Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 09:58 AM EDT

PDB ID	:	3B2Z
Title	:	Crystal Structure of ADAMTS4 (apo form)
Authors	:	Mosyak, L.; Stahl, M.; Somers, W.
Deposited on	:	2007-10-19
Resolution	:	2.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

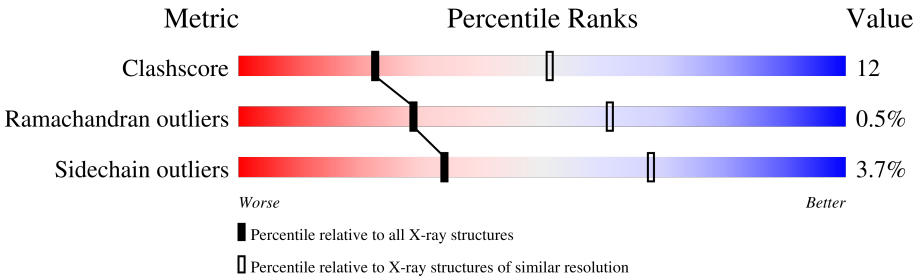
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	316	71% 21% • 8%
1	B	316	74% 16% • 9%
1	C	316	68% 22% • 9%
1	D	316	64% 26% • 9%
1	E	316	67% 21% • 11%
1	F	316	72% 19% • 7%
1	G	316	73% 18% • 8%
1	H	316	67% 20% • 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17609 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 ADAMTS-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2176	1359	386	407	24			
1	B	287	Total	C	N	O	S	0	0	0
			2158	1351	384	399	24			
1	C	289	Total	C	N	O	S	0	0	0
			2166	1353	383	406	24			
1	D	287	Total	C	N	O	S	0	0	0
			2158	1351	384	399	24			
1	E	282	Total	C	N	O	S	0	0	0
			2131	1335	381	390	25			
1	F	293	Total	C	N	O	S	0	0	0
			2195	1371	390	410	24			
1	G	291	Total	C	N	O	S	0	0	0
			2180	1361	387	408	24			
1	H	281	Total	C	N	O	S	0	0	0
			2122	1328	380	390	24			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	362	GLN	GLU	engineered mutation	UNP O75173
A	521	ASP	-	expression tag	UNP O75173
A	522	TYR	-	expression tag	UNP O75173
A	523	LYS	-	expression tag	UNP O75173
A	524	ASP	-	expression tag	UNP O75173
A	525	ASP	-	expression tag	UNP O75173
A	526	ASP	-	expression tag	UNP O75173
A	527	ASP	-	expression tag	UNP O75173
A	528	LYS	-	expression tag	UNP O75173
A	362	GLN	GLU	engineered mutation	UNP O75173
A	521	ASP	-	expression tag	UNP O75173
A	522	TYR	-	expression tag	UNP O75173
A	523	LYS	-	expression tag	UNP O75173

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Chain	Residue	Modelled	Actual	Comment	Reference
A	524	ASP	-	expression tag	UNP O75173
A	525	ASP	-	expression tag	UNP O75173
A	526	ASP	-	expression tag	UNP O75173
A	527	ASP	-	expression tag	UNP O75173
A	528	LYS	-	expression tag	UNP O75173
A	362	GLN	GLU	engineered mutation	UNP O75173
A	521	ASP	-	expression tag	UNP O75173
A	522	TYR	-	expression tag	UNP O75173
A	523	LYS	-	expression tag	UNP O75173
A	524	ASP	-	expression tag	UNP O75173
A	525	ASP	-	expression tag	UNP O75173
A	526	ASP	-	expression tag	UNP O75173
A	527	ASP	-	expression tag	UNP O75173
A	528	LYS	-	expression tag	UNP O75173
A	362	GLN	GLU	engineered mutation	UNP O75173
A	521	ASP	-	expression tag	UNP O75173
A	522	TYR	-	expression tag	UNP O75173
A	523	LYS	-	expression tag	UNP O75173
A	524	ASP	-	expression tag	UNP O75173
A	525	ASP	-	expression tag	UNP O75173
A	526	ASP	-	expression tag	UNP O75173
A	527	ASP	-	expression tag	UNP O75173
A	528	LYS	-	expression tag	UNP O75173
A	362	GLN	GLU	engineered mutation	UNP O75173
A	521	ASP	-	expression tag	UNP O75173
A	522	TYR	-	expression tag	UNP O75173
A	523	LYS	-	expression tag	UNP O75173
A	524	ASP	-	expression tag	UNP O75173
A	525	ASP	-	expression tag	UNP O75173
A	526	ASP	-	expression tag	UNP O75173
A	527	ASP	-	expression tag	UNP O75173
A	528	LYS	-	expression tag	UNP O75173
A	362	GLN	GLU	engineered mutation	UNP O75173
A	521	ASP	-	expression tag	UNP O75173
A	522	TYR	-	expression tag	UNP O75173
A	523	LYS	-	expression tag	UNP O75173
A	524	ASP	-	expression tag	UNP O75173
A	525	ASP	-	expression tag	UNP O75173
A	526	ASP	-	expression tag	UNP O75173
A	527	ASP	-	expression tag	UNP O75173
A	528	LYS	-	expression tag	UNP O75173
A	362	GLN	GLU	engineered mutation	UNP O75173

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Chain	Residue	Modelled	Actual	Comment	Reference
A	521	ASP	-	expression tag	UNP O75173
A	522	TYR	-	expression tag	UNP O75173
A	523	LYS	-	expression tag	UNP O75173
A	524	ASP	-	expression tag	UNP O75173
A	525	ASP	-	expression tag	UNP O75173
A	526	ASP	-	expression tag	UNP O75173
A	527	ASP	-	expression tag	UNP O75173
A	528	LYS	-	expression tag	UNP O75173
A	362	GLN	GLU	engineered mutation	UNP O75173
A	521	ASP	-	expression tag	UNP O75173
A	522	TYR	-	expression tag	UNP O75173
A	523	LYS	-	expression tag	UNP O75173
A	524	ASP	-	expression tag	UNP O75173
A	525	ASP	-	expression tag	UNP O75173
A	526	ASP	-	expression tag	UNP O75173
A	527	ASP	-	expression tag	UNP O75173
A	528	LYS	-	expression tag	UNP O75173

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0
2	G	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Ca 2 2	0	0
3	B	2	Total Ca 2 2	0	0
3	C	2	Total Ca 2 2	0	0
3	D	2	Total Ca 2 2	0	0
3	E	2	Total Ca 2 2	0	0
3	F	2	Total Ca 2 2	0	0
3	G	2	Total Ca 2 2	0	0
3	H	2	Total Ca 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	51	Total O 51 51	0	0
4	B	37	Total O 37 37	0	0
4	C	36	Total O 36 36	0	0
4	D	63	Total O 63 63	0	0
4	E	22	Total O 22 22	0	0
4	F	26	Total O 26 26	0	0
4	G	28	Total O 28 28	0	0
4	H	36	Total O 36 36	0	0

