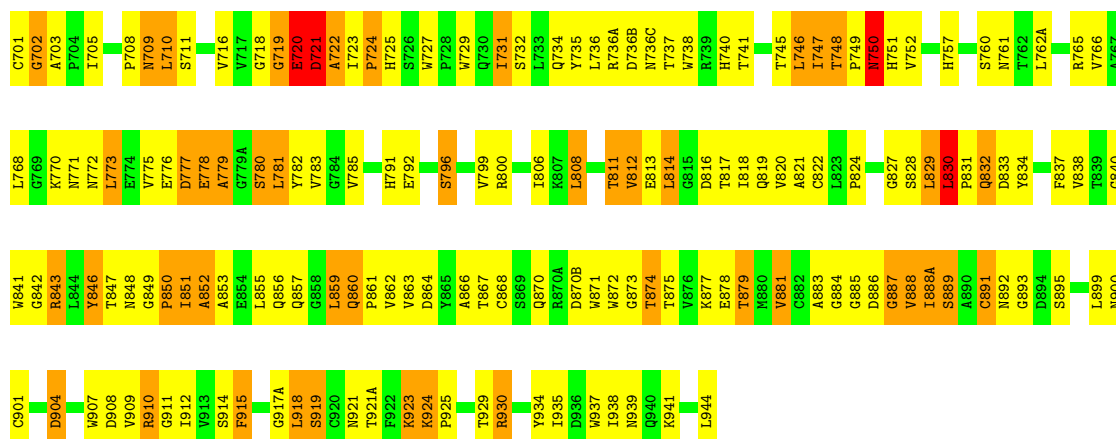
Chain C: 





● Molecule 4: CHYMOTRYPSINOGEN C

Chain D: 34% 46% 18%



4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	188.50 Å 188.50 Å 82.50 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.35	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.35)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.192 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7411	wwPDB-VP
Average B, all atoms (Å ²)	45.0	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, CA

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	0.79	1/775 (0.1%)	1.19	8/1048 (0.8%)
2	B	0.80	0/2529	1.16	19/3437 (0.6%)
3	C	0.73	2/1932 (0.1%)	1.16	19/2642 (0.7%)
4	D	0.71	1/1974 (0.1%)	1.18	18/2698 (0.7%)
All	All	0.76	4/7210 (0.1%)	1.17	64/9825 (0.7%)

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
2	B	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	580	MET	SD-CE	-7.18	1.61	1.79
3	C	506	VAL	CA-CB	5.40	1.61	1.54
4	D	747	ILE	CA-CB	5.12	1.60	1.54
1	A	17	ALA	CA-CB	-5.10	1.46	1.53

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	70	SER	N-CA-C	10.06	124.65	112.38
2	B	140	GLY	N-CA-C	9.87	123.35	112.29
1	A	40	GLY	CA-C-N	8.38	128.44	119.90
1	A	40	GLY	C-N-CA	8.38	128.44	119.90
2	B	239	LYS	N-CA-C	-8.36	97.02	109.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	553	ASP	N-CA-C	-8.23	102.84	113.12
4	D	915	PHE	N-CA-C	7.55	120.21	108.96
3	C	423	VAL	N-CA-C	-7.30	101.80	108.95
3	C	567	HIS	N-CA-C	-7.21	105.01	113.88
2	B	256	ASP	N-CA-C	-7.17	103.20	112.23
4	D	919	SER	N-CA-C	7.15	118.62	108.54
2	B	122	GLN	N-CA-C	7.09	121.62	112.12
4	D	748	THR	N-CA-C	-7.01	101.82	108.13
3	C	595	SER	N-CA-C	-6.81	101.08	110.35
4	D	863	VAL	N-CA-C	-6.64	98.87	108.17
1	A	97	GLN	N-CA-C	6.62	120.03	109.24
4	D	796	SER	N-CA-C	6.49	118.35	111.28
3	C	597	GLY	CA-C-N	6.32	126.23	119.85
3	C	597	GLY	C-N-CA	6.32	126.23	119.85
2	B	210	THR	N-CA-C	-6.30	105.60	113.28
4	D	818	ILE	N-CA-C	-6.25	98.11	107.37
2	B	254	SER	N-CA-C	6.22	117.75	110.97
4	D	912	ILE	N-CA-C	-6.16	99.25	108.12
3	C	488	LEU	N-CA-C	-6.15	102.60	110.53
2	B	69	HIS	N-CA-C	-6.13	95.37	107.69
4	D	710	LEU	N-CA-C	-6.07	97.86	110.80
3	C	542	GLY	N-CA-C	6.01	124.16	114.90
4	D	721	ASP	N-CA-C	-5.95	98.13	110.80
3	C	624	LYS	CA-C-N	5.94	125.85	119.85
3	C	624	LYS	C-N-CA	5.94	125.85	119.85
4	D	848	ASN	N-CA-C	5.89	119.30	108.58
2	B	73	TRP	N-CA-C	5.79	119.44	112.38
3	C	511	SER	N-CA-C	5.76	118.62	110.50
1	A	12	VAL	N-CA-C	-5.75	100.13	108.36
4	D	924	LYS	CA-C-N	5.75	125.73	120.21
4	D	924	LYS	C-N-CA	5.75	125.73	120.21
3	C	551	LEU	N-CA-C	5.71	118.57	110.24
1	A	67	PHE	N-CA-C	-5.68	105.00	111.07
2	B	168	LYS	N-CA-C	5.67	117.46	111.28
