



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:34 PM UTC

PDB ID : 6A29 / pdb_00006a29
Title : Crystal structure of PprA A139R mutant
Authors : Adachi, M.; Shibazaki, C.; Shimizu, R.; Arai, S.; Satoh, K.; Narumi, I.; Kuroki, R.
Deposited on : 2018-06-09
Resolution : 2.40 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:

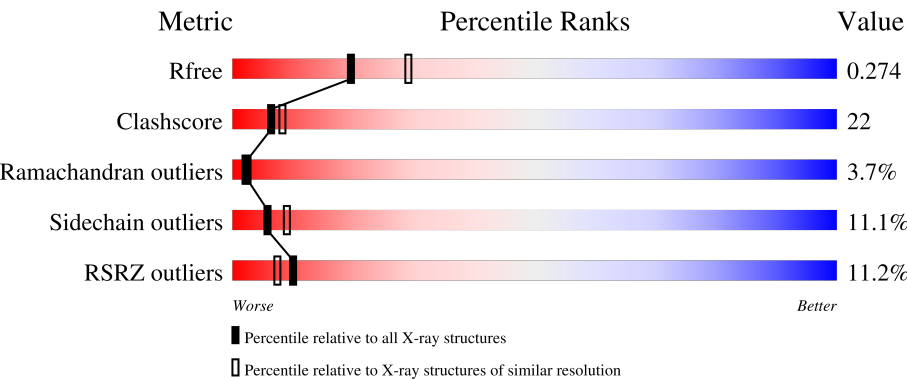
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	284	7% 60%30%6% . .
1	B	284	2% 76%18% . . .
1	C	284	7% 58%32%6% . .
1	D	284	5% 67%25%5% .
1	E	284	5% 67%23%8% .

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Mol	Chain	Length	Quality of chain
1	F	284	
1	G	284	
1	H	284	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17205 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 DNA repair protein PprA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2083	1290	383	406	4			
1	B	275	Total	C	N	O	S	0	0	0
			2083	1290	383	406	4			
1	C	275	Total	C	N	O	S	0	0	0
			2083	1290	383	406	4			
1	D	275	Total	C	N	O	S	0	0	0
			2083	1290	383	406	4			
1	E	278	Total	C	N	O	S	0	0	0
			2109	1305	388	412	4			
1	F	275	Total	C	N	O	S	0	0	0
			2083	1290	383	406	4			
1	G	275	Total	C	N	O	S	0	0	0
			2083	1290	383	406	4			
1	H	275	Total	C	N	O	S	0	0	0
			2083	1290	383	406	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	ARG	ALA	engineered mutation	UNP O32504
B	139	ARG	ALA	engineered mutation	UNP O32504
C	139	ARG	ALA	engineered mutation	UNP O32504
D	139	ARG	ALA	engineered mutation	UNP O32504
E	139	ARG	ALA	engineered mutation	UNP O32504
F	139	ARG	ALA	engineered mutation	UNP O32504
G	139	ARG	ALA	engineered mutation	UNP O32504
H	139	ARG	ALA	engineered mutation	UNP O32504

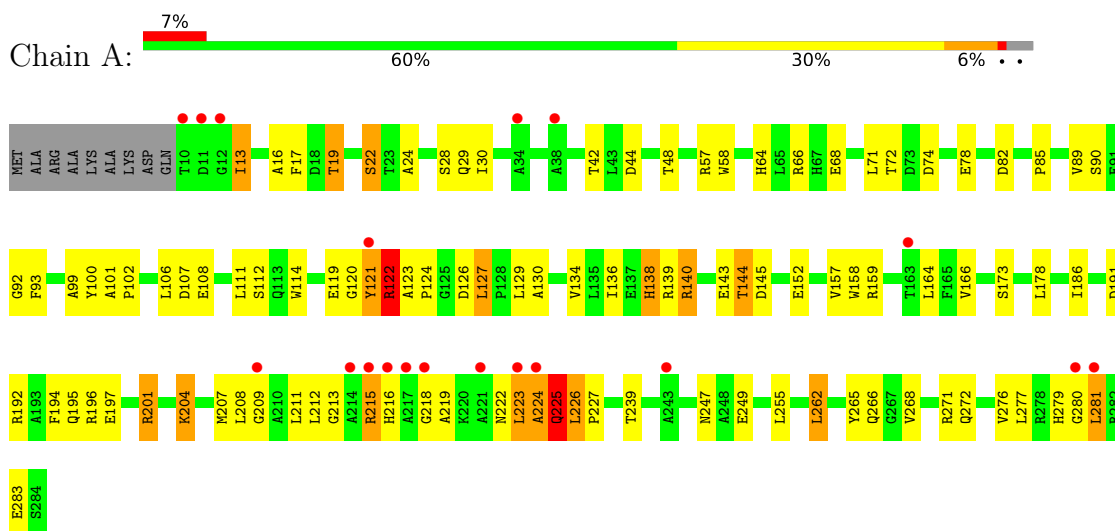
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	33	Total 33	O 33	0	0
2	B	154	Total 154	O 154	0	0
2	C	67	Total 67	O 67	0	0
2	D	75	Total 75	O 75	0	0
2	E	113	Total 113	O 113	0	0
2	F	15	Total 15	O 15	0	0
2	G	32	Total 32	O 32	0	0
2	H	26	Total 26	O 26	0	0

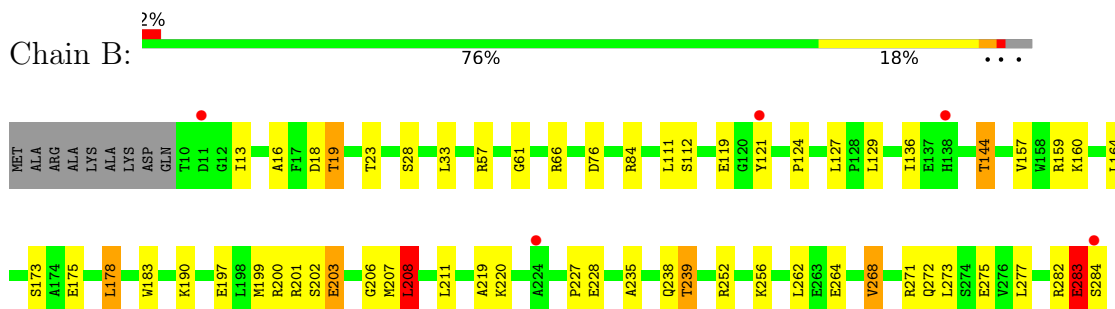
3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