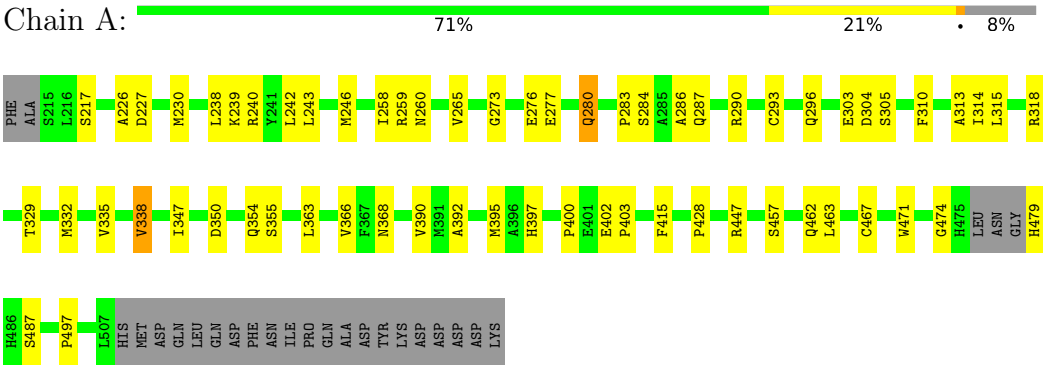
3 Residue-property plots (i)

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

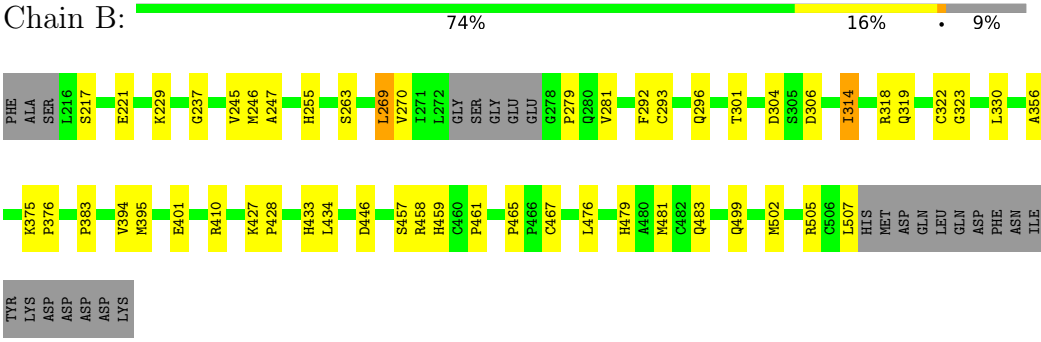
• Molecule 1: ADAMTS-4

Chain A:



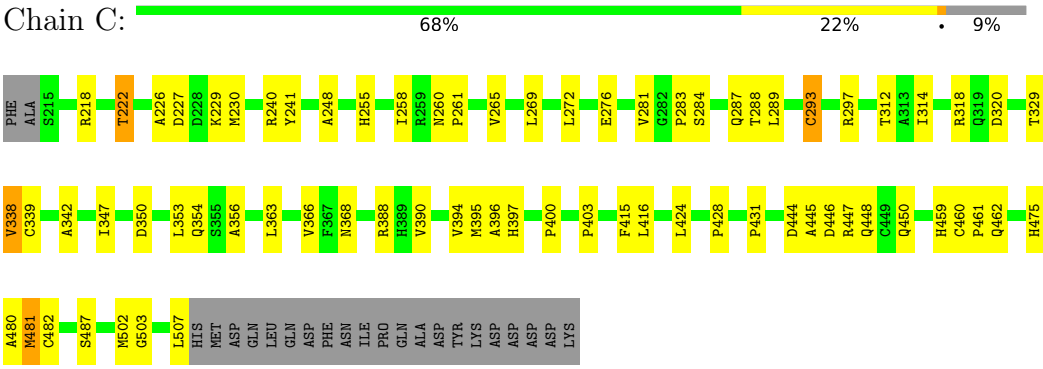
• Molecule 1: ADAMTS-4

Chain B:



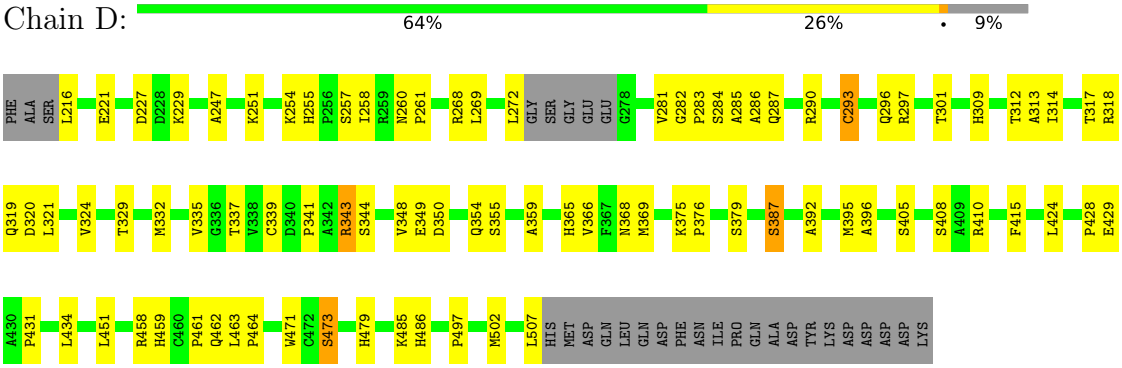
• Molecule 1: ADAMTS-4

Chain C:



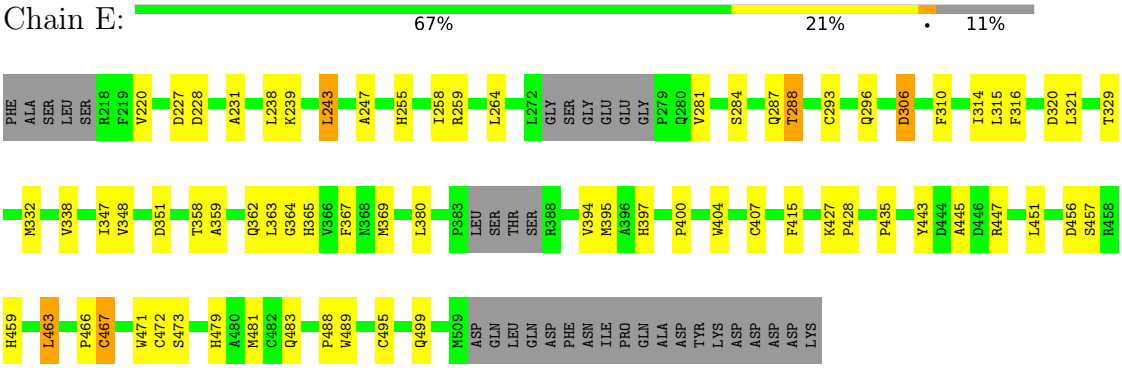
• Molecule 1: ADAMTS-4

Chain D:



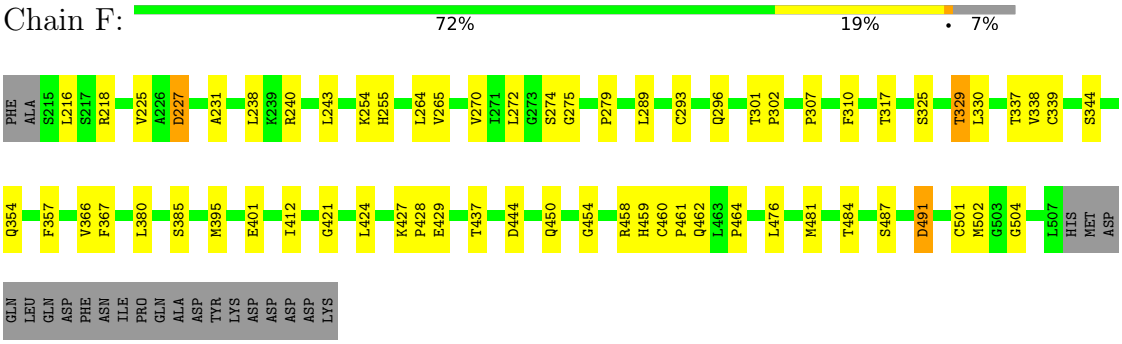
• Molecule 1: ADAMTS-4

Chain E:



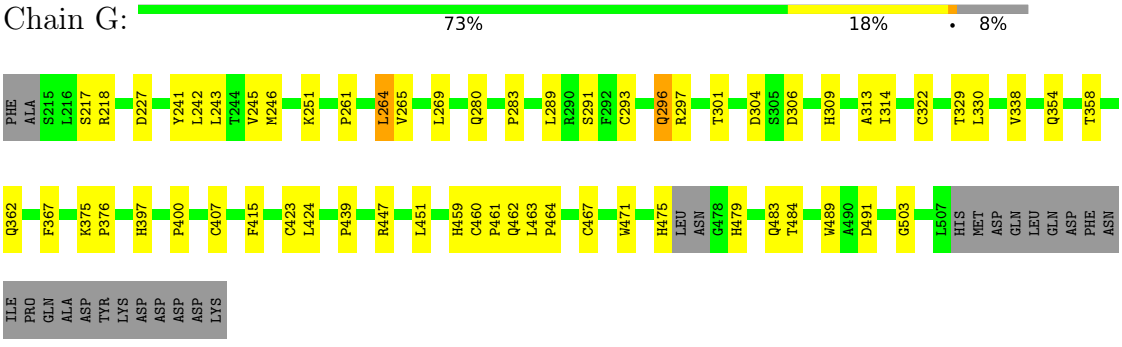
• Molecule 1: ADAMTS-4

Chain F:



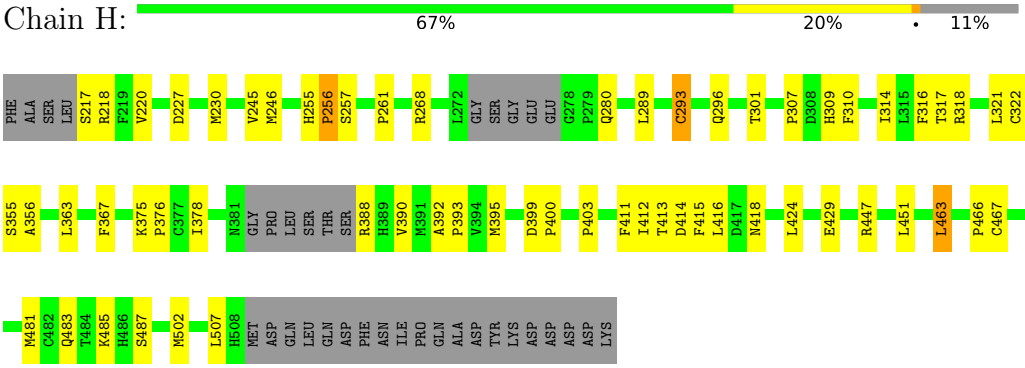
• Molecule 1: ADAMTS-4

Chain G:



• Molecule 1: ADAMTS-4

Chain H:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	128.33Å 84.31Å 150.15Å 90.00° 112.23° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80	Depositor
% Data completeness (in resolution range)	98.6 (50.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.254 , 0.312	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17609	wwPDB-VP
Average B, all atoms (Å^2)	41.0	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	0.49	0/2236	0.61	0/3049
1	B	0.49	0/2218	0.57	1/3026 (0.0%)
1	C	0.43	0/2225	0.60	0/3034
1	D	0.53	0/2218	0.64	1/3026 (0.0%)
1	E	0.61	0/2191	0.69	1/2986 (0.0%)
1	F	0.45	0/2256	0.58	0/3078
1	G	0.48	0/2240	0.60	0/3054
1	H	0.47	2/2181 (0.1%)	0.58	0/2973
All	All	0.49	2/17765 (0.0%)	0.61	3/24226 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	418	ASN	CG-OD1	5.41	1.35	1.24
1	H	280	GLN	CD-OE1	5.08	1.35	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	269	LEU	CA-CB-CG	5.82	128.69	115.30
1	E	264	LEU	CA-CB-CG	5.30	127.50	115.30
1	D	269	LEU	CA-CB-CG	5.21	127.28	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2176	0	2075	54	0
1	B	2158	0	2067	34	0
1	C	2166	0	2068	60	0
1	D	2158	0	2067	76	0
1	E	2131	0	2036	44	0
1	F	2195	0	2093	38	0
1	G	2180	0	2078	45	0
1	H	2122	0	2024	54	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
4	A	51	0	0	23	0
4	B	37	0	0	11	0
4	C	36	0	0	13	0
4	D	63	0	0	37	0
4	E	22	0	0	8	0
4	F	26	0	0	6	0
4	G	28	0	0	9	0
4	H	36	0	0	19	0
All	All	17609	0	16508	391	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 12.