4	D	830	LEU	N-CA-C	5.66	122.32	109.81
4	D	904	ASP	N-CA-C	-5.63	103.47	111.24
2	B	109	ILE	N-CA-C	5.57	116.34	110.72
1	A	29	LEU	N-CA-C	-5.56	106.85	113.97
2	B	215	ASP	N-CA-C	5.56	117.11	110.44
2	B	237	SER	N-CA-C	5.52	117.96	109.07
2	B	244	ILE	N-CA-C	5.50	116.89	110.62
3	C	598	PRO	N-CA-C	5.47	120.08	111.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	476	LEU	N-CA-C	-5.46	102.32	110.23
4	D	727	TRP	CA-C-N	5.45	126.65	119.84
4	D	727	TRP	C-N-CA	5.45	126.65	119.84
2	B	49	VAL	N-CA-C	-5.38	100.37	108.12
3	C	417	VAL	N-CA-C	-5.35	100.04	108.23
2	B	145	ARG	N-CA-C	-5.33	105.46	113.89
3	C	639	ASN	N-CA-C	5.33	117.09	111.28
1	A	47	GLN	N-CA-C	-5.29	102.78	110.08
3	C	513	GLN	N-CA-C	-5.17	98.90	107.99
1	A	61	LEU	N-CA-C	5.16	116.59	110.97
3	C	428	SER	N-CA-C	5.16	119.33	113.19
4	D	881	VAL	CB-CA-C	-5.14	103.00	110.81
2	B	61	ALA	N-CA-C	5.12	116.77	109.14
3	C	604	ALA	N-CA-C	-5.09	98.41	107.98
2	B	78	THR	N-CA-C	-5.09	106.58	112.89
4	D	727	TRP	N-CA-C	-5.09	101.44	108.76
2	B	44	GLY	N-CA-C	5.01	122.24	115.32

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	272	ARG	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	760	0	739	37	0
2	B	2462	0	2367	75	0
3	C	1880	0	1785	86	0
4	D	1926	0	1853	148	0
5	B	1	0	0	1	0
6	C	1	0	0	0	0
7	A	47	0	0	2	0
7	B	161	0	0	5	0
7	C	99	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	74	0	0	5	0
All	All	7411	0	6744	333	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (333) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:MET:HE2	2:B:50:LEU:HD13	1.49	0.93
3:C:468:LEU:HD11	3:C:483:ILE:HD12	1.53	0.91
3:C:460:SER:HB3	3:C:462(A):ARG:HG3	1.52	0.91
3:C:525:PRO:HG2	3:C:528:ASP:HB2	1.52	0.90
3:C:411:ARG:HB3	3:C:412:PRO:HD2	1.52	0.90
2:B:196:HIS:ND1	7:B:351:HOH:O	2.08	0.86
4:D:860:GLN:NE2	4:D:884:GLY:HA2	1.90	0.85
3:C:448:ALA:HB3	3:C:451:TRP:HB2	1.58	0.85
2:B:66:LEU:HD22	2:B:75:THR:O	1.77	0.84
4:D:860:GLN:HG3	4:D:884:GLY:N	1.94	0.82
4:D:860:GLN:HE21	4:D:884:GLY:HA2	1.45	0.82
4:D:830:LEU:HG	4:D:910:ARG:NH1	1.94	0.82
3:C:543:ARG:NH1	3:C:551:LEU:HD11	1.95	0.81
5:B:350:ZN:ZN	7:B:351:HOH:O	1.29	0.81
3:C:580:MET:HE3	3:C:627:VAL:HG11	1.62	0.81
4:D:921(A):THR:HB	4:D:924:LYS:HB2	1.63	0.81
4:D:881:VAL:CG2	4:D:930:ARG:HG2	2.13	0.78
3:C:410:SER:O	3:C:411:ARG:HB2	1.84	0.76
4:D:702:GLY:N	4:D:822:CYS:SG	2.58	0.76
4:D:731:ILE:HG13	4:D:766:VAL:HG13	1.68	0.75
4:D:843:ARG:HG2	4:D:843:ARG:HH11	1.53	0.74
4:D:772:ASN:OD1	4:D:775:VAL:HG23	1.89	0.73
2:B:74:ILE:O	2:B:78:THR:HG23	1.89	0.72
2:B:243:ILE:HD11	2:B:255:ILE:HD11	1.72	0.72
4:D:772:ASN:HA	4:D:853:ALA:O	1.89	0.71
1:A:62:GLN:HG3	3:C:499:VAL:HG11	1.73	0.71
3:C:510:ARG:HH11	3:C:510:ARG:HG2	1.55	0.71
1:A:14:ARG:HD2	1:A:51:PRO:HB2	1.73	0.70