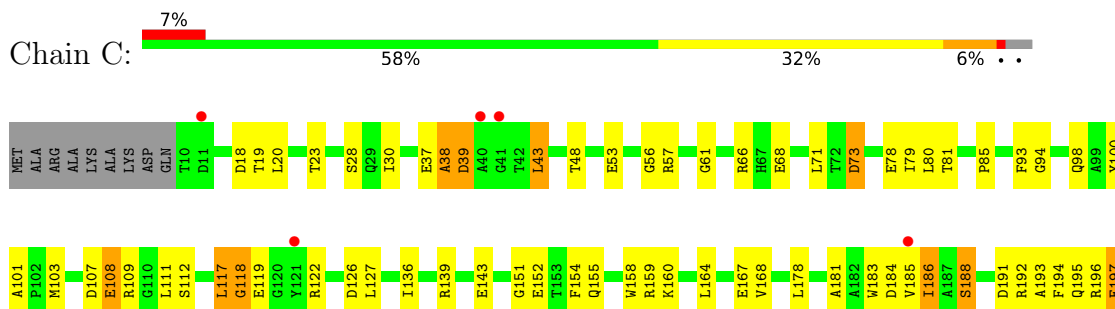
• Molecule 1: DNA repair protein PprA

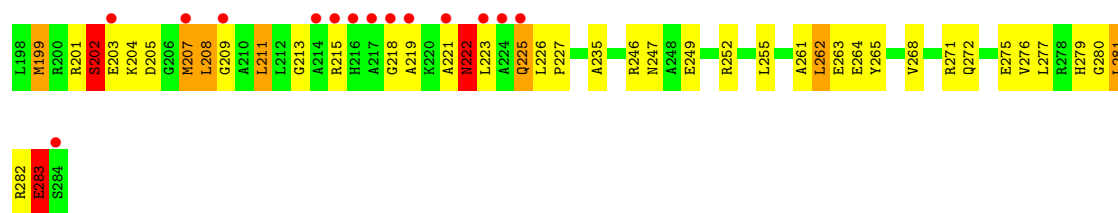


• Molecule 1: DNA repair protein PprA

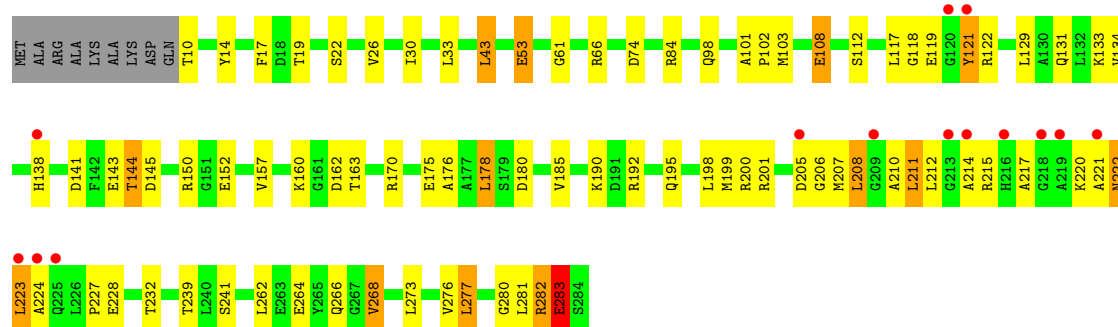


• Molecule 1: DNA repair protein PprA

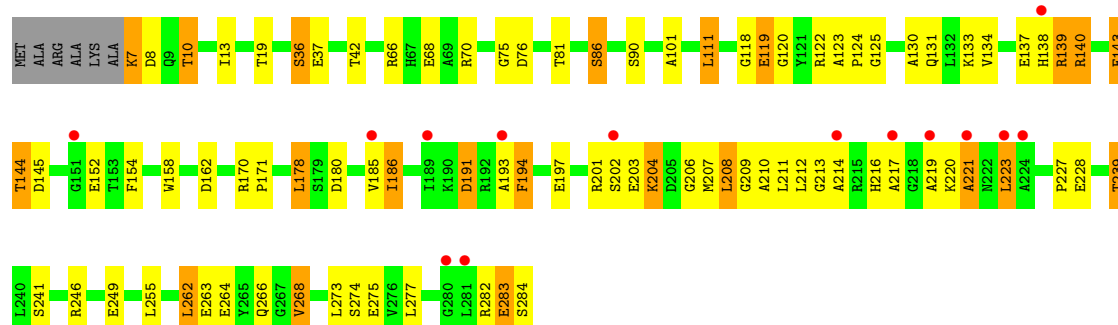




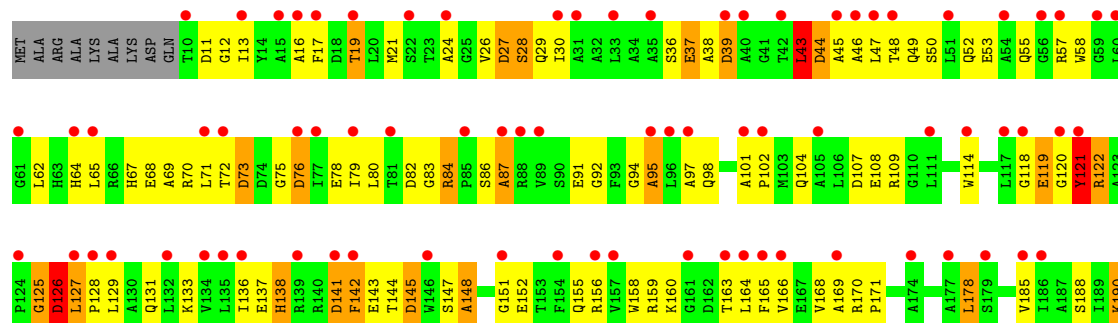
• Molecule 1: DNA repair protein PprA

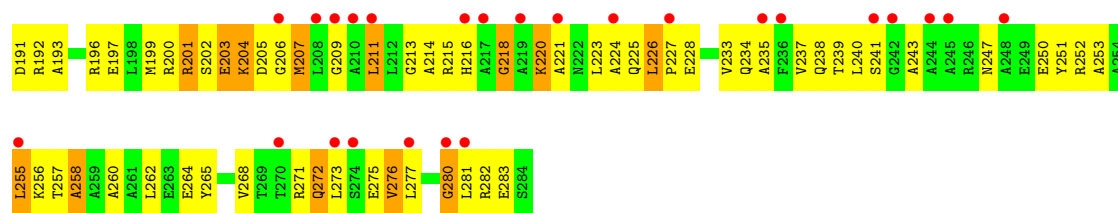


• Molecule 1: DNA repair protein PprA

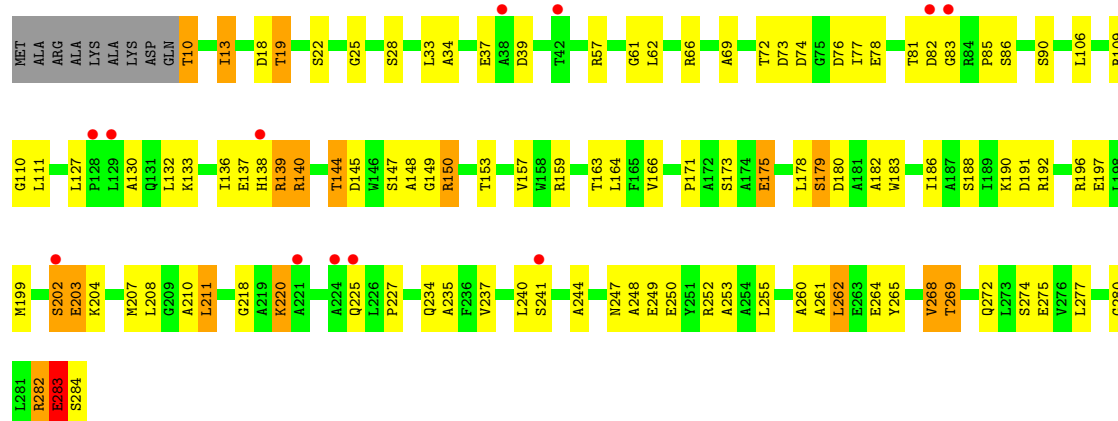


• Molecule 1: DNA repair protein PprA

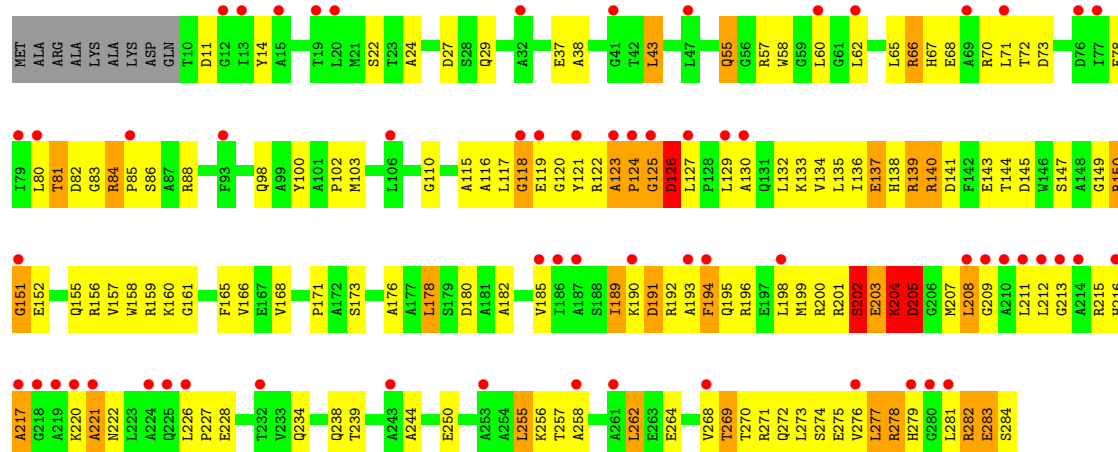




● Molecule 1: DNA repair protein PprA



● Molecule 1: DNA repair protein PprA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.19Å 272.26Å 104.89Å 90.00° 98.64° 90.00°	Depositor
Resolution (Å)	48.63 – 2.40 48.63 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.63-2.40) 95.3 (48.63-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.212 , 0.271 0.219 , 0.274	Depositor DCC
R_{free} test set	5260 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17205	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.53	0/2118	0.81	0/2866
1	B	0.80	0/2118	0.90	1/2866 (0.0%)
1	C	0.61	0/2118	0.87	2/2866 (0.1%)
1	D	0.64	0/2118	0.84	2/2866 (0.1%)
1	E	0.70	0/2144	0.93	3/2900 (0.1%)
1	F	0.35	0/2118	0.74	0/2866
1	G	0.54	0/2118	0.83	1/2866 (0.0%)
1	H	0.43	0/2118	0.81	2/2866 (0.1%)
All	All	0.59	0/16970	0.84	11/22962 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	119	GLU	N-CA-C	8.44	122.84	112.54
1	G	225	GLN	N-CA-C	-6.27	101.41	110.24
1	B	208	LEU	N-CA-C	-5.87	98.30	110.80
1	D	101	ALA	CA-C-N	-5.70	113.75	119.56
1	D	101	ALA	C-N-CA	-5.70	113.75	119.56
1	H	118	GLY	N-CA-C	-5.62	108.28	115.42
1	C	202	SER	N-CA-C	-5.35	103.07	110.35
1	E	101	ALA	CA-C-N	-5.25	114.25	119.56
1	E	101	ALA	C-N-CA	-5.25	114.25	119.56
1	C	117	LEU	N-CA-C	-5.19	107.32	113.97
1	H	269	THR	N-CA-C	-5.11	106.88	114.64