All (391) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:MET:HB3	1:C:396:ALA:HB2	1.31	1.09
1:E:259:ARG:HG2	4:E:517:HOH:O	1.52	1.08
1:E:488:PRO:O	4:E:525:HOH:O	1.76	1.03
1:C:320:ASP:HB3	4:C:527:HOH:O	1.57	1.03
1:D:332:MET:CE	4:D:545:HOH:O	2.08	1.01
1:A:259:ARG:HG2	4:A:553:HOH:O	1.66	0.95
1:A:479:HIS:HB2	4:A:554:HOH:O	1.66	0.94
1:D:332:MET:HE2	4:D:545:HOH:O	1.65	0.94
1:A:283:PRO:HD2	1:A:287:GLN:OE1	1.69	0.92
1:A:303:GLU:HG3	4:A:530:HOH:O	1.74	0.87
1:B:410:ARG:HD2	4:B:523:HOH:O	1.74	0.86
1:D:251:LYS:HB2	4:D:563:HOH:O	1.74	0.86
1:H:322:CYS:HB2	4:H:537:HOH:O	1.76	0.85
1:D:297:ARG:HD2	4:D:517:HOH:O	1.79	0.82
1:F:338:VAL:HG22	1:F:366:VAL:HG12	1.62	0.81
1:H:392:ALA:CB	4:H:529:HOH:O	2.28	0.81
1:B:458:ARG:HD2	4:B:534:HOH:O	1.80	0.80
1:E:284:SER:OG	1:E:287:GLN:HB2	1.82	0.79
1:F:274:SER:N	1:F:275:GLY:HA3	1.99	0.77
1:D:355:SER:HB2	4:D:523:HOH:O	1.82	0.77
1:E:400:PRO:HG2	4:E:516:HOH:O	1.84	0.77
1:H:476:LEU:HG	1:H:477:ASN:H	1.50	0.76
1:E:364:GLY:O	1:E:369:MET:HB2	1.84	0.76
1:E:329:THR:HG21	1:E:395:MET:HB2	1.67	0.75
1:B:237:GLY:HA2	4:B:513:HOH:O	1.87	0.74
1:D:261:PRO:HA	4:D:565:HOH:O	1.86	0.74
1:E:338:VAL:HG23	1:E:415:PHE:HE1	1.52	0.74
1:A:497:PRO:HD2	4:A:546:HOH:O	1.87	0.73
1:H:388:ARG:N	4:H:529:HOH:O	2.20	0.73
1:E:320:ASP:HB3	4:E:521:HOH:O	1.88	0.72
1:C:354:GLN:HG2	1:C:487:SER:OG	1.88	0.72
1:C:502:MET:HB2	1:C:507:LEU:HD12	1.69	0.72
1:A:322:CYS:HB2	4:A:550:HOH:O	1.88	0.72
1:E:296:GLN:HE21	1:E:310:PHE:HE1	1.38	0.72
1:A:315:LEU:HD23	1:A:347:ILE:HD12	1.72	0.71
1:F:459:HIS:O	1:F:461:PRO:HD3	1.90	0.71
1:A:329:THR:HA	4:A:529:HOH:O	1.89	0.71
1:D:251:LYS:HG3	4:D:568:HOH:O	1.90	0.71
1:D:332:MET:HE1	4:D:545:HOH:O	1.78	0.71
1:A:284:SER:HA	4:A:539:HOH:O	1.90	0.71
1:F:444:ASP:HB2	4:F:528:HOH:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:314:ILE:HD11	1:E:363:LEU:HD11	1.74	0.69
1:A:338:VAL:HG23	1:A:415:PHE:HE1	1.57	0.69
1:A:447:ARG:HD3	4:A:525:HOH:O	1.92	0.69
1:C:276:GLU:HB3	4:C:517:HOH:O	1.91	0.69
1:G:459:HIS:O	1:G:461:PRO:HD3	1.92	0.69
1:D:379:SER:CB	4:D:550:HOH:O	2.40	0.69
1:A:226:ALA:HB2	1:A:242:LEU:HD11	1.75	0.68
1:D:216:LEU:HA	4:D:536:HOH:O	1.92	0.68
1:A:286:ALA:HA	4:A:544:HOH:O	1.94	0.68
1:G:479:HIS:HA	4:G:532:HOH:O	1.93	0.68
1:H:268:ARG:HD3	4:H:514:HOH:O	1.94	0.67
1:A:240:ARG:HG2	4:A:531:HOH:O	1.93	0.67
1:H:255:HIS:ND1	1:H:257:SER:HB2	2.09	0.67
1:D:229:LYS:HD2	1:D:319:GLN:HB2	1.75	0.67
1:C:240:ARG:HD3	4:C:533:HOH:O	1.95	0.67
1:F:225:VAL:HG22	1:F:270:VAL:HG22	1.76	0.66
1:C:289:LEU:HA	1:C:347:ILE:HD12	1.77	0.66
1:E:466:PRO:O	1:E:467:CYS:HB2	1.95	0.66
1:D:281:VAL:HG12	1:D:281:VAL:O	1.96	0.65
1:D:297:ARG:HB2	4:D:557:HOH:O	1.96	0.65
1:C:281:VAL:HA	1:C:288:THR:HG23	1.78	0.65
1:D:379:SER:HB2	4:D:550:HOH:O	1.95	0.65
1:D:473:SER:HB2	4:D:544:HOH:O	1.98	0.64
1:C:395:MET:CB	1:C:396:ALA:HB2	2.18	0.64
1:C:265:VAL:HG13	1:C:431:PRO:HB3	1.80	0.64
1:G:296:GLN:HG3	1:G:313:ALA:CB	2.28	0.64
1:H:392:ALA:HB3	4:H:529:HOH:O	1.92	0.63
1:G:354:GLN:HB2	4:G:516:HOH:O	1.97	0.63
1:D:324:VAL:HG12	4:D:515:HOH:O	1.98	0.63
1:H:375:LYS:HG3	1:H:376:PRO:HD3	1.78	0.63
1:H:392:ALA:HB2	4:H:529:HOH:O	1.96	0.63
1:C:289:LEU:HA	1:C:347:ILE:CD1	2.29	0.63
1:E:255:HIS:O	1:E:258:ILE:HG22	1.99	0.63
1:G:217:SER:HA	1:G:261:PRO:HG2	1.81	0.62
1:G:246:MET:HA	1:G:246:MET:HE2	1.81	0.62
1:A:397:HIS:N	1:A:397:HIS:CD2	2.66	0.62
1:C:395:MET:HB3	1:C:396:ALA:CB	2.20	0.62
1:F:329:THR:HG22	1:F:330:LEU:N	2.13	0.62
1:H:413:THR:HG21	4:H:534:HOH:O	1.98	0.62
1:B:433:HIS:HB3	4:B:517:HOH:O	2.01	0.61
1:D:428:PRO:HG2	4:D:561:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:ARG:HD3	1:C:342:ALA:HA	1.82	0.61
1:E:281:VAL:HA	1:E:288:THR:HG23	1.83	0.61
1:A:325:SER:HB3	4:A:539:HOH:O	2.00	0.61
1:G:423:CYS:SG	1:G:424:LEU:HD12	2.40	0.61
1:A:487:SER:HB2	4:A:526:HOH:O	2.01	0.61
1:C:329:THR:HG22	1:C:330:LEU:N	2.16	0.60
1:F:357:PHE:HB3	1:F:395:MET:CE	2.32	0.60
1:D:354:GLN:HG3	4:D:546:HOH:O	2.01	0.59
1:E:457:SER:OG	1:E:472:CYS:HB3	2.00	0.59
1:D:321:LEU:HD22	4:D:542:HOH:O	2.02	0.59
1:F:338:VAL:HG23	1:F:366:VAL:O	2.03	0.59
1:B:270:VAL:HA	4:B:531:HOH:O	2.02	0.58
1:G:358:THR:O	1:G:362:GLN:HG2	2.01	0.58
1:F:462:GLN:O	1:F:464:PRO:HD3	2.04	0.58
1:A:462:GLN:HG2	1:A:463:LEU:HD12	1.84	0.58
1:G:245:VAL:HG12	1:G:246:MET:HE3	1.86	0.58
1:D:349:GLU:HG3	4:D:562:HOH:O	2.02	0.58
1:H:227:ASP:OD1	1:H:230:MET:HB2	2.02	0.58
1:E:315:LEU:HD12	1:E:316:PHE:N	2.19	0.58