3:C:411:ARG:HB3	3:C:412:PRO:CD	2.22	0.70
3:C:483:ILE:HG21	3:C:508:LEU:HB3	1.75	0.69
4:D:851:ILE:HG22	4:D:852:ALA:N	2.07	0.69
1:A:31:ASP:HB2	7:A:321:HOH:O	1.91	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:239:LYS:HD2	2:B:239:LYS:N	2.09	0.68
2:B:223:ALA:O	2:B:227:VAL:HG23	1.94	0.67
4:D:829:LEU:HD11	4:D:930:ARG:CZ	2.25	0.67
4:D:918:LEU:HD13	4:D:919:SER:OG	1.95	0.67
3:C:580:MET:HE3	3:C:627:VAL:CG1	2.25	0.67
3:C:603:ALA:HB2	3:C:608:GLN:HG3	1.78	0.66
2:B:71:ARG:HD2	7:B:364:HOH:O	1.95	0.66
2:B:198:TYR:HB2	2:B:273:ASP:H	1.58	0.66
3:C:546:TYR:HB2	3:C:591:CYS:HB3	1.79	0.65
3:C:481:GLN:NE2	3:C:518:VAL:HG21	2.12	0.65
1:A:62:GLN:OE1	3:C:457:HIS:CG	2.50	0.65
3:C:411:ARG:HH11	3:C:411:ARG:HG3	1.61	0.65
2:B:231:LYS:HG2	2:B:235:GLY:HA2	1.80	0.64
3:C:532:ASN:HB2	3:C:564:ASP:OD2	1.98	0.64
1:A:14:ARG:HD2	1:A:51:PRO:CB	2.28	0.64
3:C:534:ALA:HB3	3:C:562:VAL:HG13	1.80	0.64
4:D:935:ILE:HG22	4:D:939:ASN:ND2	2.11	0.64
4:D:881:VAL:HG22	4:D:930:ARG:HG2	1.80	0.63
4:D:881:VAL:HG23	4:D:930:ARG:HG2	1.78	0.63
2:B:199:SER:HB3	2:B:201:LEU:HG	1.81	0.63
4:D:783:VAL:HG21	4:D:808:LEU:HD13	1.81	0.63
2:B:224:LYS:O	2:B:228:GLU:HB2	1.99	0.62
2:B:73:TRP:HA	2:B:76:GLN:HE22	1.64	0.62
2:B:224:LYS:HD3	2:B:240:TYR:OH	1.99	0.62
4:D:771:ASN:ND2	4:D:855:LEU:HB3	2.14	0.62
2:B:205:PRO:HB2	2:B:213:ILE:HG21	1.81	0.61
2:B:227:VAL:HG13	2:B:238:TYR:HB2	1.82	0.61
2:B:4:THR:CG2	2:B:84:LYS:HE3	2.30	0.61
4:D:851:ILE:HG23	7:D:433:HOH:O	2.00	0.61
4:D:709:ASN:H	4:D:709:ASN:HD22	1.48	0.61
4:D:867:THR:O	4:D:870:GLN:HG3	2.01	0.60
3:C:634:PHE:O	3:C:638:ILE:HG13	2.01	0.60
4:D:757:HIS:NE2	4:D:895:SER:HB3	2.17	0.60
1:A:25:THR:HG21	1:A:71:HIS:CD2	2.37	0.59
2:B:73:TRP:HA	2:B:76:GLN:NE2	2.17	0.59
4:D:765:ARG:HD2	4:D:782:TYR:HB3	1.84	0.59
4:D:777:ASP:O	4:D:779:ALA:N	2.35	0.59
2:B:32:LEU:HD11	2:B:100:LEU:HD13	1.86	0.58
3:C:543:ARG:HH11	3:C:551:LEU:HD11	1.69	0.58
4:D:837:PHE:CE1	4:D:859:LEU:HB3	2.38	0.58
1:A:29:LEU:HD12	1:A:32:LEU:HD12	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:THR:HG23	2:B:84:LYS:HE3	1.86	0.58
4:D:736:LEU:HD13	4:D:738:TRP:CE2	2.39	0.58
2:B:62:ILE:HD12	2:B:191:ALA:HB3	1.85	0.58
4:D:879:THR:O	4:D:930:ARG:HB2	2.03	0.57
1:A:98:SER:HB2	4:D:761:ASN:CG	2.30	0.57
2:B:218:GLU:O	2:B:222:VAL:HG23	2.05	0.57
3:C:640:GLU:O	3:C:643:ALA:N	2.38	0.56
4:D:736(A):ARG:HH11	4:D:736(A):ARG:HG2	1.71	0.56
3:C:468:LEU:CD1	3:C:483:ILE:HD12	2.31	0.56
1:A:90:GLN:HA	1:A:90:GLN:HE21	1.70	0.56
2:B:284:SER:HB3	4:D:917(A):GLY:HA2	1.87	0.56
4:D:725:HIS:CD2	4:D:817:THR:HG21	2.40	0.56
3:C:543:ARG:HH11	3:C:543:ARG:HA	1.72	0.55
1:A:56:VAL:HG22	1:A:61:LEU:HD13	1.88	0.55
4:D:872:TRP:CD1	4:D:925:PRO:HD2	2.41	0.55
4:D:934:TYR:O	4:D:938:ILE:HG13	2.07	0.55