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2083	0	2024	92	1
1	B	2083	0	2024	50	0
1	C	2083	0	2024	92	0
1	D	2083	0	2024	70	1
1	E	2109	0	2049	84	0
1	F	2083	0	2024	175	3
1	G	2083	0	2024	75	1
1	H	2083	0	2024	124	1
2	A	33	0	0	2	0
2	B	154	0	0	12	1
2	C	67	0	0	11	0
2	D	75	0	0	13	0
2	E	113	0	0	16	1
2	F	15	0	0	1	0
2	G	32	0	0	1	0
2	H	26	0	0	15	0
All	All	17205	0	16217	723	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (723) 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:H:283:GLU:O	1:H:284:SER:OXT	1.65	1.15
1:H:271:ARG:HA	1:H:274:SER:OG	1.44	1.15
1:E:7:LYS:HB3	2:E:329:HOH:O	0.96	1.13
1:E:203:GLU:HB2	1:F:205:ASP:OD1	1.47	1.13
1:D:150:ARG:HD2	2:D:320:HOH:O	1.47	1.12
1:F:155:GLN:OE1	1:F:255:LEU:HD11	1.50	1.12
1:G:149:GLY:HA3	1:G:153:THR:O	1.51	1.09
1:B:271:ARG:HD3	2:B:301:HOH:O	1.52	1.08
1:B:190:LYS:HD2	1:E:241:SER:OG	1.54	1.07
1:G:163:THR:HG23	1:G:240:LEU:O	1.55	1.05
1:F:71:LEU:HD22	1:F:75:GLY:O	1.55	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:SER:O	1:C:203:GLU:HB3	1.48	1.04
1:F:126:ASP:O	1:F:127:LEU:O	1.76	1.03
1:H:200:ARG:NH2	2:H:301:HOH:O	1.90	1.03
1:H:279:HIS:HE1	2:H:310:HOH:O	1.45	1.00
1:D:282:ARG:O	1:D:283:GLU:HB2	1.62	0.99
1:H:279:HIS:CE1	2:H:310:HOH:O	2.14	0.97
1:H:122:ARG:O	1:H:123:ALA:O	1.82	0.97
1:E:202:SER:HB2	1:F:206:GLY:O	1.64	0.96
1:C:117:LEU:O	1:C:118:GLY:O	1.83	0.96
1:D:217:ALA:HB1	2:D:315:HOH:O	1.63	0.96
1:H:122:ARG:HG3	2:H:306:HOH:O	1.64	0.95
1:F:272:GLN:O	1:F:276:VAL:HG23	1.66	0.95
1:F:163:THR:HG22	1:F:241:SER:OG	1.65	0.95
1:E:137:GLU:O	1:E:246:ARG:NH2	1.97	0.95
1:F:75:GLY:O	1:F:76:ASP:O	1.85	0.95
1:F:216:HIS:HE1	1:F:224:ALA:O	1.49	0.94
1:H:220:LYS:O	1:H:220:LYS:HD3	1.66	0.94
1:H:264:GLU:O	1:H:268:VAL:HG22	1.68	0.93
1:C:68:GLU:HB2	2:C:325:HOH:O	1.69	0.92
1:E:139:ARG:O	1:E:140:ARG:HB2	1.68	0.92
1:A:191:ASP:OD2	1:A:194:PHE:N	2.01	0.92
1:D:10:THR:HG21	2:D:335:HOH:O	1.70	0.92
1:H:140:ARG:HG3	2:H:316:HOH:O	1.69	0.90
1:G:249:GLU:OE1	1:G:249:GLU:HA	1.72	0.90
1:A:271:ARG:HD2	2:A:329:HOH:O	1.72	0.90
1:H:81:THR:HG23	1:H:86:SER:OG	1.71	0.89
1:F:71:LEU:HD22	1:F:76:ASP:O	1.72	0.88
1:C:139:ARG:O	1:C:246:ARG:NH2	2.07	0.88
1:C:252:ARG:CD	2:C:302:HOH:O	2.22	0.87
1:F:215:ARG:HG2	1:F:280:GLY:O	1.74	0.87
1:B:252:ARG:HD2	2:B:430:HOH:O	1.73	0.86
1:D:281:LEU:O	1:D:282:ARG:HG3	1.75	0.86
1:F:12:GLY:O	1:F:16:ALA:HB2	1.76	0.86
1:E:219:ALA:HB1	2:E:384:HOH:O	1.76	0.85
1:G:25:GLY:HA2	2:G:315:HOH:O	1.77	0.84
1:C:215:ARG:HG2	1:C:279:HIS:O	1.78	0.84
1:F:120:GLY:O	1:F:121:TYR:HB3	1.76	0.84
1:C:202:SER:O	1:C:203:GLU:CB	2.25	0.83
1:G:106:LEU:HD22	1:G:110:GLY:O	1.78	0.83
1:G:76:ASP:OD2	1:G:90:SER:OG	1.96	0.83
1:F:57:ARG:HA	1:F:235:ALA:O	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:MET:HE1	1:D:208:LEU:HB2	1.61	0.83
1:A:140:ARG:O	1:A:159:ARG:NH1	2.12	0.82
1:H:83:GLY:O	1:H:84:ARG:O	1.97	0.82
1:E:138:HIS:CE1	2:E:373:HOH:O	2.32	0.81
1:F:118:GLY:O	1:F:119:GLU:O	1.97	0.81
1:D:264:GLU:O	1:D:268:VAL:HG12	1.79	0.81
1:F:216:HIS:CE1	1:F:224:ALA:O	2.34	0.80
1:E:138:HIS:O	1:E:139:ARG:O	2.00	0.80
1:H:189:ILE:HG22	1:H:189:ILE:O	1.82	0.79
1:F:260:ALA:O	1:F:264:GLU:HG3	1.82	0.79
1:H:180:ASP:OD2	2:H:302:HOH:O	2.01	0.79
1:E:10:THR:HB	2:E:329:HOH:O	1.82	0.78
1:F:72:THR:O	1:F:73:ASP:HB2	1.83	0.78
1:H:140:ARG:CG	2:H:316:HOH:O	2.24	0.78
1:A:120:GLY:O	1:A:122:ARG:N	2.16	0.78
1:F:141:ASP:O	1:F:142:PHE:HB3	1.81	0.78
1:F:144:THR:HG22	1:F:145:ASP:O	1.83	0.77
1:F:204:LYS:O	1:F:204:LYS:HG3	1.82	0.77
1:E:220:LYS:HG3	2:E:395:HOH:O	1.84	0.77
1:F:191:ASP:OD2	1:F:193:ALA:HB3	1.85	0.76
1:F:250:GLU:OE1	1:F:250:GLU:HA	1.84	0.76
1:F:257:THR:O	1:F:260:ALA:N	2.18	0.76
1:F:209:GLY:O	1:F:213:GLY:N	2.19	0.75
1:A:212:LEU:O	1:A:215:ARG:HB2	1.87	0.75
1:H:140:ARG:CB	2:H:316:HOH:O	2.34	0.75
1:F:252:ARG:O	1:F:256:LYS:HG2	1.86	0.74
1:A:191:ASP:O	1:A:195:GLN:HG3	1.87	0.74
1:H:211:LEU:O	1:H:215:ARG:HG3	1.86	0.74
1:C:48:THR:HG23	1:C:68:GLU:HA	1.67	0.74
1:A:225:GLN:O	1:A:226:LEU:C	2.30	0.74
1:F:30:ILE:HG22	1:F:30:ILE:O	1.87	0.74
1:C:207:MET:HB3	1:D:207:MET:HE2	1.69	0.74
1:C:252:ARG:NE	2:C:302:HOH:O	2.17	0.74
1:F:237:VAL:HG12	1:F:237:VAL:O	1.87	0.74
1:H:73:ASP:OD1	2:H:303:HOH:O	2.04	0.73
1:G:139:ARG:O	1:G:159:ARG:NH1	2.21	0.73
1:G:202:SER:O	1:G:203:GLU:CB	2.36	0.73
1:F:272:GLN:O	1:F:276:VAL:CG2	2.35	0.73
1:G:66:ARG:HB3	1:G:82:ASP:HA	1.70	0.73
1:H:198:LEU:O	1:H:202:SER:OG	2.06	0.73
1:F:43:LEU:O	1:F:44:ASP:OD1	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:VAL:O	1:D:138:HIS:ND1	2.21	0.73
1:H:140:ARG:HH11	1:H:141:ASP:H	1.37	0.73
1:B:190:LYS:CD	1:E:241:SER:OG	2.36	0.72
1:E:282:ARG:O	1:E:284:SER:N	2.21	0.72
1:H:78:GLU:OE1	1:H:80:LEU:HD11	1.88	0.72
1:H:129:LEU:HB3	1:H:133:LYS:HE3	1.70	0.72
1:F:133:LYS:NZ	1:F:137:GLU:OE2	2.23	0.72
1:A:216:HIS:ND1	1:A:222:ASN:OD1	2.22	0.72
1:A:215:ARG:HE	1:A:279:HIS:HB3	1.54	0.72
1:A:215:ARG:HH22	1:A:222:ASN:HA	1.55	0.71
1:A:224:ALA:O	1:A:226:LEU:N	2.23	0.71
1:G:140:ARG:O	1:G:159:ARG:NH1	2.24	0.71
1:F:239:THR:O	1:F:240:LEU:HD23	1.89	0.71
1:H:120:GLY:O	2:H:304:HOH:O	2.08	0.71
1:C:282:ARG:O	1:C:283:GLU:HB3	1.90	0.71
1:E:139:ARG:O	1:E:140:ARG:CB	2.38	0.71
1:D:228:GLU:OE2	2:D:301:HOH:O	2.09	0.71
1:C:196:ARG:HE	1:D:176:ALA:HB1	1.54	0.71
1:B:200:ARG:O	1:B:203:GLU:HB2	1.90	0.71
1:G:191:ASP:HB2	1:G:284:SER:OG	1.91	0.71
1:E:207:MET:O	1:E:210:ALA:HB3	1.91	0.71
1:A:207:MET:HG3	1:B:202:SER:OG	1.90	0.70
1:H:98:GLN:O	1:H:102:PRO:CD	2.40	0.70
1:E:203:GLU:O	1:E:204:LYS:HB2	1.89	0.70
1:H:273:LEU:O	1:H:277:LEU:HD12	1.91	0.70
1:F:27:ASP:O	1:F:29:GLN:N	2.25	0.70
1:C:191:ASP:O	1:C:195:GLN:HG3	1.92	0.70
1:F:168:VAL:O	1:F:235:ALA:CB	2.40	0.70
1:F:19:THR:HG22	1:F:227:PRO:HG3	1.73	0.69
1:F:178:LEU:HD11	1:F:226:LEU:HD13	1.73	0.69
1:G:202:SER:O	1:G:203:GLU:HG3	1.92	0.69
1:B:271:ARG:NH2	2:B:303:HOH:O	2.24	0.69
1:E:37:GLU:HA	1:E:37:GLU:OE1	1.93	0.69
1:F:83:GLY:O	1:F:84:ARG:O	2.10	0.69
1:C:139:ARG:CB	2:C:357:HOH:O	2.40	0.69
1:E:220:LYS:O	1:E:221:ALA:HB2	1.93	0.69
1:F:168:VAL:O	1:F:235:ALA:HB1	1.93	0.69
1:A:209:GLY:O	1:A:213:GLY:N	2.15	0.69
1:D:232:THR:OG1	2:D:303:HOH:O	2.10	0.69
1:D:103:MET:O	2:D:302:HOH:O	2.09	0.69
1:E:81:THR:HG23	1:E:86:SER:OG	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:218:GLY:O	1:F:282:ARG:NH2	2.26	0.69
1:H:138:HIS:O	1:H:139:ARG:O	2.11	0.68
1:A:30:ILE:HG22	1:A:30:ILE:O	1.92	0.68
1:F:91:GLU:HG2	1:F:91:GLU:O	1.91	0.68
1:B:19:THR:HG23	1:B:227:PRO:HG3	1.75	0.68
1:F:121:TYR:O	1:F:122:ARG:O	2.11	0.68
1:G:76:ASP:OD1	1:G:77:ILE:N	2.23	0.68
1:F:13:ILE:HG21	1:F:76:ASP:OD1	1.93	0.68
1:F:188:SER:O	1:F:190:LYS:HG2	1.94	0.68
1:F:84:ARG:HG2	2:F:307:HOH:O	1.94	0.68
1:C:117:LEU:O	1:C:118:GLY:C	2.37	0.68
1:E:66:ARG:NH1	1:E:68:GLU:OE1	2.27	0.68
1:F:13:ILE:CG2	1:F:76:ASP:OD1	2.42	0.68
1:A:66:ARG:NH1	1:A:68:GLU:OE2	2.26	0.67
1:F:268:VAL:HG12	1:F:271:ARG:HH21	1.60	0.67
1:F:52:GLN:NE2	1:F:67:HIS:O	2.26	0.67
1:H:204:LYS:O	1:H:205:ASP:CB	2.42	0.67
1:H:122:ARG:HG2	1:H:145:ASP:OD1	1.95	0.67
1:C:126:ASP:OD1	1:C:126:ASP:N	2.26	0.67
1:C:159:ARG:CD	2:C:326:HOH:O	2.42	0.67
1:F:192:ARG:O	1:F:196:ARG:HG3	1.94	0.67
1:A:276:VAL:O	1:A:279:HIS:HB2	1.93	0.67
1:G:13:ILE:HD11	1:G:90:SER:HB3	1.77	0.67
1:H:124:PRO:O	1:H:125:GLY:O	2.13	0.67
1:H:220:LYS:O	1:H:221:ALA:CB	2.42	0.67
1:A:19:THR:O	1:A:22:SER:HB2	1.95	0.67
1:C:56:GLY:O	2:C:301:HOH:O	2.11	0.67
1:A:134:VAL:O	1:A:138:HIS:O	2.13	0.67
1:F:94:GLY:O	1:F:97:ALA:HB3	1.95	0.67
1:G:220:LYS:O	1:G:220:LYS:HD3	1.95	0.67
1:F:215:ARG:CG	1:F:280:GLY:O	2.42	0.66
1:C:38:ALA:O	1:C:39:ASP:O	2.13	0.66
1:F:48:THR:O	1:F:48:THR:HG22	1.93	0.66
1:B:160:LYS:CE	2:B:307:HOH:O	2.43	0.66
1:D:150:ARG:NH2	2:D:304:HOH:O	2.28	0.66
1:F:151:GLY:O	1:F:170:ARG:NH2	2.28	0.66
1:H:83:GLY:O	1:H:84:ARG:C	2.39	0.66
1:G:202:SER:O	1:G:203:GLU:HB2	1.96	0.66
1:A:218:GLY:HA3	1:A:280:GLY:O	1.95	0.66
1:C:215:ARG:HH22	1:C:223:LEU:HD12	1.60	0.66
1:H:70:ARG:HH21	1:H:72:THR:HG22	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:MET:C	1:B:208:LEU:O	2.34	0.65
1:F:144:THR:CG2	1:F:145:ASP:O	2.44	0.65
1:H:270:THR:O	1:H:274:SER:OG	2.13	0.65
1:H:283:GLU:O	1:H:284:SER:C	2.38	0.65
1:B:160:LYS:HE2	2:B:307:HOH:O	1.94	0.65
1:A:99:ALA:O	1:A:102:PRO:HD2	1.97	0.65
1:E:138:HIS:HE1	2:E:373:HOH:O	1.74	0.65
1:D:10:THR:CG2	2:D:335:HOH:O	2.34	0.65
1:H:168:VAL:HG12	1:H:262:LEU:HD12	1.79	0.65
1:A:192:ARG:O	1:A:196:ARG:HG3	1.96	0.64
1:C:197:GLU:OE2	1:C:201:ARG:HD2	1.97	0.64
1:E:203:GLU:HG3	1:F:204:LYS:H	1.62	0.64
1:H:66:ARG:NH2	1:H:68:GLU:OE2	2.30	0.64
1:A:207:MET:HG2	1:B:207:MET:HG2	1.80	0.64
1:F:44:ASP:HA	1:F:47:LEU:HB2	1.77	0.64
1:F:197:GLU:O	1:F:201:ARG:HG3	1.96	0.64
1:B:283:GLU:O	1:B:284:SER:CB	2.45	0.64
1:F:69:ALA:HA	1:F:78:GLU:O	1.97	0.64
1:C:94:GLY:O	1:C:98:GLN:HG3	1.96	0.64
1:C:280:GLY:O	1:C:281:LEU:O	2.16	0.64
1:F:26:VAL:HG12	1:F:28:SER:H	1.62	0.64
1:F:55:GLN:OE1	1:F:62:LEU:HD12	1.97	0.64
1:F:126:ASP:O	1:F:127:LEU:C	2.41	0.64
1:C:81:THR:OG1	1:C:103:MET:HE1	1.98	0.64
1:G:132:LEU:O	1:G:136:ILE:HG12	1.97	0.64
1:H:132:LEU:O	1:H:136:ILE:HG12	1.97	0.64
1:F:272:GLN:HA	1:F:275:GLU:HG2	1.80	0.64
1:D:205:ASP:OD1	1:D:206:GLY:N	2.31	0.64
1:E:19:THR:HG22	1:E:227:PRO:HG3	1.80	0.64
1:F:240:LEU:HD11	1:F:250:GLU:O	1.98	0.64
1:H:200:ARG:O	1:H:202:SER:O	2.16	0.64
1:G:202:SER:O	1:G:203:GLU:CG	2.47	0.63
1:H:204:LYS:O	1:H:205:ASP:HB2	1.98	0.63
1:F:137:GLU:O	1:F:138:HIS:HB2	1.97	0.63
1:B:16:ALA:O	1:B:19:THR:HG22	1.97	0.63
1:A:64:HIS:HE2	1:A:114:TRP:CD1	2.16	0.63
1:C:23:THR:HG21	1:C:227:PRO:HB2	1.81	0.63
1:A:78:GLU:OE2	1:A:85:PRO:HB3	1.99	0.63
1:B:136:ILE:O	1:B:159:ARG:NH2	2.32	0.63
1:E:197:GLU:O	1:E:201:ARG:HG3	1.99	0.63
1:C:207:MET:SD	1:D:207:MET:HG2	2.39	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:THR:HG21	2:B:416:HOH:O	1.98	0.62
1:E:203:GLU:O	1:E:204:LYS:CB	2.47	0.62
1:A:215:ARG:O	1:A:219:ALA:HB3	1.99	0.62
1:C:219:ALA:HB2	1:C:280:GLY:HA2	1.80	0.62
1:H:78:GLU:HG3	1:H:88:ARG:HG2	1.82	0.62
1:H:122:ARG:N	2:H:306:HOH:O	2.32	0.62
1:A:208:LEU:HG	1:B:199:MET:HE1	1.82	0.61
1:F:204:LYS:O	1:F:204:LYS:CG	2.47	0.61
1:F:126:ASP:OD1	1:F:126:ASP:N	2.33	0.61
1:H:201:ARG:O	1:H:205:ASP:HB2	2.00	0.61
1:G:220:LYS:O	1:G:220:LYS:CG	2.48	0.61
1:C:196:ARG:NH2	1:D:180:ASP:OD2	2.33	0.61
1:E:76:ASP:OD2	1:E:90:SER:OG	2.11	0.61
1:F:43:LEU:O	1:F:44:ASP:CG	2.43	0.61
1:F:227:PRO:HG2	1:F:228:GLU:OE1	2.01	0.61
1:B:275:GLU:OE2	2:B:302:HOH:O	2.15	0.61
1:H:98:GLN:O	1:H:102:PRO:HD3	1.98	0.61
1:H:157:VAL:HG23	1:H:165:PHE:O	2.00	0.61
1:H:220:LYS:O	1:H:221:ALA:HB2	2.01	0.61
1:C:28:SER:HB2	1:C:30:ILE:HG12	1.81	0.61