1:F:385:SER:HA	4:F:530:HOH:O	2.03	0.57
1:E:348:VAL:HG21	1:E:359:ALA:HA	1.86	0.57
1:D:321:LEU:HA	4:D:512:HOH:O	2.03	0.57
1:A:481:MET:HB3	4:A:533:HOH:O	2.04	0.57
1:C:318:ARG:HD2	1:C:350:ASP:HB3	1.85	0.57
1:A:296:GLN:HE21	1:A:310:PHE:HE1	1.52	0.57
1:H:399:ASP:OD1	1:H:400:PRO:HD2	2.04	0.57
1:D:254:LYS:HG3	4:D:570:HOH:O	2.05	0.56
1:C:481:MET:HG2	1:C:482:CYS:N	2.19	0.56
1:F:255:HIS:CE1	1:F:401:GLU:O	2.58	0.56
1:G:463:LEU:HD12	1:G:471:TRP:CD1	2.41	0.56
1:H:246:MET:CE	1:H:246:MET:HA	2.36	0.56
1:E:362:GLN:O	1:E:365:HIS:HB2	2.05	0.56
1:D:410:ARG:HG3	4:D:554:HOH:O	2.04	0.56
1:C:329:THR:HG21	1:C:395:MET:HG3	1.87	0.55
1:D:463:LEU:HG	1:D:471:TRP:CD1	2.41	0.55
1:D:502:MET:HB2	1:D:507:LEU:HD12	1.87	0.55
1:A:296:GLN:HG3	1:A:313:ALA:CB	2.37	0.55
1:D:329:THR:HG21	1:D:395:MET:HG2	1.89	0.55
1:A:428:PRO:HB2	4:A:528:HOH:O	2.05	0.55
1:B:481:MET:HE3	1:F:481:MET:SD	2.46	0.55
1:D:349:GLU:CG	4:D:562:HOH:O	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:459:HIS:CE1	1:D:461:PRO:HA	2.42	0.55
1:B:465:PRO:HG3	4:B:539:HOH:O	2.07	0.55
1:H:217:SER:N	4:H:540:HOH:O	2.40	0.54
1:G:322:CYS:SG	1:G:330:LEU:HA	2.46	0.54
1:G:367:PHE:HE2	1:G:424:LEU:HD21	1.72	0.54
1:D:348:VAL:HG21	1:D:359:ALA:HA	1.89	0.54
1:D:387:SER:OG	1:D:392:ALA:HB1	2.08	0.54
1:H:477:ASN:HB3	4:H:521:HOH:O	2.07	0.54
1:A:338:VAL:CG2	1:A:415:PHE:HE1	2.21	0.54
1:D:290:ARG:HG3	4:D:513:HOH:O	2.08	0.53
1:A:332:MET:CE	4:A:544:HOH:O	2.56	0.53
1:A:354:GLN:HG3	1:A:395:MET:HE1	1.89	0.53
1:A:463:LEU:HD11	1:E:463:LEU:HD21	1.90	0.53
1:H:261:PRO:HD3	4:H:531:HOH:O	2.07	0.53
1:A:276:GLU:HG2	1:B:383:PRO:HG2	1.90	0.53
1:E:463:LEU:HD13	1:E:471:TRP:CG	2.43	0.53
1:F:307:PRO:HG3	1:F:429:GLU:OE1	2.08	0.53
1:E:314:ILE:HD11	1:E:363:LEU:CD1	2.37	0.53
1:F:437:THR:HG23	4:F:517:HOH:O	2.09	0.53
1:E:231:ALA:HA	1:E:238:LEU:HD22	1.90	0.53
1:F:502:MET:C	1:F:504:GLY:H	2.12	0.53
1:C:338:VAL:HG23	1:C:415:PHE:HE1	1.73	0.53
1:B:427:LYS:HE2	4:B:516:HOH:O	2.09	0.52
1:C:388:ARG:HG2	1:C:397:HIS:CD2	2.44	0.52
1:D:283:PRO:HD2	1:D:287:GLN:OE1	2.09	0.52
1:A:258:ILE:HG23	1:A:260:ASN:H	1.74	0.52
1:B:323:GLY:N	4:B:525:HOH:O	2.42	0.52
1:D:485:LYS:O	1:D:486:HIS:HB2	2.08	0.52
1:G:251:LYS:HE3	4:G:517:HOH:O	2.09	0.52
1:G:367:PHE:CE2	1:G:424:LEU:HD21	2.45	0.52
1:D:339:CYS:O	1:D:341:PRO:HD3	2.10	0.52
1:F:272:LEU:HD21	1:F:279:PRO:HD2	1.92	0.52
1:D:318:ARG:NH1	1:D:350:ASP:OD2	2.42	0.52
1:E:481:MET:CE	1:E:483:GLN:HB3	2.40	0.52
1:C:222:THR:HG23	1:C:312:THR:HG23	1.92	0.52
1:D:431:PRO:HD2	4:D:548:HOH:O	2.09	0.52
1:E:380:LEU:HB2	1:E:407:CYS:HB3	1.91	0.52
1:A:397:HIS:CD2	1:A:397:HIS:H	2.27	0.51
1:G:242:LEU:HD13	1:G:269:LEU:HD11	1.92	0.51
1:D:216:LEU:N	4:D:521:HOH:O	2.43	0.51
1:E:258:ILE:HB	1:E:404:TRP:CD1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:ARG:HD2	4:C:534:HOH:O	2.11	0.51
1:E:220:VAL:HG21	1:E:367:PHE:HZ	1.75	0.51
1:E:348:VAL:HG22	1:E:358:THR:HG22	1.92	0.51
1:A:338:VAL:HG23	1:A:415:PHE:CE1	2.44	0.51
1:B:281:VAL:HG22	4:B:521:HOH:O	2.09	0.51
1:C:400:PRO:HD3	1:C:503:GLY:HA3	1.93	0.51
1:E:247:ALA:HB2	1:E:435:PRO:HD2	1.93	0.51
1:C:255:HIS:O	1:C:258:ILE:HG22	2.10	0.51
1:G:296:GLN:HG3	1:G:313:ALA:HB2	1.93	0.51
1:H:355:SER:HA	4:H:512:HOH:O	2.11	0.51
1:F:450:GLN:HE21	1:F:458:ARG:NH1	2.09	0.50
1:H:393:PRO:HB2	4:H:518:HOH:O	2.11	0.50
1:B:375:LYS:HB3	1:B:376:PRO:HD3	1.92	0.50
1:A:246:MET:HE1	1:A:314:ILE:HD12	1.94	0.50
1:B:304:ASP:HB2	4:B:510:HOH:O	2.10	0.50
1:C:276:GLU:CB	4:C:517:HOH:O	2.55	0.50
1:H:476:LEU:O	1:H:477:ASN:C	2.49	0.50
1:C:284:SER:HA	4:C:528:HOH:O	2.12	0.50
1:H:301:THR:OG1	1:H:309:HIS:HB2	2.10	0.50
1:C:218:ARG:HD2	1:C:416:LEU:HD13	1.94	0.50
1:C:446:ASP:O	1:C:450:GLN:HG3	2.11	0.50
1:E:427:LYS:HG2	1:E:428:PRO:HD2	1.93	0.50
1:G:264:LEU:HD23	1:G:265:VAL:N	2.26	0.50
1:H:218:ARG:NH2	1:H:416:LEU:HB3	2.26	0.50
1:H:227:ASP:OD1	1:H:317:THR:HA	2.11	0.50
1:G:218:ARG:HB3	1:G:424:LEU:HD23	1.94	0.49
1:C:329:THR:CG2	1:C:395:MET:HG3	2.42	0.49
1:B:229:LYS:HB3	1:B:318:ARG:HB2	1.94	0.49
1:G:246:MET:HA	1:G:246:MET:CE	2.42	0.49
1:C:289:LEU:HD22	1:C:332:MET:HG3	1.94	0.49
1:D:284:SER:N	4:D:543:HOH:O	2.46	0.49
1:C:447:ARG:NH2	4:C:520:HOH:O	2.05	0.49
1:H:255:HIS:CE1	1:H:403:PRO:HD2	2.47	0.49
1:H:393:PRO:CB	4:H:518:HOH:O	2.61	0.49
1:D:285:ALA:HB1	1:D:332:MET:HG3	1.94	0.49
1:D:464:PRO:HD2	1:G:462:GLN:HB3	1.93	0.49
1:E:239:LYS:O	1:E:243:LEU:HD22	2.13	0.49
1:A:332:MET:HG3	4:A:544:HOH:O	2.13	0.49