1:A:34(B):LEU:HD22	1:A:60:SER:HB3	1.89	0.55
4:D:731:ILE:HG13	4:D:766:VAL:CG1	2.37	0.55
3:C:435:TYR:O	3:C:438:PHE:HA	2.07	0.55
4:D:716:VAL:HG11	4:D:720:GLU:HG2	1.88	0.55
4:D:778:GLU:HB2	4:D:780:SER:OG	2.07	0.54
2:B:157:SER:O	2:B:166:HIS:ND1	2.41	0.54
4:D:705:ILE:HG12	4:D:705:ILE:O	2.07	0.54
3:C:481:GLN:HE21	3:C:518:VAL:HG21	1.72	0.54
1:A:74:ARG:HD2	7:A:479:HOH:O	2.08	0.54
2:B:127:ARG:NH1	2:B:142:ASP:OD2	2.41	0.54
2:B:291:GLN:O	2:B:294:TRP:HB3	2.07	0.54
3:C:416:VAL:HG12	3:C:418:ASN:ND2	2.23	0.54
3:C:564:ASP:OD1	3:C:567:HIS:HB2	2.07	0.54
4:D:775:VAL:HG12	4:D:776:GLU:N	2.23	0.54
4:D:883:ALA:O	4:D:925:PRO:HB3	2.08	0.54
3:C:566:GLU:H	3:C:566:GLU:CD	2.15	0.54
3:C:639:ASN:HB3	7:C:651:HOH:O	2.08	0.53
4:D:941:LYS:HD3	4:D:944:LEU:HD11	1.89	0.53
4:D:747:ILE:HA	4:D:820:VAL:HG13	1.89	0.53
1:A:12:VAL:HA	1:A:54:VAL:O	2.08	0.53
3:C:636:ASP:HB2	7:C:736:HOH:O	2.09	0.53
4:D:721:ASP:HA	4:D:856:GLN:OE1	2.08	0.53
2:B:146:ASN:HA	2:B:151:PHE:HE2	1.74	0.52
3:C:468:LEU:O	3:C:480:GLU:HA	2.09	0.52
4:D:842:GLY:HA2	4:D:891:CYS:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:729:TRP:CG	4:D:821:ALA:HB2	2.45	0.52
3:C:560:LEU:HD22	3:C:584:GLY:HA3	1.92	0.52
4:D:830:LEU:HG	4:D:910:ARG:HH12	1.71	0.52
4:D:849:GLY:O	4:D:851:ILE:N	2.42	0.52
4:D:831:PRO:HG2	4:D:834:TYR:HB2	1.92	0.52
3:C:462:SER:C	3:C:462(A):ARG:HG2	2.34	0.52
3:C:432:SER:O	3:C:466:VAL:HA	2.10	0.52
4:D:736(C):ASN:O	4:D:736(C):ASN:ND2	2.43	0.52
1:A:97:GLN:O	4:D:760:SER:HB3	2.10	0.51
3:C:538:ILE:HG21	3:C:560:LEU:HD12	1.90	0.51
2:B:287:ILE:HB	2:B:288:PRO:HD3	1.92	0.51
4:D:822:CYS:O	4:D:908:ASP:HA	2.10	0.51
1:A:29:LEU:HD21	1:A:64:VAL:HG13	1.93	0.51
4:D:811:THR:HA	7:D:435:HOH:O	2.10	0.51
4:D:870(B):ASP:HB2	4:D:923:LYS:NZ	2.25	0.51
4:D:824:PRO:HB3	4:D:910:ARG:NH2	2.25	0.51
4:D:860:GLN:HG3	4:D:884:GLY:CA	2.41	0.51
4:D:888:VAL:O	4:D:888:VAL:HG13	2.11	0.51
1:A:39:ARG:HB3	1:A:53:ASP:H	1.76	0.51
2:B:272:ARG:HE	2:B:285:GLN:NE2	2.09	0.51
4:D:705:ILE:HG21	4:D:816:ASP:OD2	2.11	0.51
4:D:770:LYS:HA	4:D:778:GLU:OE1	2.10	0.51
4:D:843:ARG:HG2	4:D:843:ARG:NH1	2.23	0.51
2:B:186:HIS:CE1	2:B:188:ASN:HB3	2.46	0.50
4:D:910:ARG:HH11	4:D:910:ARG:CG	2.24	0.50
4:D:941:LYS:HD3	4:D:944:LEU:CD1	2.40	0.50
4:D:885:GLY:O	4:D:887:GLY:N	2.44	0.50
2:B:51:LYS:HD2	2:B:106:PHE:CE1	2.46	0.50
4:D:828:SER:CB	4:D:910:ARG:HH22	2.25	0.50
3:C:574:ILE:HA	7:C:737:HOH:O	2.10	0.50
4:D:828:SER:O	4:D:829:LEU:HD12	2.11	0.50
4:D:843:ARG:O	4:D:843:ARG:HG3	2.11	0.50
2:B:288:PRO:O	2:B:292:GLU:HG2	2.12	0.50
4:D:851:ILE:HG22	4:D:852:ALA:H	1.77	0.50
2:B:186:HIS:HE1	2:B:188:ASN:HB3	1.76	0.49
4:D:746:LEU:HD22	4:D:748:THR:O	2.11	0.49
2:B:297:VAL:HG12	2:B:301:MET:HE2	1.95	0.49
2:B:208:TYR:O	2:B:249:GLN:HG3	2.12	0.49
