



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 07:56 PM UTC

PDB ID : 8TUB / pdb_00008tub
Title : HLA B7:02 with HPNGYKSLSTL
Authors : Littler, D.R.; Rossjohn, J.; Chaurasia, P.; Petersen, J.
Deposited on : 2023-08-16
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
Mogul : 2022.3.0, CSD as543be (2022)
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

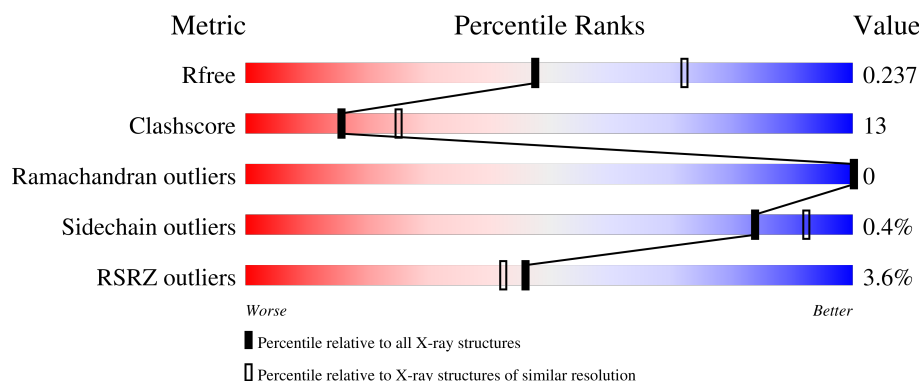
1 Overall quality at a glance

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	99	80% 18% .
1	B	99	87% 13% .
1	E	99	74% 25% .
1	I	99	73% 27% .
2	C	275	77% 22% .

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Mol	Chain	Length	Quality of chain
2	F	275	 3% 77% 23%
2	G	275	 % 80% 20%
2	J	275	 9% 72% 27%
3	D	11	 91% 9%
3	H	11	 73% 18% 9%
3	K	11	 82% 18%
3	Q	11	 73% 27%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PEG	F	301	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13263 atoms, of which 46 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 Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
1	B	99	Total	C	N	O	S	0	0	0
			813	518	138	154	3			
1	E	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
1	I	99	Total	C	N	O	S	0	0	0
			823	525	137	158	3			

- Molecule 2 is a protein called HLA class I histocompatibility antigen, B-7 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	275	Total	C	N	O	S	0	1	0
			2248	1396	411	434	7			
2	C	275	Total	C	N	O	S	0	0	0
			2247	1395	412	434	6			
2	G	275	Total	C	N	O	S	0	0	0
			2249	1396	410	437	6			
2	J	275	Total	C	N	O	S	0	0	0
			2247	1395	413	433	6			

- Molecule 3 is a protein called HIS-PRO-ASN-GLY-TYR-LYS-SER-LEU-SER-THR-LEU.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	11	Total	C	N	O	0	0	0
			85	54	15	16			
3	D	11	Total	C	N	O	0	0	0
			85	54	15	16			
3	H	11	Total	C	N	O	0	0	0
			86	54	15	17			
3	K	11	Total	C	N	O	0	0	0
			86	54	15	17			

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	F	1	Total	C	H	O	0	0
			10	2	6	2		
4	Q	1	Total	C	H	O	0	0
			10	2	6	2		
4	E	1	Total	C	H	O	0	0
			10	2	6	2		
4	E	1	Total	C	H	O	0	0
			10	2	6	2		
4	H	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	F	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	48	Total	O	0	0
			48	48		
6	F	114	Total	O	0	0
			114	114		
6	Q	2	Total	O	0	0
			2	2		
6	B	30	Total	O	0	0
			30	30		
6	C	92	Total	O	0	0
			92	92		
6	D	4	Total	O	0	0
			4	4		
6	E	32	Total	O	0	0
			32	32		
6	G	138	Total	O	0	0
			138	138		
6	H	7	Total	O	0	0
			7	7		
6	I	22	Total	O	0	0
			22	22		
6	J	64	Total	O	0	0
			64	64		

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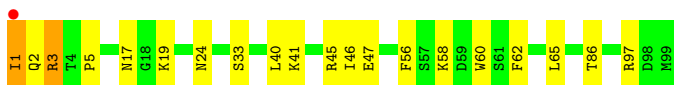
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	K	6	Total	O	0	0
			6	6		

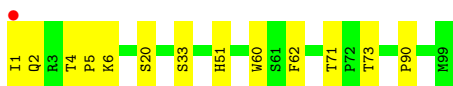
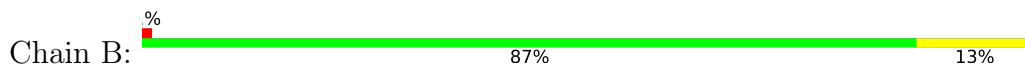
3 Residue-property plots [i](#)

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 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.