1:B:459:HIS:CE1	1:B:461:PRO:HA	2.48	0.49
1:D:410:ARG:CG	4:D:554:HOH:O	2.60	0.49
1:F:329:THR:HG22	1:F:330:LEU:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:296:GLN:HG3	1:D:313:ALA:CB	2.43	0.48
1:D:429:GLU:HB3	1:E:394:VAL:HG11	1.95	0.48
1:C:248:ALA:HB3	1:C:356:ALA:HB1	1.95	0.48
1:E:306:ASP:N	1:E:306:ASP:OD1	2.46	0.48
1:G:322:CYS:HB2	4:G:523:HOH:O	2.12	0.48
1:H:314:ILE:HD11	1:H:363:LEU:HD21	1.95	0.48
1:H:414:ASP:HB3	4:H:516:HOH:O	2.13	0.48
1:F:296:GLN:HE21	1:F:310:PHE:HE1	1.62	0.48
1:D:319:GLN:HA	4:D:538:HOH:O	2.11	0.48
1:E:481:MET:HE1	1:E:483:GLN:HB3	1.95	0.48
1:F:218:ARG:NH1	1:F:421:GLY:O	2.47	0.48
1:C:338:VAL:HG23	1:C:415:PHE:CE1	2.49	0.48
1:D:463:LEU:HD13	1:G:463:LEU:HD21	1.95	0.48
1:F:337:THR:O	1:F:344:SER:HB2	2.14	0.48
1:A:230:MET:HE1	1:A:350:ASP:HB2	1.95	0.48
1:D:255:HIS:CE1	1:D:257:SER:HG	2.29	0.48
1:D:355:SER:CB	4:D:523:HOH:O	2.48	0.47
1:H:447:ARG:HD2	4:H:527:HOH:O	2.15	0.47
1:E:489:TRP:CD1	1:E:489:TRP:N	2.82	0.47
1:F:367:PHE:HB3	1:F:412:ILE:HG13	1.95	0.47
1:G:301:THR:OG1	1:G:309:HIS:HB2	2.14	0.47
1:B:476:LEU:HD13	1:F:476:LEU:HD13	1.96	0.47
1:C:450:GLN:CD	4:C:520:HOH:O	2.52	0.47
1:B:330:LEU:HD13	1:B:395:MET:HE3	1.95	0.47
1:C:289:LEU:O	1:C:293:CYS:HB2	2.14	0.47
1:A:400:PRO:HG3	4:A:518:HOH:O	2.15	0.47
1:B:217:SER:HB2	4:B:520:HOH:O	2.15	0.47
1:B:322:CYS:SG	1:B:330:LEU:HA	2.55	0.47
1:B:502:MET:HB3	1:B:507:LEU:HD12	1.97	0.47
1:C:258:ILE:HG23	1:C:260:ASN:H	1.80	0.47
1:D:293:CYS:SG	1:D:343:ARG:HA	2.54	0.47
1:F:339:CYS:SG	1:F:424:LEU:HD13	2.55	0.47
1:G:447:ARG:HD2	4:G:510:HOH:O	2.14	0.47
1:A:395:MET:CE	4:A:548:HOH:O	2.62	0.47
1:C:241:TYR:OH	1:C:350:ASP:OD1	2.28	0.47
1:F:450:GLN:HA	1:F:454:GLY:O	2.15	0.47
1:B:479:HIS:HB2	1:F:484:THR:O	2.15	0.47
1:G:304:ASP:HA	1:G:309:HIS:CD2	2.49	0.47
1:E:400:PRO:CD	4:E:516:HOH:O	2.63	0.46
1:F:265:VAL:HG11	1:F:428:PRO:HG2	1.98	0.46
1:H:268:ARG:CD	4:H:514:HOH:O	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:378:ILE:HG13	4:H:522:HOH:O	2.13	0.46
1:A:474:GLY:HA3	1:A:481:MET:HE3	1.97	0.46
1:B:247:ALA:HA	1:B:434:LEU:HD13	1.98	0.46
1:D:462:GLN:HG2	1:D:463:LEU:HD22	1.97	0.46
1:A:280:GLN:HG2	4:A:549:HOH:O	2.16	0.46
1:F:231:ALA:HA	1:F:238:LEU:HD22	1.96	0.46
1:E:400:PRO:CG	4:E:516:HOH:O	2.53	0.46
1:C:428:PRO:HB2	4:C:536:HOH:O	2.14	0.46
1:D:368:ASN:HB2	1:D:415:PHE:CD2	2.51	0.46
1:G:309:HIS:HB3	4:G:521:HOH:O	2.16	0.46
1:H:318:ARG:NH2	1:H:451:LEU:O	2.40	0.46
1:A:390:VAL:HG23	1:A:403:PRO:O	2.16	0.46
1:C:339:CYS:SG	1:C:424:LEU:HD13	2.56	0.46
1:D:297:ARG:N	4:D:557:HOH:O	2.43	0.46
1:D:479:HIS:HB2	1:G:484:THR:O	2.17	0.45
1:A:335:VAL:HG12	1:A:368:ASN:HA	1.98	0.45
1:C:265:VAL:CG1	1:C:431:PRO:HB3	2.46	0.45
1:H:354:GLN:HG2	1:H:487:SER:CB	2.47	0.45
1:A:463:LEU:HD22	1:A:471:TRP:CD2	2.52	0.45
1:D:282:GLY:C	4:D:543:HOH:O	2.54	0.45
1:G:280:GLN:HG3	4:G:519:HOH:O	2.15	0.45
1:C:445:ALA:HB1	1:C:459:HIS:CG	2.51	0.45
1:F:427:LYS:HE2	4:F:524:HOH:O	2.16	0.45
1:A:290:ARG:HD3	1:A:290:ARG:HA	1.62	0.45
1:D:369:MET:CE	1:D:408:SER:HB3	2.47	0.45
1:H:255:HIS:HA	1:H:256:PRO:HD2	1.81	0.45
1:B:476:LEU:HD13	1:F:476:LEU:CD1	2.47	0.44
1:C:314:ILE:HD11	1:C:363:LEU:HD11	1.99	0.44
1:D:335:VAL:HA	1:D:365:HIS:O	2.17	0.44
1:F:301:THR:HB	1:F:302:PRO:HD2	1.99	0.44
1:H:463:LEU:HD13	1:H:471:TRP:CG	2.53	0.44
1:H:481:MET:HE2	1:H:483:GLN:HB3	1.98	0.44
1:C:354:GLN:HG2	1:C:487:SER:CB	2.46	0.44
1:G:400:PRO:HG3	1:G:503:GLY:HA3	1.99	0.44
1:A:273:GLY:H	1:A:276:GLU:HB2	1.83	0.44
1:E:443:TYR:HB3	1:E:447:ARG:HB2	1.98	0.44
1:G:471:TRP:HA	1:G:483:GLN:O	2.17	0.44
1:A:230:MET:HE2	1:A:318:ARG:HG3	1.99	0.44
1:A:246:MET:CE	1:A:314:ILE:HD12	2.48	0.44
1:C:394:VAL:HG23	1:C:394:VAL:O	2.18	0.44
1:B:246:MET:CE	1:B:314:ILE:HD12	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:227:ASP:OD1	1:F:317:THR:HA	2.17	0.44
1:H:289:LEU:O	1:H:293:CYS:HB2	2.18	0.44
1:D:286:ALA:HA	4:D:545:HOH:O	2.16	0.44
1:G:375:LYS:N	1:G:376:PRO:HD2	2.33	0.44
1:A:303:GLU:C	1:A:305:SER:H	2.20	0.44
1:D:337:THR:HG22	1:D:366:VAL:HG13	2.00	0.44
1:D:255:HIS:ND1	1:D:257:SER:OG	2.36	0.44
1:E:397:HIS:CE1	4:E:513:HOH:O	2.71	0.44
1:H:220:VAL:HG21	1:H:367:PHE:HZ	1.83	0.44
1:B:245:VAL:HG13	1:B:356:ALA:HA	1.99	0.43
1:B:481:MET:HE1	1:B:483:GLN:HG3	2.00	0.43
1:H:390:VAL:HG23	1:H:403:PRO:O	2.17	0.43
1:H:502:MET:HB2	1:H:507:LEU:HD12	2.00	0.43
1:C:329:THR:HG22	1:C:330:LEU:H	1.80	0.43
1:H:296:GLN:HE21	1:H:310:PHE:HE1	1.66	0.43