1:A:224:ALA:O	1:A:225:GLN:C	2.42	0.60
1:D:201:ARG:HH22	1:D:214:ALA:HB2	1.66	0.60
1:E:202:SER:CB	1:F:206:GLY:O	2.46	0.60
1:C:276:VAL:O	1:C:279:HIS:HB3	2.00	0.60
1:F:71:LEU:CD2	1:F:76:ASP:O	2.47	0.60
1:C:159:ARG:HD2	2:C:326:HOH:O	2.01	0.60
1:G:163:THR:CG2	1:G:240:LEU:O	2.43	0.60
1:E:170:ARG:NH2	1:E:263:GLU:OE1	2.33	0.60
1:C:122:ARG:O	1:C:122:ARG:HG3	2.01	0.60
1:G:175:GLU:CD	1:G:175:GLU:H	2.09	0.60
1:D:221:ALA:O	1:D:222:ASN:CB	2.49	0.60
1:F:257:THR:O	1:F:258:ALA:C	2.45	0.60
1:A:108:GLU:CD	1:A:108:GLU:H	2.10	0.60
1:G:159:ARG:HB2	1:G:164:LEU:HD12	1.83	0.60
1:H:140:ARG:HB3	2:H:316:HOH:O	2.00	0.60
1:D:117:LEU:O	1:D:119:GLU:N	2.26	0.60
1:E:220:LYS:O	1:E:221:ALA:CB	2.49	0.60
1:H:110:GLY:O	1:H:171:PRO:HB3	2.01	0.60
1:E:7:LYS:HA	1:E:7:LYS:HZ3	1.66	0.59
1:H:151:GLY:O	1:H:152:GLU:HB2	2.01	0.59
1:E:170:ARG:HH12	1:E:263:GLU:CD	2.10	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:141:ASP:O	1:F:142:PHE:CB	2.51	0.59
1:D:26:VAL:HG22	1:D:53:GLU:HG2	1.85	0.59
1:F:125:GLY:O	1:F:127:LEU:N	2.35	0.59
1:F:143:GLU:HG3	1:F:158:TRP:HB3	1.83	0.59
1:H:281:LEU:O	1:H:283:GLU:N	2.35	0.59
1:A:140:ARG:H	1:A:140:ARG:HD2	1.68	0.59
1:C:271:ARG:NH2	2:C:303:HOH:O	2.29	0.59
1:F:216:HIS:O	1:F:221:ALA:O	2.21	0.59
1:F:92:GLY:O	1:F:95:ALA:HB3	2.03	0.59
1:H:204:LYS:O	1:H:205:ASP:OD1	2.21	0.59
1:G:173:SER:HB2	1:G:175:GLU:HG2	1.85	0.59
1:G:197:GLU:OE1	1:G:282:ARG:NH1	2.36	0.59
1:H:137:GLU:HG2	2:H:309:HOH:O	2.02	0.59
1:C:209:GLY:O	1:C:213:GLY:N	2.36	0.58
1:E:130:ALA:O	1:E:133:LYS:HG2	2.03	0.58
1:H:98:GLN:O	1:H:102:PRO:HD2	2.03	0.58
1:D:280:GLY:O	1:D:281:LEU:HD23	2.03	0.58
1:G:207:MET:O	1:G:210:ALA:HB3	2.03	0.58
1:A:262:LEU:O	1:A:266:GLN:HG3	2.03	0.58
1:D:10:THR:HG22	1:D:10:THR:O	2.04	0.58
1:D:19:THR:HG22	1:D:227:PRO:HG3	1.86	0.58
1:F:86:SER:O	1:F:87:ALA:HB2	2.04	0.58
1:H:122:ARG:CG	1:H:145:ASP:OD1	2.52	0.58
1:H:276:VAL:HG12	1:H:276:VAL:O	2.03	0.58
1:C:263:GLU:O	1:C:264:GLU:C	2.45	0.58
1:E:68:GLU:CD	2:E:302:HOH:O	2.46	0.58
1:E:144:THR:HG23	1:E:145:ASP:O	2.03	0.57
1:H:173:SER:OG	1:H:176:ALA:HB2	2.04	0.57
1:E:209:GLY:O	1:E:213:GLY:N	2.36	0.57
1:F:192:ARG:O	1:F:196:ARG:CG	2.52	0.57
1:D:152:GLU:HG3	2:D:360:HOH:O	2.04	0.57
1:G:220:LYS:O	1:G:220:LYS:CD	2.53	0.57
1:F:46:ALA:HA	1:F:49:GLN:HG3	1.85	0.57
1:D:268:VAL:HG11	1:G:268:VAL:HG11	1.86	0.57
1:B:197:GLU:OE2	1:B:201:ARG:NH1	2.38	0.57
1:A:66:ARG:N	1:A:82:ASP:OD1	2.36	0.57
1:A:71:LEU:HD12	1:A:71:LEU:H	1.69	0.57
1:F:21:MET:HB3	1:F:26:VAL:HB	1.86	0.57
1:H:27:ASP:OD1	1:H:29:GLN:HG2	2.04	0.57
1:H:209:GLY:O	1:H:213:GLY:N	2.38	0.57
1:C:43:LEU:HD23	1:C:71:LEU:HD11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:122:ARG:O	1:H:123:ALA:C	2.48	0.57
1:H:244:ALA:HB1	1:H:250:GLU:OE1	2.04	0.57
1:B:283:GLU:O	1:B:284:SER:HB2	2.03	0.57
1:G:136:ILE:O	1:G:159:ARG:NH2	2.37	0.57
1:F:47:LEU:O	1:F:69:ALA:HB3	2.05	0.56
1:E:70:ARG:HD2	2:E:362:HOH:O	2.05	0.56
1:E:191:ASP:OD2	1:E:193:ALA:HB3	2.06	0.56
1:F:17:PHE:O	1:F:21:MET:HG2	2.06	0.56
1:G:260:ALA:O	1:G:264:GLU:HG3	2.06	0.56
1:A:28:SER:O	1:A:29:GLN:HG2	2.04	0.56
1:D:163:THR:HG23	1:D:239:THR:OG1	2.06	0.56
1:A:72:THR:OG1	1:A:74:ASP:OD1	2.22	0.56
1:E:144:THR:CG2	1:E:145:ASP:O	2.53	0.56
1:H:123:ALA:O	1:H:125:GLY:N	2.39	0.56
1:C:107:ASP:OD1	1:C:109:ARG:N	2.39	0.56
1:F:215:ARG:O	1:F:216:HIS:C	2.48	0.56
1:H:122:ARG:C	1:H:123:ALA:O	2.50	0.55
1:B:124:PRO:HD2	1:B:127:LEU:HD21	1.89	0.55
1:C:215:ARG:CG	1:C:279:HIS:O	2.52	0.55
1:E:7:LYS:HD3	1:E:8:ASP:H	1.69	0.55
1:H:211:LEU:O	1:H:281:LEU:HD21	2.06	0.55
1:C:37:GLU:OE2	1:C:37:GLU:HA	2.05	0.55
1:C:191:ASP:OD1	1:C:193:ALA:N	2.38	0.55
1:H:55:GLN:NE2	1:H:60:LEU:HD12	2.22	0.55
1:A:121:TYR:O	1:A:122:ARG:CG	2.55	0.55
1:G:272:GLN:O	1:G:275:GLU:HG2	2.06	0.55
1:D:74:ASP:OD1	1:D:74:ASP:N	2.39	0.55
1:E:214:ALA:O	1:E:217:ALA:HB2	2.07	0.55
1:G:147:SER:O	1:G:148:ALA:C	2.49	0.55
1:A:272:GLN:O	1:A:276:VAL:HG23	2.07	0.55
1:C:265:TYR:HA	1:C:268:VAL:HG22	1.89	0.55
1:H:173:SER:OG	1:H:176:ALA:CB	2.55	0.55
1:C:57:ARG:HA	1:C:235:ALA:O	2.06	0.54
1:F:27:ASP:O	1:F:29:GLN:HG2	2.06	0.54
1:F:101:ALA:HB3	1:F:102:PRO:HD3	1.89	0.54
1:E:208:LEU:HD22	1:E:212:LEU:HG	1.89	0.54
1:F:36:SER:O	1:F:37:GLU:HB2	2.07	0.54
1:F:70:ARG:O	1:F:71:LEU:HD23	2.07	0.54
1:H:149:GLY:O	1:H:150:ARG:C	2.50	0.54
1:B:178:LEU:HD13	1:B:208:LEU:HD11	1.89	0.54
1:F:83:GLY:O	1:F:84:ARG:C	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:164:LEU:HD21	1:F:251:TYR:HD2	1.71	0.54
1:F:104:GLN:HA	1:F:114:TRP:HE1	1.72	0.54
1:B:119:GLU:HG3	1:B:119:GLU:O	2.07	0.54
1:D:33:LEU:HD23	1:D:43:LEU:HD13	1.89	0.54
1:F:214:ALA:HA	1:F:218:GLY:HA3	1.89	0.54
1:H:182:ALA:O	1:H:185:VAL:HB	2.07	0.54
1:F:272:GLN:O	1:F:276:VAL:CB	2.55	0.54
1:G:218:GLY:HA3	1:G:280:GLY:O	2.08	0.54
1:A:265:TYR:HA	1:A:268:VAL:HG22	1.89	0.54
1:E:170:ARG:NH1	1:E:263:GLU:OE1	2.41	0.54
1:A:225:GLN:OE1	1:A:225:GLN:HA	2.08	0.54
1:G:139:ARG:O	1:G:140:ARG:O	2.26	0.54
1:A:191:ASP:OD2	1:A:194:PHE:CB	2.56	0.54
1:C:38:ALA:O	1:C:39:ASP:C	2.49	0.54
1:D:178:LEU:HD23	1:D:273:LEU:HD21	1.90	0.54
1:F:75:GLY:O	1:F:76:ASP:C	2.51	0.54
1:H:192:ARG:O	1:H:196:ARG:HG2	2.06	0.54
1:C:203:GLU:N	1:C:205:ASP:O	2.41	0.54
1:C:208:LEU:HB2	1:D:199:MET:HE3	1.89	0.54
1:E:239:THR:HB	2:E:371:HOH:O	2.07	0.54
1:F:148:ALA:O	1:F:155:GLN:HG2	2.08	0.53
1:H:58:TRP:O	1:H:234:GLN:HB2	2.08	0.53
1:F:48:THR:O	1:F:48:THR:CG2	2.56	0.53
1:G:130:ALA:HA	1:G:133:LYS:HD2	1.89	0.53
1:H:125:GLY:O	1:H:126:ASP:C	2.51	0.53
1:B:173:SER:OG	1:B:175:GLU:HG2	2.08	0.53
1:D:61:GLY:HA3	1:D:112:SER:HB2	1.89	0.53
1:A:122:ARG:HG3	1:A:122:ARG:O	2.08	0.53
1:A:276:VAL:O	1:A:279:HIS:CB	2.57	0.53
1:F:281:LEU:HD23	1:F:282:ARG:HD2	1.90	0.53
1:E:119:GLU:O	1:E:122:ARG:HB3	2.08	0.53
1:F:17:PHE:HE1	1:F:79:ILE:HD11	1.73	0.53
1:C:268:VAL:O	1:C:272:GLN:HG3	2.07	0.53
1:D:190:LYS:HG3	1:G:241:SER:HB2	1.89	0.53
1:D:220:LYS:HD2	1:G:39:ASP:HB3	1.90	0.53
1:G:171:PRO:HA	1:G:234:GLN:OE1	2.08	0.53
1:G:247:ASN:OD1	1:G:249:GLU:HB2	2.09	0.53
1:A:157:VAL:HG23	1:A:166:VAL:HG22	1.90	0.53
1:G:138:HIS:O	1:G:139:ARG:C	2.51	0.53
1:F:12:GLY:O	1:F:16:ALA:CB	2.53	0.52
1:B:160:LYS:NZ	2:B:307:HOH:O	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:ILE:O	1:C:159:ARG:NH2	2.40	0.52
1:F:78:GLU:O	1:F:80:LEU:HD12	2.08	0.52
1:F:125:GLY:C	1:F:126:ASP:OD1	2.53	0.52
1:H:244:ALA:CB	1:H:250:GLU:OE1	2.57	0.52
1:F:166:VAL:HB	1:F:238:GLN:HB3	1.90	0.52
1:G:192:ARG:O	1:G:196:ARG:HG3	2.10	0.52
1:D:144:THR:HG23	1:D:145:ASP:O	2.09	0.52
1:F:152:GLU:O	1:F:152:GLU:HG2	2.09	0.52
1:C:122:ARG:O	1:C:122:ARG:CG	2.58	0.52
1:D:282:ARG:O	1:D:283:GLU:CB	2.45	0.52
1:D:212:LEU:O	1:D:215:ARG:HB2	2.09	0.52
1:G:57:ARG:HA	1:G:235:ALA:O	2.08	0.52
1:G:61:GLY:O	1:G:62:LEU:HD23	2.10	0.52
1:A:126:ASP:O	1:A:127:LEU:C	2.53	0.52
1:B:282:ARG:HG2	2:B:363:HOH:O	2.10	0.52
1:E:7:LYS:HD3	1:E:8:ASP:N	2.25	0.52
1:G:109:ARG:O	1:G:171:PRO:HG2	2.09	0.52
1:H:117:LEU:C	1:H:119:GLU:H	2.18	0.51
1:C:222:ASN:CG	1:C:222:ASN:O	2.52	0.51
1:F:136:ILE:HG23	1:F:159:ARG:NH2	2.24	0.51
1:F:200:ARG:O	1:F:202:SER:O	2.28	0.51
1:H:199:MET:O	1:H:202:SER:OG	2.27	0.51
1:A:123:ALA:N	1:A:143:GLU:O	2.35	0.51
1:A:124:PRO:HB2	1:A:126:ASP:OD1	2.11	0.51
1:F:202:SER:O	1:F:203:GLU:HB3	2.11	0.51
1:H:275:GLU:HA	1:H:278:ARG:HB2	1.93	0.51
1:C:204:LYS:O	1:E:120:GLY:HA3	2.09	0.51
1:C:215:ARG:NE	1:C:276:VAL:O	2.43	0.51
1:G:19:THR:HG23	1:G:227:PRO:HG3	1.92	0.51
1:B:190:LYS:HD2	1:E:241:SER:HG	1.70	0.51
1:C:282:ARG:O	1:C:283:GLU:CB	2.58	0.51
1:E:219:ALA:CB	2:E:384:HOH:O	2.46	0.51
1:C:143:GLU:HB2	1:C:158:TRP:HB3	1.93	0.51
1:E:216:HIS:CE1	1:E:223:LEU:HD22	2.46	0.51
1:F:62:LEU:HD22	1:F:65:LEU:HD12	1.93	0.51
1:B:61:GLY:HA3	1:B:112:SER:HB2	1.92	0.51
1:C:159:ARG:HD3	2:C:326:HOH:O	2.09	0.51
1:E:178:LEU:HD13	1:E:208:LEU:HD11	1.93	0.51
1:D:223:LEU:HD23	1:D:224:ALA:O	2.10	0.50
1:E:139:ARG:H	1:E:246:ARG:NH2	2.09	0.50
1:H:24:ALA:HB1	1:H:57:ARG:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:PHE:CZ	1:A:281:LEU:HB3	2.47	0.50
1:C:192:ARG:HB3	1:C:196:ARG:NH1	2.26	0.50
1:H:273:LEU:O	1:H:273:LEU:HG	2.10	0.50
1:E:131:GLN:O	1:E:134:VAL:HB	2.11	0.50
1:B:228:GLU:HG2	1:B:273:LEU:HD22	1.94	0.50
1:F:276:VAL:O	1:F:276:VAL:CG1	2.59	0.50
1:G:265:TYR:O	1:G:269:THR:OG1	2.23	0.50
1:B:159:ARG:HB2	1:B:164:LEU:HD12	1.92	0.50
1:F:64:HIS:CE1	1:F:65:LEU:HG	2.46	0.50
1:F:243:ALA:O	1:F:247:ASN:HB2	2.12	0.50
1:G:204:LYS:O	1:H:203:GLU:OE1	2.30	0.50
1:B:268:VAL:O	1:B:272:GLN:HG3	2.12	0.50
1:H:269:THR:HA	1:H:272:GLN:HB2	1.94	0.50
1:E:122:ARG:NH2	2:E:306:HOH:O	2.44	0.49
1:H:282:ARG:O	1:H:282:ARG:HG3	2.11	0.49
1:A:207:MET:HG2	1:B:207:MET:CG	2.41	0.49
1:D:53:GLU:OE1	1:G:275:GLU:OE1	2.30	0.49
1:F:121:TYR:O	1:F:122:ARG:C	2.55	0.49
1:H:276:VAL:O	1:H:276:VAL:CG1	2.59	0.49
1:A:16:ALA:O	1:A:17:PHE:C	2.54	0.49
1:F:240:LEU:CD1	1:F:250:GLU:O	2.60	0.49
1:G:182:ALA:HB1	1:G:211:LEU:HD12	1.94	0.49
1:A:191:ASP:OD2	1:A:194:PHE:HB2	2.12	0.49
1:H:116:ALA:H	1:H:143:GLU:CD	2.20	0.49
1:H:204:LYS:O	1:H:205:ASP:CG	2.55	0.49
1:E:13:ILE:HD13	1:E:76:ASP:HA	1.94	0.49
1:A:24:ALA:O	1:A:57:ARG:HD2	2.13	0.49
1:F:215:ARG:CB	1:F:280:GLY:O	2.60	0.49
1:A:283:GLU:HG3	1:A:283:GLU:O	2.13	0.49
1:G:144:THR:HG23	1:G:145:ASP:O	2.12	0.49
1:H:220:LYS:O	1:H:220:LYS:CD	2.50	0.49
1:A:213:GLY:C	1:A:215:ARG:H	2.21	0.49
1:B:144:THR:HG22	1:B:157:VAL:H	1.78	0.49
1:C:66:ARG:O	1:C:81:THR:HA	2.12	0.49
1:H:123:ALA:HB1	1:H:124:PRO:HD2	1.94	0.49
1:F:75:GLY:C	1:F:76:ASP:O	2.51	0.49
1:C:155:GLN:HA	1:C:167:GLU:O	2.13	0.48
1:E:143:GLU:HB2	1:E:158:TRP:HB3	1.95	0.48
1:H:178:LEU:HD23	1:H:273:LEU:HD21	1.94	0.48
1:A:30:ILE:O	1:A:30:ILE:CG2	2.60	0.48
1:D:144:THR:HG21	2:D:347:HOH:O	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:220:LYS:O	1:G:220:LYS:HG2	2.12	0.48
1:F:98:GLN:O	1:F:102:PRO:HD3	2.14	0.48
1:G:34:ALA:O	1:G:37:GLU:N	2.40	0.48
1:E:119:GLU:N	1:E:120:GLY:HA3	2.28	0.48
1:F:147:SER:O	1:F:148:ALA:O	2.31	0.48
1:G:69:ALA:HA	1:G:78:GLU:O	2.14	0.48
1:A:225:GLN:NE2	2:A:303:HOH:O	2.46	0.48
1:F:207:MET:HE1	1:F:211:LEU:HD12	1.94	0.48
1:G:81:THR:O	1:G:82:ASP:HB2	2.14	0.48
1:A:136:ILE:O	1:A:159:ARG:NH2	2.46	0.48
1:C:38:ALA:C	1:C:39:ASP:O	2.56	0.48
1:D:163:THR:HG23	1:D:239:THR:HG1	1.79	0.48
1:G:72:THR:OG1	1:G:74:ASP:OD1	2.16	0.48
1:G:144:THR:HG22	1:G:157:VAL:H	1.78	0.48
1:G:261:ALA:O	1:G:262:LEU:C	2.57	0.48
1:H:238:GLN:HB2	1:H:258:ALA:HB2	1.95	0.48
1:A:13:ILE:HD11	1:A:90:SER:HB3	1.96	0.48
1:A:247:ASN:OD1	1:A:249:GLU:N	2.47	0.48
1:E:203:GLU:CG	1:F:204:LYS:H	2.26	0.48
1:C:181:ALA:O	1:C:185:VAL:HG23	2.14	0.47
1:D:121:TYR:HD1	1:D:121:TYR:H	1.62	0.47