4:D:840:GLY:HA3	4:D:893:GLY:HA2	1.93	0.49
3:C:534:ALA:O	3:C:561:PRO:HA	2.12	0.49
1:A:36:ASP:HB3	1:A:55:ARG:HB3	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:TRP:HH2	2:B:280:LEU:HD12	1.77	0.49
3:C:576:VAL:HA	3:C:580:MET:HE1	1.95	0.49
4:D:757:HIS:C	4:D:757:HIS:CD2	2.90	0.49
4:D:781:LEU:HD23	4:D:783:VAL:CG1	2.43	0.49
3:C:510:ARG:HG2	3:C:510:ARG:NH1	2.27	0.48
4:D:901:CYS:O	4:D:907:TRP:HA	2.12	0.48
4:D:838:VAL:O	4:D:892:ASN:ND2	2.46	0.48
2:B:2:ARG:NH1	2:B:2:ARG:HB3	2.29	0.48
4:D:724:PRO:O	4:D:725:HIS:HB2	2.13	0.48
4:D:812:VAL:O	4:D:814:LEU:N	2.46	0.48
3:C:604:ALA:O	3:C:605:ASP:HB2	2.14	0.48
4:D:885:GLY:C	4:D:887:GLY:H	2.21	0.48
2:B:203:LEU:HA	2:B:241:GLY:O	2.13	0.48
4:D:918:LEU:HB2	7:D:376:HOH:O	2.13	0.48
1:A:8:VAL:HG13	3:C:462(A):ARG:CD	2.44	0.48
4:D:748:THR:C	4:D:750:ASN:H	2.21	0.48
2:B:203:LEU:HD11	2:B:247:ILE:HD11	1.95	0.48
4:D:870:GLN:NE2	4:D:871:TRP:CD1	2.82	0.48
2:B:198:TYR:O	2:B:199:SER:CB	2.62	0.48
2:B:292:GLU:HG3	2:B:293:THR:N	2.29	0.48
3:C:436:GLU:HB2	3:C:463:THR:HB	1.96	0.48
3:C:560:LEU:HB3	3:C:583:ALA:HB1	1.95	0.48
4:D:838:VAL:O	4:D:838:VAL:HG23	2.14	0.48
2:B:161:CYS:HB2	7:B:481:HOH:O	2.13	0.47
4:D:701:CYS:O	4:D:703:ALA:N	2.47	0.47
4:D:827:GLY:O	4:D:829:LEU:HD13	2.13	0.47
2:B:272:ARG:HE	2:B:285:GLN:HE21	1.62	0.47
4:D:719:GLY:O	4:D:856:GLN:NE2	2.48	0.47
2:B:45:ARG:NH1	2:B:114:ASP:OD1	2.46	0.47
4:D:731:ILE:HG12	4:D:732:SER:N	2.29	0.47
4:D:851:ILE:O	4:D:852:ALA:CB	2.62	0.47
4:D:800:ARG:CZ	4:D:877:LYS:HE3	2.45	0.47
4:D:846:TYR:HD1	4:D:846:TYR:H	1.61	0.47
2:B:114:ASP:HB3	2:B:130:ARG:HG3	1.95	0.47
2:B:211:GLN:NE2	2:B:212:SER:O	2.47	0.47
4:D:748:THR:OG1	4:D:751:HIS:HB2	2.15	0.47
4:D:750:ASN:O	4:D:751:HIS:ND1	2.48	0.47
3:C:525:PRO:CG	3:C:528:ASP:HB2	2.35	0.46
3:C:530:LEU:HD13	3:C:562:VAL:HG11	1.96	0.46
4:D:735:TYR:HB2	4:D:762(A):LEU:HD12	1.96	0.46
4:D:860:GLN:NE2	4:D:860:GLN:HA	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:888:VAL:O	4:D:888(A):ILE:HB	2.14	0.46
1:A:98:SER:HB2	4:D:761:ASN:ND2	2.30	0.46
3:C:482:VAL:HG23	3:C:482:VAL:O	2.15	0.46
4:D:888:VAL:C	4:D:889:SER:H	2.24	0.46
1:A:64:VAL:O	1:A:67:PHE:HB3	2.16	0.46
2:B:103:MET:HE1	2:B:304:THR:CG2	2.45	0.46
4:D:747:ILE:HG13	4:D:748:THR:HG23	1.97	0.46
1:A:38:TRP:CH2	2:B:280:LEU:HD12	2.51	0.46
3:C:495:ASN:O	3:C:497:ASN:N	2.49	0.46
3:C:528:ASP:O	3:C:529:ILE:HG13	2.15	0.46
4:D:871:TRP:CE2	4:D:923:LYS:HG3	2.51	0.46
1:A:11:GLN:HG2	1:A:80:GLU:O	2.16	0.46
4:D:864:ASP:OD1	4:D:866:ALA:HB3	2.16	0.45
2:B:85:LYS:HE3	2:B:89:ASP:OD2	2.16	0.45
3:C:521:ALA:HB1	3:C:609:VAL:HG23	1.97	0.45
4:D:734:GLN:OE1	4:D:765:ARG:NH2	2.41	0.45
3:C:538:ILE:CG2	3:C:560:LEU:HD12	2.47	0.45
1:A:78:MET:HE3	1:A:78:MET:HA	1.98	0.45
1:A:4:LYS:NZ	1:A:4:LYS:HB3	2.31	0.45