1:B:221:GLU:HG2	1:B:428:PRO:HB3	1.99	0.43
1:D:463:LEU:HD13	1:G:463:LEU:CD2	2.49	0.43
1:G:280:GLN:HG2	1:G:291:SER:OG	2.18	0.43
1:C:261:PRO:HA	4:C:529:HOH:O	2.17	0.43
1:C:368:ASN:HB2	1:C:415:PHE:CD2	2.53	0.43
1:E:332:MET:HB2	1:E:347:ILE:HG22	2.01	0.43
1:D:281:VAL:O	1:D:281:VAL:CG1	2.65	0.43
1:G:475:HIS:HA	1:G:479:HIS:O	2.19	0.43
1:C:444:ASP:O	1:C:448:GLN:HG3	2.19	0.43
1:D:258:ILE:HG23	1:D:260:ASN:H	1.83	0.43
1:H:463:LEU:HD13	1:H:471:TRP:CD2	2.53	0.43
1:E:445:ALA:HB1	1:E:459:HIS:CG	2.54	0.43
1:H:353:LEU:HD13	1:H:451:LEU:HD13	2.00	0.43
1:D:216:LEU:CA	4:D:536:HOH:O	2.60	0.43
1:D:321:LEU:HD11	4:D:526:HOH:O	2.18	0.43
1:D:375:LYS:HB3	1:D:376:PRO:HD3	2.00	0.43
1:G:329:THR:HG22	1:G:330:LEU:N	2.34	0.43
1:D:247:ALA:HA	1:D:434:LEU:HD13	2.00	0.43
1:D:301:THR:OG1	1:D:309:HIS:HB2	2.18	0.43
1:H:338:VAL:HG23	1:H:415:PHE:HE1	1.83	0.43
1:F:255:HIS:HE1	1:F:401:GLU:O	1.99	0.42
1:F:338:VAL:CG1	1:F:424:LEU:HD11	2.49	0.42
1:G:338:VAL:HG12	1:G:415:PHE:HE1	1.84	0.42
1:H:307:PRO:HB3	1:H:429:GLU:HG2	2.01	0.42
1:A:485:LYS:HE2	1:E:479:HIS:NE2	2.34	0.42
1:A:497:PRO:CD	4:A:546:HOH:O	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:THR:O	1:B:362:GLN:HG2	2.19	0.42
1:H:230:MET:HE3	1:H:316:PHE:HB3	1.99	0.42
1:H:481:MET:CE	1:H:483:GLN:HB3	2.49	0.42
1:C:481:MET:HG3	1:H:481:MET:CE	2.49	0.42
1:H:475:HIS:CE1	4:H:542:HOH:O	2.72	0.42
1:H:466:PRO:O	1:H:467:CYS:HB2	2.19	0.42
1:B:255:HIS:CE1	1:B:401:GLU:O	2.72	0.42
1:C:338:VAL:HG22	1:C:366:VAL:HG12	2.02	0.42
1:C:480:ALA:HB3	4:C:535:HOH:O	2.20	0.42
1:D:227:ASP:OD1	1:D:317:THR:HA	2.20	0.42
1:B:229:LYS:HE2	1:B:319:GLN:HG3	2.02	0.42
1:G:245:VAL:HG12	1:G:246:MET:CE	2.49	0.42
1:G:397:HIS:CD2	4:G:530:HOH:O	2.72	0.42
1:A:332:MET:HE2	4:A:544:HOH:O	2.18	0.42
1:F:491:ASP:HA	1:F:501:CYS:O	2.19	0.42
1:D:458:ARG:NE	4:D:534:HOH:O	2.53	0.42
1:E:473:SER:HA	1:E:481:MET:O	2.20	0.42
1:C:265:VAL:HG11	1:C:428:PRO:HG3	2.02	0.41
1:C:480:ALA:N	4:C:512:HOH:O	2.52	0.41
1:C:227:ASP:HA	1:C:272:LEU:HD12	2.01	0.41
1:C:283:PRO:HD2	1:C:287:GLN:HG2	2.02	0.41
1:G:462:GLN:O	1:G:464:PRO:HD3	2.20	0.41
1:A:363:LEU:O	1:A:366:VAL:HB	2.21	0.41
1:H:245:VAL:HG12	1:H:246:MET:HE3	2.01	0.41
1:B:467:CYS:HB2	1:B:505:ARG:HA	2.02	0.41
1:D:285:ALA:HB1	1:D:332:MET:CG	2.49	0.41
1:E:400:PRO:HD2	4:E:516:HOH:O	2.20	0.41
1:G:289:LEU:O	1:G:293:CYS:HB2	2.21	0.41
1:H:485:LYS:HE3	4:H:533:HOH:O	2.20	0.41
1:D:296:GLN:HG3	1:D:313:ALA:HB3	2.01	0.41
1:F:254:LYS:HE3	4:F:514:HOH:O	2.20	0.41
1:G:251:LYS:CE	4:G:517:HOH:O	2.66	0.41
1:B:246:MET:HE3	1:B:314:ILE:HD12	2.03	0.41
1:C:226:ALA:HB1	1:C:230:MET:HG2	2.03	0.41
1:D:312:THR:HB	4:D:551:HOH:O	2.21	0.41
1:E:447:ARG:O	1:E:451:LEU:HG	2.21	0.41
1:G:241:TYR:CE2	1:G:451:LEU:HD22	2.56	0.41
1:G:439:PRO:HD2	1:G:491:ASP:O	2.21	0.41
1:H:245:VAL:HG13	1:H:356:ALA:HA	2.03	0.41
1:A:335:VAL:CG1	1:A:368:ASN:HA	2.51	0.41
1:G:467:CYS:HA	1:G:489:TRP:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:GLU:N	1:A:403:PRO:HD3	2.36	0.40
1:F:354:GLN:HG2	1:F:487:SER:OG	2.20	0.40
1:H:476:LEU:HG	1:H:477:ASN:N	2.25	0.40
1:C:390:VAL:HG23	1:C:403:PRO:O	2.21	0.40
1:D:337:THR:HG23	1:D:344:SER:HA	2.02	0.40
1:A:217:SER:HB3	4:A:538:HOH:O	2.21	0.40
1:A:238:LEU:O	1:A:239:LYS:C	2.60	0.40
1:B:301:THR:HG21	1:B:306:ASP:OD2	2.22	0.40
1:C:460:CYS:HB3	1:C:462:GLN:NE2	2.37	0.40
1:C:475:HIS:HA	4:C:512:HOH:O	2.20	0.40
1:H:255:HIS:ND1	1:H:403:PRO:HD2	2.37	0.40
1:H:367:PHE:HB3	1:H:412:ILE:HG13	2.03	0.40
1:F:240:ARG:HB2	4:F:516:HOH:O	2.20	0.40
1:A:392:ALA:HB2	4:A:557:HOH:O	2.21	0.40
1:B:279:PRO:HG3	1:B:292:PHE:HD1	1.86	0.40
1:C:229:LYS:H	1:C:229:LYS:HG2	1.64	0.40
1:C:459:HIS:O	1:C:461:PRO:HD3	2.21	0.40
1:D:284:SER:HB2	1:D:287:GLN:HB2	2.02	0.40
1:D:287:GLN:HG3	4:D:552:HOH:O	2.21	0.40
1:D:387:SER:O	1:D:396:ALA:HB3	2.22	0.40
1:D:463:LEU:CD1	1:G:463:LEU:HD21	2.50	0.40
1:E:481:MET:HB2	1:E:481:MET:HE3	1.83	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	286/316 (90%)	258 (90%)	26 (9%)	2 (1%)	22 53
1	B	283/316 (90%)	259 (92%)	24 (8%)	0	100 100
1	C	285/316 (90%)	262 (92%)	23 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	283/316 (90%)	255 (90%)	25 (9%)	3 (1%)	14	41
1	E	276/316 (87%)	255 (92%)	19 (7%)	2 (1%)	22	53
1	F	291/316 (92%)	259 (89%)	31 (11%)	1 (0%)	41	72
1	G	287/316 (91%)	269 (94%)	16 (6%)	2 (1%)	22	53
1	H	275/316 (87%)	255 (93%)	18 (6%)	2 (1%)	22	53
All	All	2266/2528 (90%)	2072 (91%)	182 (8%)	12 (0%)	29	61