1:D:170:ARG:HB3	1:D:266:GLN:HE22	1.79	0.47
1:E:197:GLU:OE2	1:E:201:ARG:HD2	2.14	0.47
1:F:282:ARG:O	1:F:283:GLU:HB3	2.13	0.47
1:G:183:TRP:CE2	1:H:195:GLN:HG2	2.49	0.47
1:D:221:ALA:O	1:D:222:ASN:HB2	2.13	0.47
1:F:119:GLU:O	1:F:120:GLY:C	2.55	0.47
1:G:166:VAL:O	1:G:237:VAL:HA	2.12	0.47
1:A:186:ILE:HG23	1:B:183:TRP:CH2	2.49	0.47
1:C:37:GLU:O	1:C:38:ALA:HB2	2.14	0.47
1:E:118:GLY:C	1:E:120:GLY:HA3	2.40	0.47
1:F:202:SER:O	1:F:203:GLU:CB	2.62	0.47
1:H:191:ASP:OD1	1:H:191:ASP:O	2.32	0.47
1:C:191:ASP:OD1	1:C:191:ASP:C	2.58	0.47
1:E:37:GLU:OE1	1:E:37:GLU:CA	2.58	0.47
1:D:66:ARG:NH2	2:D:312:HOH:O	2.47	0.47
1:E:111:LEU:HD21	1:E:154:PHE:CD2	2.50	0.47
1:H:122:ARG:NE	1:H:145:ASP:OD1	2.47	0.47
1:A:194:PHE:O	1:A:197:GLU:HB3	2.14	0.47
1:C:158:TRP:O	1:C:164:LEU:HD12	2.15	0.47
1:D:84:ARG:NH2	2:D:313:HOH:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:ARG:NH2	1:D:214:ALA:HB2	2.28	0.47
1:E:111:LEU:HD13	1:E:171:PRO:HG3	1.96	0.47
1:E:180:ASP:OD1	1:F:196:ARG:NE	2.46	0.47
1:F:107:ASP:OD2	1:F:109:ARG:NH2	2.48	0.47
1:G:78:GLU:OE2	1:G:85:PRO:HB3	2.15	0.47
1:A:216:HIS:CG	1:A:222:ASN:OD1	2.68	0.47
1:G:248:ALA:O	1:G:252:ARG:HG2	2.15	0.47
1:A:212:LEU:O	1:A:215:ARG:CB	2.61	0.47
1:F:185:VAL:HB	1:F:211:LEU:HD11	1.96	0.47
1:H:212:LEU:O	1:H:216:HIS:N	2.31	0.47
1:F:121:TYR:C	1:F:122:ARG:O	2.58	0.47
1:A:78:GLU:OE2	1:A:85:PRO:HG3	2.15	0.46
1:G:133:LYS:O	1:G:137:GLU:HG3	2.15	0.46
1:D:141:ASP:OD2	1:D:160:LYS:HA	2.15	0.46
1:F:38:ALA:O	1:F:39:ASP:O	2.34	0.46
1:H:136:ILE:O	1:H:159:ARG:NH2	2.45	0.46
1:D:207:MET:O	1:D:210:ALA:HB3	2.15	0.46
1:H:37:GLU:O	1:H:38:ALA:C	2.57	0.46
1:F:30:ILE:HG21	1:F:47:LEU:HD21	1.97	0.46
1:F:243:ALA:O	1:F:247:ASN:CB	2.64	0.46
1:C:252:ARG:HB3	1:C:252:ARG:NH1	2.31	0.46
1:C:261:ALA:O	1:C:262:LEU:C	2.55	0.46
1:D:133:LYS:HD2	2:D:368:HOH:O	2.15	0.46
1:G:244:ALA:HA	1:G:250:GLU:HG3	1.97	0.46
1:A:19:THR:HG22	1:A:227:PRO:HG3	1.97	0.46
1:E:186:ILE:HD13	1:E:211:LEU:HD12	1.97	0.46
1:F:58:TRP:O	1:F:234:GLN:NE2	2.44	0.46
1:F:199:MET:O	1:F:202:SER:HB2	2.14	0.46
1:D:117:LEU:HD12	1:D:143:GLU:HB2	1.98	0.46
1:H:126:ASP:CG	1:H:147:SER:HB3	2.41	0.46
1:H:129:LEU:H	1:H:129:LEU:HD12	1.81	0.46
1:A:138:HIS:HA	1:A:139:ARG:HA	1.66	0.46
1:C:183:TRP:CZ3	1:D:195:GLN:O	2.69	0.46
1:G:19:THR:CG2	1:G:227:PRO:HG3	2.46	0.46
1:A:218:GLY:CA	1:A:280:GLY:O	2.63	0.45
1:F:91:GLU:O	1:F:91:GLU:CG	2.62	0.45
1:E:219:ALA:CA	2:E:384:HOH:O	2.63	0.45
1:C:107:ASP:OD1	1:C:107:ASP:C	2.60	0.45
1:F:252:ARG:O	1:F:256:LYS:CG	2.60	0.45
1:H:62:LEU:HD22	1:H:65:LEU:HD12	1.98	0.45
1:H:65:LEU:O	1:H:67:HIS:CD2	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:GLU:CD	1:D:108:GLU:H	2.24	0.45
1:F:206:GLY:HA3	1:F:207:MET:HA	1.83	0.45
1:H:121:TYR:CA	2:H:306:HOH:O	2.64	0.45
1:B:219:ALA:HA	1:E:42:THR:OG1	2.17	0.45
1:C:199:MET:HB3	1:C:199:MET:HE3	1.48	0.45
1:F:128:PRO:HD2	1:F:131:GLN:HB2	1.98	0.45
1:F:125:GLY:O	1:F:126:ASP:C	2.60	0.45
1:F:265:TYR:HA	1:F:268:VAL:HG22	1.98	0.45
1:A:201:ARG:HA	1:A:201:ARG:HD2	1.75	0.45
1:G:199:MET:SD	1:H:208:LEU:HB2	2.56	0.45
1:H:115:ALA:HB1	1:H:143:GLU:OE1	2.17	0.45
1:H:270:THR:O	1:H:270:THR:HG22	2.16	0.45
1:A:106:LEU:HD23	1:A:112:SER:HA	1.98	0.44
1:A:120:GLY:O	1:A:121:TYR:C	2.59	0.44
1:D:134:VAL:O	1:D:138:HIS:CE1	2.70	0.44
1:D:220:LYS:O	1:D:220:LYS:HG2	2.17	0.44
1:F:253:ALA:O	1:F:256:LYS:HB2	2.16	0.44
1:A:143:GLU:HG3	1:A:158:TRP:HB3	1.99	0.44
1:B:18:ASP:HA	1:B:28:SER:OG	2.17	0.44
1:B:183:TRP:CZ3	1:B:207:MET:HE1	2.52	0.44
1:B:197:GLU:OE1	1:B:282:ARG:NH1	2.46	0.44
1:C:61:GLY:HA3	1:C:112:SER:HB2	1.99	0.44
1:E:185:VAL:CG2	1:E:274:SER:O	2.65	0.44
1:F:276:VAL:O	1:F:276:VAL:HG13	2.16	0.44
1:G:10:THR:HA	1:G:13:ILE:HD12	1.99	0.44
1:G:282:ARG:O	1:G:283:GLU:C	2.61	0.44
1:F:24:ALA:HB3	1:F:26:VAL:HG23	1.98	0.44
1:G:188:SER:O	1:G:190:LYS:HG2	2.18	0.44
1:A:44:ASP:OD1	1:A:71:LEU:HD12	2.18	0.44
1:E:130:ALA:O	1:E:133:LYS:CG	2.66	0.44
1:H:166:VAL:HG11	1:H:255:LEU:HA	2.00	0.44
1:C:203:GLU:CD	1:C:203:GLU:O	2.61	0.44
1:C:247:ASN:OD1	1:C:249:GLU:N	2.51	0.44
1:F:156:ARG:HG3	1:F:158:TRP:HZ3	1.81	0.44
1:H:14:TYR:HE1	1:H:71:LEU:HD21	1.81	0.44
1:H:129:LEU:O	1:H:133:LYS:HG3	2.17	0.44
1:C:78:GLU:OE2	1:C:85:PRO:HB3	2.17	0.44
1:D:14:TYR:N	1:D:14:TYR:CD1	2.86	0.44
1:F:27:ASP:O	1:F:28:SER:C	2.60	0.44
1:B:264:GLU:O	1:B:268:VAL:HG13	2.18	0.43
1:F:200:ARG:O	1:F:201:ARG:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:43:LEU:HD12	1:H:43:LEU:HA	1.89	0.43
1:H:121:TYR:HA	2:H:306:HOH:O	2.17	0.43
1:D:185:VAL:HG21	1:D:277:LEU:HB3	2.00	0.43
1:A:121:TYR:O	1:A:122:ARG:HG3	2.18	0.43
1:F:45:ALA:O	1:F:49:GLN:HG2	2.18	0.43
1:F:80:LEU:HB3	1:F:84:ARG:O	2.18	0.43
1:G:138:HIS:O	1:G:138:HIS:ND1	2.49	0.43
1:A:216:HIS:CE1	1:A:222:ASN:OD1	2.71	0.43
1:B:256:LYS:CE	2:B:333:HOH:O	2.65	0.43
1:F:24:ALA:HA	1:F:233:VAL:HG22	2.01	0.43
1:E:206:GLY:CA	1:F:202:SER:HB3	2.48	0.43
1:G:283:GLU:HB3	1:G:284:SER:H	1.56	0.43
1:H:100:TYR:O	1:H:103:MET:HG3	2.18	0.43
1:B:121:TYR:HA	2:B:319:HOH:O	2.19	0.43
1:F:30:ILE:O	1:F:30:ILE:CG2	2.59	0.43
1:F:48:THR:HG23	1:F:68:GLU:HA	2.00	0.43
1:F:281:LEU:HD23	1:F:283:GLU:H	1.83	0.43
1:A:225:GLN:O	1:A:226:LEU:O	2.37	0.43
1:E:264:GLU:O	1:E:268:VAL:HG13	2.19	0.43
1:F:199:MET:HE3	1:F:199:MET:HB3	1.91	0.43
1:A:48:THR:HG23	1:A:68:GLU:HA	2.01	0.43
1:A:100:TYR:O	1:A:101:ALA:C	2.61	0.43
1:D:162:ASP:O	1:D:241:SER:HA	2.19	0.43
1:A:92:GLY:O	1:A:93:PHE:C	2.60	0.43
1:A:204:LYS:H	1:A:204:LYS:HG3	1.76	0.43
1:F:118:GLY:C	1:F:119:GLU:O	2.61	0.43
1:F:169:ALA:O	1:F:171:PRO:HD3	2.18	0.43
1:E:228:GLU:HG2	1:E:273:LEU:HD22	2.01	0.42
1:F:28:SER:HB2	1:F:30:ILE:HG12	2.01	0.42
1:G:186:ILE:HG13	1:G:211:LEU:HG	2.01	0.42
1:H:216:HIS:O	1:H:217:ALA:HB2	2.18	0.42
1:E:216:HIS:HD2	2:E:316:HOH:O	2.02	0.42
1:F:86:SER:O	1:F:87:ALA:CB	2.67	0.42
1:F:209:GLY:O	1:F:213:GLY:CA	2.66	0.42
1:G:18:ASP:OD1	1:G:28:SER:OG	2.29	0.42
1:H:158:TRP:NE1	1:H:165:PHE:CD1	2.88	0.42
1:B:238:GLN:NE2	1:B:239:THR:H	2.17	0.42
1:C:184:ASP:CG	1:D:192:ARG:HH22	2.27	0.42
1:F:272:GLN:O	1:F:276:VAL:HB	2.19	0.42
1:C:226:LEU:HA	1:C:227:PRO:HD2	1.85	0.42
1:C:252:ARG:NH1	2:C:304:HOH:O	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:THR:HG22	1:D:157:VAL:H	1.84	0.42
1:F:204:LYS:N	1:F:205:ASP:HA	2.33	0.42
1:H:228:GLU:CD	1:H:273:LEU:HD13	2.45	0.42
1:C:194:PHE:HD1	1:C:282:ARG:HH21	1.67	0.42
1:C:196:ARG:NH1	1:D:180:ASP:OD1	2.52	0.42
1:C:226:LEU:HA	1:C:226:LEU:HD23	1.76	0.42
1:D:264:GLU:HG2	1:G:264:GLU:HA	2.02	0.42
1:A:17:PHE:CD2	1:A:30:ILE:HG13	2.54	0.42
1:A:78:GLU:OE2	1:A:85:PRO:CG	2.67	0.42
1:A:159:ARG:HG3	1:A:164:LEU:HB2	2.00	0.42
1:C:73:ASP:OD2	1:C:73:ASP:N	2.23	0.42
1:F:228:GLU:HG2	1:F:273:LEU:HD22	2.01	0.42
1:H:122:ARG:CD	1:H:145:ASP:OD1	2.67	0.42
1:A:249:GLU:OE2	1:D:103:MET:HG2	2.20	0.42
1:C:108:GLU:CD	1:C:108:GLU:H	2.27	0.42
1:C:186:ILE:C	1:C:188:SER:H	2.28	0.42
1:D:198:LEU:HD22	1:D:211:LEU:HD13	2.01	0.42
1:F:104:GLN:C	1:F:114:TRP:HE1	2.28	0.42
1:H:132:LEU:O	1:H:135:LEU:HB3	2.20	0.42
1:H:140:ARG:O	1:H:159:ARG:HD2	2.20	0.42
1:A:215:ARG:HB3	1:A:215:ARG:NH1	2.34	0.42
1:A:223:LEU:O	1:A:224:ALA:O	2.38	0.42
1:B:57:ARG:HA	1:B:235:ALA:O	2.20	0.42
1:C:20:LEU:HB2	1:C:93:PHE:CE1	2.55	0.42
1:C:154:PHE:O	1:C:168:VAL:HA	2.19	0.42
1:D:17:PHE:CD2	1:D:30:ILE:HG13	2.55	0.42
1:A:24:ALA:HB2	1:A:58:TRP:NE1	2.35	0.42
1:E:208:LEU:HB2	2:E:354:HOH:O	2.20	0.42
1:E:262:LEU:HD22	1:E:266:GLN:HG3	2.02	0.42
1:F:215:ARG:HB2	1:F:216:HIS:H	1.71	0.42
1:C:18:ASP:OD1	1:C:30:ILE:HB	2.20	0.41
1:C:100:TYR:O	1:C:101:ALA:C	2.63	0.41
1:H:140:ARG:HD3	1:H:141:ASP:N	2.34	0.41
1:H:271:ARG:CA	1:H:274:SER:OG	2.38	0.41
1:A:215:ARG:HD2	1:A:276:VAL:O	2.20	0.41
1:D:222:ASN:CG	1:D:223:LEU:H	2.28	0.41
1:A:129:LEU:O	1:A:130:ALA:C	2.63	0.41
1:C:151:GLY:O	1:C:152:GLU:HB2	2.20	0.41
1:E:246:ARG:HE	1:E:246:ARG:HB3	1.59	0.41
1:H:124:PRO:O	1:H:125:GLY:C	2.62	0.41
1:A:13:ILE:HG23	1:A:89:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:GLU:OE2	1:A:85:PRO:CB	2.67	0.41
1:A:207:MET:CG	1:B:207:MET:HG2	2.50	0.41
1:B:13:ILE:HD13	1:B:76:ASP:HA	2.02	0.41
1:F:43:LEU:O	1:F:44:ASP:CB	2.68	0.41
1:B:256:LYS:HE2	2:B:333:HOH:O	2.21	0.41
1:C:225:GLN:HA	2:C:306:HOH:O	2.19	0.41
1:D:220:LYS:O	1:D:221:ALA:HB3	2.20	0.41
1:A:144:THR:CG2	1:A:145:ASP:O	2.68	0.41
1:E:13:ILE:HD12	1:E:75:GLY:O	2.20	0.41
1:D:98:GLN:O	1:D:102:PRO:HD3	2.20	0.41
1:F:226:LEU:HD22	1:F:228:GLU:HB2	2.01	0.41
1:G:179:SER:O	1:G:180:ASP:C	2.62	0.41
1:F:197:GLU:OE1	1:F:201:ARG:NH1	2.54	0.41
1:H:80:LEU:HG	1:H:85:PRO:HA	2.03	0.41
1:H:227:PRO:HG2	1:H:228:GLU:OE1	2.20	0.41
1:B:206:GLY:O	1:B:208:LEU:O	2.39	0.41
1:E:162:ASP:O	1:E:241:SER:HA	2.21	0.41
1:F:120:GLY:O	1:F:121:TYR:CB	2.55	0.41
1:F:121:TYR:O	1:F:121:TYR:CD2	2.73	0.41
1:F:136:ILE:HG23	1:F:159:ARG:HH22	1.85	0.41
1:F:152:GLU:O	1:F:152:GLU:CG	2.69	0.41
1:F:207:MET:HE2	1:F:207:MET:HB3	1.82	0.41
1:G:149:GLY:CA	1:G:153:THR:O	2.44	0.41
1:H:118:GLY:C	1:H:120:GLY:H	2.28	0.41
1:H:155:GLN:O	1:H:156:ARG:HB3	2.21	0.41
1:H:244:ALA:HA	1:H:250:GLU:OE1	2.21	0.41
1:A:207:MET:SD	1:B:207:MET:HG2	2.61	0.41
1:B:283:GLU:HB3	1:B:284:SER:H	1.36	0.41
1:E:282:ARG:O	1:E:283:GLU:C	2.63	0.41
1:F:158:TRP:HE1	1:F:165:PHE:HD2	1.68	0.41
1:H:141:ASP:CG	1:H:160:LYS:HA	2.45	0.41
1:E:123:ALA:HB1	1:E:124:PRO:HD2	2.02	0.40
1:F:107:ASP:C	1:F:109:ARG:H	2.29	0.40
1:H:130:ALA:O	1:H:134:VAL:HG23	2.21	0.40
1:H:226:LEU:HD22	1:H:228:GLU:OE1	2.21	0.40
1:B:23:THR:HG22	1:B:228:GLU:CD	2.45	0.40
1:C:117:LEU:CD2	1:C:160:LYS:HB2	2.51	0.40
1:E:36:SER:O	1:E:37:GLU:HB2	2.21	0.40
1:F:50:SER:HA	1:F:53:GLU:OE1	2.21	0.40
1:F:282:ARG:O	1:F:283:GLU:CB	2.68	0.40
1:H:191:ASP:O	1:H:192:ARG:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:MET:HA	1:D:207:MET:HE3	2.03	0.40
1:E:194:PHE:HD1	1:E:194:PHE:HA	1.80	0.40
1:E:201:ARG:NH2	2:E:316:HOH:O	2.53	0.40
1:E:220:LYS:HA	2:E:395:HOH:O	2.21	0.40
1:F:44:ASP:OD2	1:F:69:ALA:O	2.40	0.40
1:H:194:PHE:CE2	1:H:281:LEU:HB3	2.57	0.40
1:C:215:ARG:NE	1:C:279:HIS:O	2.55	0.40
1:A:107:ASP:OD1	1:A:107:ASP:C	2.62	0.40
1:C:211:LEU:HD23	1:C:281:LEU:HD21	2.04	0.40
1:C:271:ARG:O	1:C:275:GLU:HG2	2.21	0.40
1:E:206:GLY:HA2	1:F:202:SER:HB3	2.03	0.40
1:F:50:SER:O	1:F:53:GLU:HG2	2.22	0.40
1:F:128:PRO:O	1:F:129:LEU:C	2.64	0.40
1:F:129:LEU:H	1:F:129:LEU:HD12	1.86	0.40
1:G:250:GLU:O	1:G:253:ALA:N	2.55	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:TYR:OH	1:F:118:GLY:O[2_445]	1.95	0.25
1:F:11:ASP:OD2	1:H:222:ASN:ND2[2_556]	1.96	0.24
2:B:420:HOH:O	2:E:339:HOH:O[1_655]	2.14	0.06
1:G:73:ASP:OD1	1:G:150:ARG:NH2[1_655]	2.15	0.05
1:D:131:GLN:NE2	1:F:137:GLU:OE1[2_445]	2.19	0.01