3:C:546:TYR:HD1	3:C:547:THR:N	2.15	0.45
2:B:204:TYR:O	2:B:242:SER:HA	2.17	0.45
4:D:829:LEU:HD12	4:D:829:LEU:HA	1.76	0.45
3:C:630:ARG:NH1	3:C:632:SER:OG	2.46	0.45
4:D:808:LEU:HD12	4:D:812:VAL:HG21	1.99	0.45
4:D:830:LEU:HG	4:D:910:ARG:HH11	1.76	0.45
4:D:900:ASN:C	4:D:901:CYS:SG	2.99	0.45
3:C:431:VAL:HG22	3:C:468:LEU:HD23	1.99	0.45
3:C:571:TRP:HA	3:C:623:LYS:O	2.16	0.45
4:D:791:HIS:HD1	4:D:937:TRP:NE1	2.15	0.45
2:B:287:ILE:O	2:B:290:ALA:HB3	2.17	0.45
3:C:567:HIS:O	3:C:570:GLN:HG2	2.17	0.45
4:D:851:ILE:O	4:D:852:ALA:HB2	2.17	0.45
1:A:76:ARG:HE	1:A:76:ARG:HB2	1.55	0.45
3:C:491:HIS:HD2	3:C:493:LEU:HB2	1.81	0.44
4:D:768:LEU:O	4:D:780:SER:HA	2.17	0.44
4:D:930:ARG:NH1	4:D:930:ARG:HG3	2.32	0.44
4:D:830:LEU:HD22	4:D:831:PRO:HD2	1.99	0.44
4:D:867:THR:HG23	4:D:870:GLN:NE2	2.32	0.44
4:D:930:ARG:HG3	4:D:930:ARG:HH11	1.81	0.44
1:A:39:ARG:O	1:A:52:ILE:HA	2.17	0.44
3:C:546:TYR:CD1	3:C:546:TYR:C	2.95	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:870(B):ASP:HB2	4:D:923:LYS:HZ2	1.81	0.44
4:D:729:TRP:O	4:D:745:THR:HA	2.17	0.44
3:C:433:LEU:O	3:C:441:THR:HG22	2.16	0.44
4:D:860:GLN:HG3	4:D:884:GLY:H	1.80	0.44
2:B:208:TYR:HD1	2:B:256:ASP:OD2	2.00	0.44
2:B:273:ASP:HB2	2:B:281:LEU:HD13	1.99	0.44
4:D:738:TRP:HD1	7:D:247:HOH:O	2.01	0.44
3:C:495:ASN:C	3:C:497:ASN:H	2.26	0.44
4:D:710:LEU:HG	4:D:711:SER:H	1.83	0.44
1:A:94:PHE:CZ	4:D:736(A):ARG:HG3	2.53	0.43
1:A:94:PHE:O	1:A:97:GLN:HG2	2.17	0.43
4:D:757:HIS:HE1	4:D:914:SER:O	2.01	0.43
4:D:861:PRO:O	4:D:862:VAL:C	2.60	0.43
2:B:233:LEU:HD12	2:B:233:LEU:HA	1.79	0.43
3:C:570(A):TYR:CD1	3:C:570(A):TYR:C	2.94	0.43
3:C:421:ASP:HB3	3:C:471:TYR:OH	2.18	0.43
3:C:521:ALA:HB1	3:C:609:VAL:CG2	2.48	0.43
3:C:562:VAL:HG23	3:C:563:VAL:N	2.33	0.43
4:D:709:ASN:HD22	4:D:709:ASN:N	2.12	0.43
4:D:910:ARG:HH11	4:D:910:ARG:HG2	1.83	0.43
2:B:80:VAL:O	2:B:83:ALA:HB3	2.18	0.43
4:D:832:GLN:O	4:D:833:ASP:HB2	2.18	0.43
3:C:411:ARG:N	3:C:411:ARG:CZ	2.82	0.43
2:B:295:LEU:HD12	2:B:295:LEU:HA	1.82	0.43
4:D:851:ILE:CG2	4:D:852:ALA:N	2.77	0.43
3:C:534:ALA:HB3	3:C:562:VAL:CG1	2.48	0.43
4:D:828:SER:HB3	4:D:910:ARG:HH22	1.84	0.43
2:B:144:ASN:HD21	2:B:254:SER:H	1.66	0.42
4:D:748:THR:O	4:D:750:ASN:N	2.52	0.42
2:B:203:LEU:CD1	2:B:247:ILE:HD11	2.49	0.42
3:C:522:ASN:O	3:C:608:GLN:HA	2.19	0.42
4:D:718:GLY:O	4:D:720:GLU:N	2.52	0.42
2:B:273:ASP:CG	2:B:274:THR:N	2.78	0.42
3:C:503:ILE:HG12	3:C:504:ALA:N	2.35	0.42
1:A:85:LEU:HA	1:A:85:LEU:HD23	1.67	0.42
4:D:785:VAL:HG13	4:D:806:ILE:HG23	2.01	0.42
4:D:791:HIS:HE1	7:D:292:HOH:O	2.02	0.42
4:D:808:LEU:CD1	4:D:812:VAL:HG21	2.48	0.42
1:A:6:ASP:HA	3:C:436(A):LYS:HE3	2.00	0.42
1:A:56:VAL:HG22	1:A:61:LEU:CD1	2.49	0.42