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	351	ASP
1	A	304	ASP
1	E	467	CYS
1	H	395	MET
1	A	467	CYS
1	D	221	GLU
1	D	320	ASP
1	D	497	PRO
1	H	256	PRO
1	F	460	CYS
1	G	460	CYS
1	G	283	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	238/261 (91%)	229 (96%)	9 (4%)	33	67
1	B	236/261 (90%)	227 (96%)	9 (4%)	33	67
1	C	237/261 (91%)	231 (98%)	6 (2%)	47	80
1	D	236/261 (90%)	226 (96%)	10 (4%)	30	63
1	E	232/261 (89%)	221 (95%)	11 (5%)	26	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	239/261 (92%)	229 (96%)	10 (4%)	30 63
1	G	238/261 (91%)	230 (97%)	8 (3%)	37 71
1	H	231/261 (88%)	225 (97%)	6 (3%)	46 79
All	All	1887/2088 (90%)	1818 (96%)	69 (4%)	34 68

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	227	ASP
1	A	243	LEU
1	A	265	VAL
1	A	277	GLU
1	A	280	GLN
1	A	293	CYS
1	A	338	VAL
1	A	355	SER
1	A	457	SER
1	B	263	SER
1	B	269	LEU
1	B	293	CYS
1	B	296	GLN
1	B	314	ILE
1	B	394	VAL
1	B	446	ASP
1	B	457	SER
1	B	499	GLN
1	C	222	THR
1	C	269	LEU
1	C	293	CYS
1	C	338	VAL
1	C	353	LEU
1	C	481	MET
1	D	268	ARG
1	D	272	LEU
1	D	293	CYS
1	D	314	ILE
1	D	343	ARG
1	D	387	SER
1	D	405	SER
1	D	424	LEU
1	D	451	LEU

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Mol	Chain	Res	Type
1	D	473	SER
1	E	227	ASP
1	E	228	ASP
1	E	243	LEU
1	E	288	THR
1	E	293	CYS
1	E	306	ASP
1	E	321	LEU
1	E	456	ASP
1	E	463	LEU
1	E	495	CYS
1	E	499	GLN
1	F	216	LEU
1	F	227	ASP
1	F	243	LEU
1	F	264	LEU
1	F	289	LEU
1	F	293	CYS
1	F	325	SER
1	F	329	THR
1	F	380	LEU
1	F	491	ASP
1	G	227	ASP
1	G	243	LEU
1	G	264	LEU
1	G	296	GLN
1	G	297	ARG
1	G	306	ASP
1	G	314	ILE
1	G	407	CYS
1	H	293	CYS
1	H	321	LEU
1	H	353	LEU
1	H	411	PHE
1	H	424	LEU
1	H	463	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	433	HIS
1	E	499	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 24 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.