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	273/284 (96%)	243 (89%)	25 (9%)	5 (2%)	6 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	273/284 (96%)	267 (98%)	5 (2%)	1 (0%)	30	43
1	C	273/284 (96%)	236 (86%)	29 (11%)	8 (3%)	3	3
1	D	273/284 (96%)	256 (94%)	13 (5%)	4 (2%)	8	12
1	E	276/284 (97%)	256 (93%)	13 (5%)	7 (2%)	4	5
1	F	273/284 (96%)	207 (76%)	38 (14%)	28 (10%)	0	0
1	G	273/284 (96%)	247 (90%)	21 (8%)	5 (2%)	6	9
1	H	273/284 (96%)	220 (81%)	31 (11%)	22 (8%)	1	0
All	All	2187/2272 (96%)	1932 (88%)	175 (8%)	80 (4%)	2	2

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	TYR
1	A	224	ALA
1	A	225	GLN
1	C	39	ASP
1	C	118	GLY
1	C	281	LEU
1	D	222	ASN
1	D	283	GLU
1	E	139	ARG
1	E	140	ARG
1	E	204	LYS
1	E	221	ALA
1	E	283	GLU
1	F	28	SER
1	F	39	ASP
1	F	44	ASP
1	F	73	ASP
1	F	76	ASP
1	F	84	ARG
1	F	119	GLU
1	F	121	TYR
1	F	122	ARG
1	F	126	ASP
1	F	127	LEU
1	F	142	PHE
1	F	148	ALA
1	G	140	ARG
1	G	203	GLU