4:D:875:THR:HG22	4:D:915:PHE:HZ	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:ASN:HB3	7:B:477:HOH:O	2.20	0.42
4:D:773:LEU:HD13	4:D:841:TRP:CE2	2.55	0.42
4:D:861:PRO:HD2	4:D:884:GLY:H	1.85	0.42
1:A:36:ASP:OD1	2:B:71:ARG:NH2	2.51	0.42
2:B:103:MET:HE1	2:B:304:THR:HG22	2.01	0.42
4:D:870:GLN:HB2	4:D:871:TRP:CD1	2.55	0.42
4:D:750:ASN:O	4:D:751:HIS:CG	2.73	0.41
4:D:791:HIS:HA	4:D:937:TRP:CZ2	2.55	0.41
2:B:205:PRO:O	2:B:242:SER:HB2	2.20	0.41
3:C:621:ASN:C	3:C:621:ASN:HD22	2.28	0.41
4:D:832:GLN:HB2	4:D:864:ASP:HB3	2.01	0.41
4:D:935:ILE:O	4:D:939:ASN:ND2	2.53	0.41
3:C:429:TRP:HB3	3:C:519:GLN:O	2.20	0.41
2:B:24:LEU:HD23	2:B:24:LEU:HA	1.76	0.41
4:D:721:ASP:O	4:D:722:ALA:HB2	2.20	0.41
4:D:924:LYS:N	4:D:925:PRO:HD3	2.35	0.41
2:B:205:PRO:HA	2:B:206:TYR:HA	1.87	0.41
3:C:551:LEU:HA	3:C:552:PRO:HD3	1.94	0.41
4:D:723:ILE:O	4:D:724:PRO:C	2.64	0.41
3:C:434:GLN:HB3	3:C:438:PHE:HB3	2.03	0.41
3:C:640:GLU:O	3:C:641:THR:C	2.63	0.41
4:D:878:GLU:O	4:D:930:ARG:NH1	2.54	0.41
2:B:84:LYS:O	2:B:85:LYS:C	2.64	0.41
3:C:630:ARG:HG2	3:C:630:ARG:HH11	1.86	0.41
2:B:95:SER:HB3	2:B:302:GLU:OE2	2.21	0.41
2:B:156:ALA:HB1	2:B:166:HIS:HB3	2.02	0.41
3:C:447:ILE:C	3:C:447:ILE:HD12	2.46	0.41
3:C:573:GLY:O	3:C:576:VAL:HG12	2.21	0.41
2:B:59:ARG:C	2:B:188:ASN:HD22	2.28	0.41
2:B:160:PRO:HA	2:B:165:TYR:CD2	2.56	0.41
2:B:168:LYS:HG3	2:B:169:TYR:CE1	2.55	0.41
3:C:411:ARG:HG3	3:C:411:ARG:NH1	2.32	0.41
3:C:528:ASP:C	3:C:529:ILE:HG13	2.46	0.41
3:C:570(A):TYR:CZ	3:C:570(B):ASP:HB3	2.56	0.41
4:D:725:HIS:HD2	4:D:817:THR:HG21	1.83	0.41
4:D:736(A):ARG:HH11	4:D:736(A):ARG:CG	2.33	0.41
4:D:911:GLY:HA2	4:D:929:THR:O	2.21	0.41
1:A:5:GLU:HG3	2:B:123:ASN:CG	2.46	0.41
1:A:65:LYS:O	1:A:68:LEU:HB2	2.21	0.41
3:C:609:VAL:O	3:C:631:VAL:HG11	2.20	0.41
4:D:783:VAL:HG11	4:D:812:VAL:HG22	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:PHE:CE1	4:D:736(A):ARG:HG3	2.56	0.40
2:B:31:GLN:CD	2:B:31:GLN:H	2.29	0.40
2:B:66:LEU:HD23	2:B:195:ILE:HB	2.03	0.40
2:B:264:LYS:HB2	2:B:264:LYS:NZ	2.36	0.40
3:C:434:GLN:HG2	3:C:440:HIS:HA	2.02	0.40
4:D:874:THR:O	4:D:875:THR:C	2.63	0.40
1:A:19:ASP:O	1:A:22:GLU:N	2.55	0.40
3:C:530:LEU:HG	3:C:610:HIS:CD2	2.57	0.40
3:C:446:LEU:HD13	3:C:468:LEU:CD2	2.51	0.40
3:C:612:VAL:O	3:C:612:VAL:HG12	2.20	0.40
4:D:746:LEU:HG	4:D:768:LEU:HD21	2.03	0.40
4:D:899:LEU:HB3	4:D:911:GLY:N	2.37	0.40
4:D:766:VAL:O	4:D:782:TYR:HA	2.21	0.40
4:D:792:GLU:CD	4:D:792:GLU:H	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	92/94 (98%)	87 (95%)	4 (4%)	1 (1%)	11	11
2	B	307/309 (99%)	281 (92%)	23 (8%)	3 (1%)	12	12
3	C	246/253 (97%)	215 (87%)	25 (10%)	6 (2%)	4	3
4	D	249/251 (99%)	179 (72%)	42 (17%)	28 (11%)	0	0
All	All	894/907 (99%)	762 (85%)	94 (10%)	38 (4%)	2	1