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Mol	Chain	Res	Type
1	H	84	ARG
1	H	123	ALA
1	H	124	PRO
1	H	125	GLY
1	H	139	ARG
1	H	191	ASP
1	H	217	ALA
1	H	221	ALA
1	H	282	ARG
1	C	38	ALA
1	E	125	GLY
1	F	87	ALA
1	F	125	GLY
1	F	141	ASP
1	F	223	LEU
1	G	283	GLU
1	H	126	ASP
1	H	151	GLY
1	H	161	GLY
1	H	203	GLU
1	H	205	ASP
1	B	283	GLU
1	C	221	ALA
1	C	222	ASN
1	D	118	GLY
1	F	138	HIS
1	F	218	GLY
1	F	220	LYS
1	F	258	ALA
1	F	280	GLY
1	H	11	ASP
1	H	204	LYS
1	A	226	LEU
1	C	218	GLY
1	C	283	GLU
1	D	282	ARG
1	F	37	GLU
1	F	108	GLU
1	G	83	GLY
1	H	127	LEU
1	H	189	ILE
1	H	193	ALA

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Mol	Chain	Res	Type
1	H	283	GLU
1	F	43	LEU
1	F	82	ASP
1	F	95	ALA
1	F	203	GLU
1	G	139	ARG
1	H	202	SER
1	A	122	ARG
1	E	191	ASP
1	H	150	ARG

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	199/206 (97%)	174 (87%)	25 (13%)	4	6
1	B	199/206 (97%)	182 (92%)	17 (8%)	10	16
1	C	199/206 (97%)	174 (87%)	25 (13%)	4	6
1	D	199/206 (97%)	180 (90%)	19 (10%)	8	13
1	E	202/206 (98%)	182 (90%)	20 (10%)	7	11
1	F	199/206 (97%)	178 (89%)	21 (11%)	6	10
1	G	199/206 (97%)	174 (87%)	25 (13%)	4	6
1	H	199/206 (97%)	174 (87%)	25 (13%)	4	6
All	All	1595/1648 (97%)	1418 (89%)	177 (11%)	6	9

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	19	THR
1	A	22	SER
1	A	42	THR
1	A	111	LEU

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Mol	Chain	Res	Type
1	A	119	GLU
1	A	122	ARG
1	A	127	LEU
1	A	138	HIS
1	A	140	ARG
1	A	144	THR
1	A	152	GLU
1	A	173	SER
1	A	178	LEU
1	A	201	ARG
1	A	204	LYS
1	A	211	LEU
1	A	215	ARG
1	A	223	LEU
1	A	225	GLN
1	A	239	THR
1	A	255	LEU
1	A	262	LEU
1	A	277	LEU
1	A	281	LEU
1	B	19	THR
1	B	33	LEU
1	B	66	ARG
1	B	84	ARG
1	B	111	LEU
1	B	129	LEU
1	B	144	THR
1	B	178	LEU
1	B	203	GLU
1	B	208	LEU
1	B	211	LEU
1	B	220	LYS
1	B	239	THR
1	B	262	LEU
1	B	268	VAL
1	B	277	LEU
1	B	283	GLU
1	C	19	THR
1	C	43	LEU
1	C	53	GLU
1	C	73	ASP
1	C	79	ILE

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Mol	Chain	Res	Type
1	C	80	LEU
1	C	108	GLU
1	C	111	LEU
1	C	119	GLU
1	C	127	LEU
1	C	178	LEU
1	C	186	ILE
1	C	188	SER
1	C	197	GLU
1	C	199	MET
1	C	202	SER
1	C	207	MET
1	C	208	LEU
1	C	211	LEU
1	C	222	ASN
1	C	225	GLN
1	C	255	LEU
1	C	262	LEU
1	C	277	LEU
1	C	283	GLU
1	D	22	SER
1	D	43	LEU
1	D	53	GLU
1	D	108	GLU
1	D	121	TYR
1	D	122	ARG
1	D	129	LEU
1	D	144	THR
1	D	175	GLU
1	D	178	LEU
1	D	200	ARG
1	D	208	LEU
1	D	211	LEU
1	D	223	LEU
1	D	262	LEU
1	D	268	VAL
1	D	276	VAL
1	D	277	LEU
1	D	283	GLU
1	E	7	LYS
1	E	10	THR
1	E	36	SER