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	199	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	411	ARG
3	C	605	ASP
4	D	702	GLY
4	D	721	ASP
4	D	778	GLU
4	D	813	GLU
4	D	830	LEU
4	D	843	ARG
4	D	850	PRO
4	D	851	ILE
4	D	852	ALA
4	D	886	ASP
4	D	888	VAL
2	B	271	LEU
3	C	496	SER
3	C	570(A)	TYR
3	C	573	GLY
4	D	719	GLY
4	D	847	THR
4	D	887	GLY
4	D	888(A)	ILE
3	C	486(A)	ALA
4	D	708	PRO
4	D	808	LEU
4	D	921	ASN
1	A	20	GLU
2	B	205	PRO
4	D	736(B)	ASP
4	D	750	ASN
4	D	779	ALA
4	D	724	PRO
4	D	812	VAL
4	D	889	SER
4	D	720	GLU
4	D	722	ALA
4	D	749	PRO
4	D	873	GLY

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	83/83 (100%)	71 (86%)	12 (14%)	3	2
2	B	266/266 (100%)	241 (91%)	25 (9%)	8	8
3	C	205/210 (98%)	174 (85%)	31 (15%)	3	2
4	D	209/209 (100%)	174 (83%)	35 (17%)	2	2
All	All	763/768 (99%)	660 (86%)	103 (14%)	4	3

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	20	GLU
1	A	35	LEU
1	A	56	VAL
1	A	60	SER
1	A	62	GLN
1	A	68	LEU
1	A	76	ARG
1	A	86	LEU
1	A	90	GLN
1	A	91	GLU
1	A	99	ARG
2	B	4	THR
2	B	15	LEU
2	B	31	GLN
2	B	33	VAL
2	B	34	SER
2	B	50	LEU
2	B	59	ARG
2	B	71	ARG
2	B	76	GLN
2	B	84	LYS
2	B	95	SER
2	B	125	LEU
2	B	131	SER
2	B	133	THR
2	B	141	VAL
2	B	197	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	210	THR
2	B	211	GLN
2	B	221	GLN
2	B	248	TYR
2	B	264	LYS
2	B	272	ARG
2	B	288	PRO
2	B	295	LEU
2	B	298	LEU
3	C	411	ARG
3	C	413	SER
3	C	418	ASN
3	C	431	VAL
3	C	450	ASP
3	C	460	SER
3	C	466	VAL
3	C	468	LEU
3	C	488	LEU
3	C	496	SER
3	C	497	ASN
3	C	506	VAL
3	C	510	ARG
3	C	522	ASN
3	C	543	ARG
3	C	562	VAL
3	C	566	GLU
3	C	567	HIS
3	C	570	GLN
3	C	570(A)	TYR
3	C	570(B)	ASP
3	C	574	ILE
3	C	578	LYS
3	C	579	THR
3	C	588	ARG
3	C	621	ASN
3	C	621(A)	THR
3	C	631	VAL
3	C	639	ASN
3	C	640	GLU
3	C	644	SER
4	D	709	ASN
4	D	720	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	731	ILE
4	D	737	THR
4	D	740	HIS
4	D	741	THR
4	D	746	LEU
4	D	750	ASN
4	D	752	VAL
4	D	773	LEU
4	D	777	ASP
4	D	780	SER
4	D	781	LEU
4	D	796	SER
4	D	799	VAL
4	D	811	THR
4	D	814	LEU
4	D	819	GLN
4	D	829	LEU
4	D	832	GLN
4	D	846	TYR
4	D	850	PRO
4	D	857	GLN
4	D	859	LEU
4	D	860	GLN
4	D	868	CYS
4	D	874	THR
4	D	879	THR
4	D	891	CYS
4	D	904	ASP
4	D	909	VAL
4	D	910	ARG
4	D	918	LEU
4	D	923	LYS
4	D	930	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	90	GLN
2	B	76	GLN
2	B	122	GLN
2	B	144	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	166	HIS
2	B	188	ASN
2	B	211	GLN
2	B	220	ASN
2	B	285	GLN
3	C	418	ASN
3	C	434	GLN
3	C	495	ASN
3	C	570	GLN
3	C	608	GLN
3	C	610	HIS
3	C	639	ASN
4	D	709	ASN
4	D	725	HIS
4	D	736(C)	ASN
4	D	771	ASN
4	D	832	GLN
4	D	856	GLN
4	D	857	GLN
4	D	870	GLN
4	D	939	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.