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Mol	Chain	Res	Type
1	E	86	SER
1	E	111	LEU
1	E	143	GLU
1	E	144	THR
1	E	152	GLU
1	E	178	LEU
1	E	186	ILE
1	E	194	PHE
1	E	208	LEU
1	E	223	LEU
1	E	239	THR
1	E	249	GLU
1	E	255	LEU
1	E	262	LEU
1	E	268	VAL
1	E	275	GLU
1	E	277	LEU
1	F	19	THR
1	F	27	ASP
1	F	43	LEU
1	F	121	TYR
1	F	126	ASP
1	F	145	ASP
1	F	160	LYS
1	F	178	LEU
1	F	190	LYS
1	F	201	ARG
1	F	204	LYS
1	F	207	MET
1	F	211	LEU
1	F	220	LYS
1	F	225	GLN
1	F	226	LEU
1	F	255	LEU
1	F	262	LEU
1	F	272	GLN
1	F	276	VAL
1	F	277	LEU
1	G	10	THR
1	G	13	ILE
1	G	19	THR
1	G	22	SER

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Mol	Chain	Res	Type
1	G	33	LEU
1	G	86	SER
1	G	111	LEU
1	G	127	LEU
1	G	144	THR
1	G	150	ARG
1	G	175	GLU
1	G	178	LEU
1	G	179	SER
1	G	202	SER
1	G	208	LEU
1	G	211	LEU
1	G	220	LYS
1	G	255	LEU
1	G	262	LEU
1	G	268	VAL
1	G	269	THR
1	G	274	SER
1	G	277	LEU
1	G	282	ARG
1	G	283	GLU
1	H	22	SER
1	H	43	LEU
1	H	55	GLN
1	H	66	ARG
1	H	81	THR
1	H	82	ASP
1	H	126	ASP
1	H	137	GLU
1	H	140	ARG
1	H	144	THR
1	H	178	LEU
1	H	190	LYS
1	H	194	PHE
1	H	202	SER
1	H	204	LYS
1	H	205	ASP
1	H	207	MET
1	H	208	LEU
1	H	239	THR
1	H	255	LEU
1	H	256	LYS

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Mol	Chain	Res	Type
1	H	257	THR
1	H	262	LEU
1	H	277	LEU
1	H	278	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	B	98	GLN
1	B	230	HIS
1	B	238	GLN
1	C	230	HIS
1	D	49	GLN
1	D	113	GLN
1	D	131	GLN
1	D	216	HIS
1	D	266	GLN
1	D	279	HIS
1	E	216	HIS
1	E	230	HIS
1	F	104	GLN
1	F	113	GLN
1	F	216	HIS
1	F	230	HIS
1	G	230	HIS
1	H	29	GLN
1	H	55	GLN
1	H	138	HIS
1	H	272	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	275/284 (96%)	0.68	19 (6%) 23 19	47, 61, 91, 112	0
1	B	275/284 (96%)	-0.01	5 (1%) 67 63	27, 36, 59, 79	0
1	C	275/284 (96%)	0.59	19 (6%) 23 19	38, 55, 96, 130	0
1	D	275/284 (96%)	0.35	14 (5%) 33 30	34, 48, 89, 123	0
1	E	278/284 (97%)	0.35	14 (5%) 34 30	28, 45, 86, 104	0
1	F	275/284 (96%)	1.71	102 (37%) 1 0	67, 112, 140, 160	0
1	G	275/284 (96%)	0.58	12 (4%) 39 34	42, 63, 83, 97	0
1	H	275/284 (96%)	1.28	62 (22%) 2 2	63, 83, 132, 157	0
All	All	2203/2272 (96%)	0.69	247 (11%) 10 7	27, 60, 120, 160	0

All (247) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	46	ALA	6.9
1	A	281	LEU	6.6
1	F	45	ALA	6.4
1	D	224	ALA	5.0
1	C	217	ALA	4.8
1	C	223	LEU	4.7
1	A	224	ALA	4.7
1	E	217	ALA	4.7
1	C	221	ALA	4.5
1	D	209	GLY	4.4
1	A	10	THR	4.3
1	A	280	GLY	4.3
1	F	135	LEU	4.2
1	E	151	GLY	4.2
1	H	224	ALA	4.2
1	F	280	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	223	LEU	4.1
1	C	224	ALA	4.1
1	F	132	LEU	4.1
1	F	85	PRO	4.0
1	F	72	THR	4.0
1	B	138	HIS	3.9
1	C	215	ARG	3.8
1	H	220	LYS	3.8
1	E	224	ALA	3.8
1	H	214	ALA	3.8
1	H	124	PRO	3.8
1	A	223	LEU	3.8
1	B	224	ALA	3.7
1	D	219	ALA	3.7
1	H	85	PRO	3.7
1	F	42	THR	3.6
1	D	121	TYR	3.6
1	F	65	LEU	3.6
1	H	121	TYR	3.6
1	F	30	ILE	3.6
1	F	208	LEU	3.6
1	F	174	ALA	3.6
1	F	242	GLY	3.5
1	C	219	ALA	3.5
1	D	214	ALA	3.5
1	F	177	ALA	3.4
1	C	41	GLY	3.4
1	H	218	GLY	3.4
1	C	216	HIS	3.4
1	C	203	GLU	3.4
1	G	83	GLY	3.4
1	H	118	GLY	3.4
1	F	186	ILE	3.4
1	H	60	LEU	3.4
1	A	216	HIS	3.4
1	D	213	GLY	3.4
1	F	179	SER	3.3
1	A	121	TYR	3.3
1	A	221	ALA	3.2
1	F	89	VAL	3.3
1	F	241	SER	3.2
1	H	208	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	214	ALA	3.2
1	F	235	ALA	3.2
1	H	187	ALA	3.2
1	H	221	ALA	3.2
1	F	81	THR	3.2
1	F	59	GLY	3.2
1	F	281	LEU	3.2
1	F	31	ALA	3.1
1	C	121	TYR	3.1
1	D	138	HIS	3.1
1	B	121	TYR	3.0
1	F	166	VAL	3.0
1	F	24	ALA	3.0
1	F	77	ILE	3.0
1	F	22	SER	3.0
1	H	193	ALA	2.9
1	H	194	PHE	2.9
1	D	223	LEU	2.9
1	F	13	ILE	2.9
1	A	11	ASP	2.9
1	D	205	ASP	2.9
1	H	69	ALA	2.9
1	F	19	THR	2.9
1	F	117	LEU	2.8
1	H	127	LEU	2.8
1	F	210	ALA	2.8
1	H	212	LEU	2.8
1	F	245	ALA	2.8
1	H	219	ALA	2.8
1	F	56	GLY	2.8
1	A	214	ALA	2.8
1	F	217	ALA	2.8
1	H	209	GLY	2.7
1	F	165	PHE	2.7
1	H	79	ILE	2.7
1	H	125	GLY	2.7
1	F	96	LEU	2.7
1	H	268	VAL	2.7
1	F	136	ILE	2.7
1	F	209	GLY	2.7
1	H	151	GLY	2.7
1	F	111	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	123	ALA	2.7
1	H	216	HIS	2.7
1	F	156	ARG	2.7
1	F	47	LEU	2.7
1	H	119	GLU	2.6
1	D	120	GLY	2.6
1	F	277	LEU	2.6
1	F	120	GLY	2.6
1	D	221	ALA	2.6
1	H	77	ILE	2.6
1	H	226	LEU	2.6
1	E	214	ALA	2.6
1	F	105	ALA	2.6
1	F	142	PHE	2.6
1	F	64	HIS	2.6
1	F	114	TRP	2.5
1	A	209	GLY	2.5
1	G	138	HIS	2.5
1	F	71	LEU	2.5
1	H	62	LEU	2.5
1	H	41	GLY	2.5
1	F	33	LEU	2.4
1	H	106	LEU	2.4
1	E	221	ALA	2.4
1	F	224	ALA	2.4
1	F	151	GLY	2.4
1	E	202	SER	2.4
1	H	93	PHE	2.4
1	F	216	HIS	2.4
1	C	11	ASP	2.4
1	F	57	ARG	2.4
1	H	76	ASP	2.4
1	E	280	GLY	2.4
1	F	87	ALA	2.4
1	H	279	HIS	2.4
1	D	225	GLN	2.4
1	F	270	THR	2.4
1	E	185	VAL	2.4
1	H	71	LEU	2.4
1	D	216	HIS	2.4
1	A	34	ALA	2.3
1	F	40	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	221	ALA	2.3
1	F	244	ALA	2.3
1	H	47	LEU	2.3
1	F	124	PRO	2.3
1	F	128	PRO	2.3
1	E	219	ALA	2.3
1	H	130	ALA	2.3
1	F	134	VAL	2.3
1	E	281	LEU	2.3
1	F	102	PRO	2.3
1	E	193	ALA	2.3
1	H	243	ALA	2.3
1	F	10	THR	2.3
1	B	284	SER	2.3
1	E	138	HIS	2.3
1	F	154	PHE	2.3
1	F	236	PHE	2.3
1	H	281	LEU	2.3
1	B	11	ASP	2.3
1	C	40	ALA	2.3
1	F	95	ALA	2.3
1	G	221	ALA	2.3
1	H	210	ALA	2.3
1	G	42	THR	2.3
1	H	225	GLN	2.3
1	C	209	GLY	2.2
1	H	280	GLY	2.2
1	A	38	ALA	2.2
1	F	16	ALA	2.2
1	F	54	ALA	2.2
1	H	15	ALA	2.2
1	F	273	LEU	2.2
1	H	80	LEU	2.2
1	D	218	GLY	2.2
1	F	161	GLY	2.2
1	F	206	GLY	2.2
1	A	217	ALA	2.2
1	F	35	ALA	2.2
1	F	97	ALA	2.2
1	G	38	ALA	2.2
1	F	121	TYR	2.2
1	H	211	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	218	GLY	2.2
1	F	48	THR	2.2
1	F	163	THR	2.2
1	H	19	THR	2.2
1	H	217	ALA	2.2
1	G	202	SER	2.2
1	F	255	LEU	2.2
1	G	129	LEU	2.2
1	A	12	GLY	2.2
1	C	218	GLY	2.2
1	C	207	MET	2.1
1	F	146	TRP	2.1
1	C	185	VAL	2.1
1	F	17	PHE	2.1
1	F	61	GLY	2.1
1	A	163	THR	2.1
1	C	284	SER	2.1
1	F	248	ALA	2.1
1	G	241	SER	2.1
1	H	258	ALA	2.1
1	H	261	ALA	2.1
1	A	215	ARG	2.1
1	F	139	ARG	2.1
1	F	79	ILE	2.1
1	F	127	LEU	2.1
1	F	164	LEU	2.1
1	G	128	PRO	2.1
1	H	276	VAL	2.1
1	A	243	ALA	2.1
1	F	219	ALA	2.1
1	F	274	SER	2.1
1	E	189	ILE	2.1
1	F	51	LEU	2.1
1	F	129	LEU	2.1
1	G	82	ASP	2.1
1	H	13	ILE	2.1
1	C	225	GLN	2.1
1	F	227	PRO	2.1
1	H	185	VAL	2.1
1	H	213	GLY	2.1
1	F	101	ALA	2.1
1	F	211	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	198	LEU	2.1
1	F	76	ASP	2.1
1	F	141	ASP	2.1
1	H	186	ILE	2.1
1	F	118	GLY	2.1
1	H	12	GLY	2.1
1	H	32	ALA	2.0
1	H	253	ALA	2.0
1	G	225	GLN	2.0
1	F	60	LEU	2.0
1	H	20	LEU	2.0
1	F	157	VAL	2.0
1	F	185	VAL	2.0
1	H	232	THR	2.0
1	F	15	ALA	2.0
1	F	169	ALA	2.0
1	G	224	ALA	2.0
1	F	39	ASP	2.0
1	H	129	LEU	2.0
1	F	88	ARG	2.0
1	H	190	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.