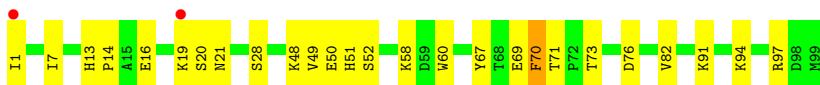
- Molecule 1: Beta-2-microglobulin



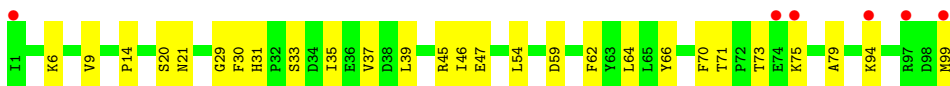
- Molecule 1: Beta-2-microglobulin



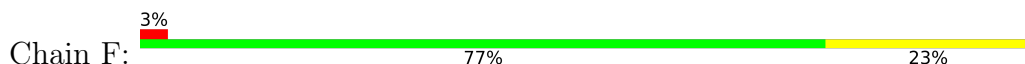
- Molecule 1: Beta-2-microglobulin

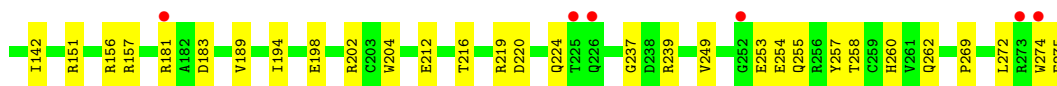


- Molecule 1: Beta-2-microglobulin

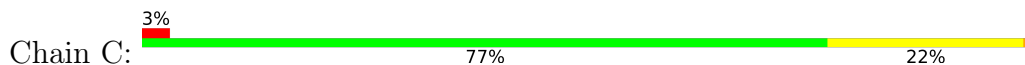


- Molecule 2: HLA class I histocompatibility antigen, B-7 alpha chain

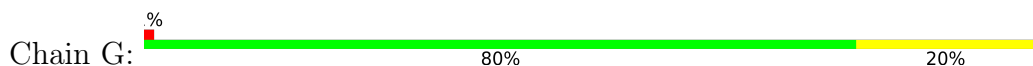




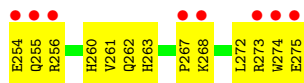
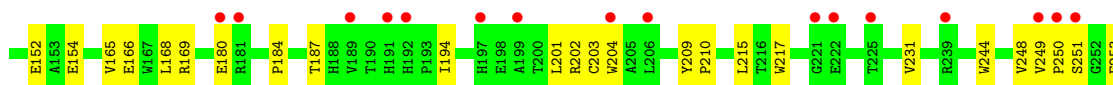
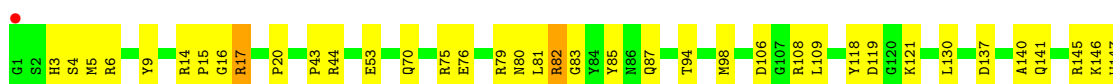
- Molecule 2: HLA class I histocompatibility antigen, B-7 alpha chain



- Molecule 2: HLA class I histocompatibility antigen, B-7 alpha chain



- Molecule 2: HLA class I histocompatibility antigen, B-7 alpha chain



- Molecule 3: HIS-PRO-ASN-GLY-TYR-LYS-SER-LEU-SER-THR-LEU



- Molecule 3: HIS-PRO-ASN-GLY-TYR-LYS-SER-LEU-SER-THR-LEU





- Molecule 3: HIS-PRO-ASN-GLY-TYR-LYS-SER-LEU-SER-THR-LEU

Chain H:  73% 18% 9%



- Molecule 3: HIS-PRO-ASN-GLY-TYR-LYS-SER-LEU-SER-THR-LEU

Chain K:  82% 18%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	49.21Å 90.67Å 104.56Å 97.54° 93.83° 90.23°	Depositor
Resolution (Å)	43.00 – 2.40 43.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.5 (43.00-2.40) 94.4 (43.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.197 , 0.238 0.199 , 0.237	Depositor DCC
R_{free} test set	3320 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13263	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% 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

5.1 Standard geometry

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

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	0.60	1/852 (0.1%)	0.69	2/1152 (0.2%)
1	B	0.52	1/836 (0.1%)	0.70	1/1134 (0.1%)
1	E	0.37	0/852	0.61	0/1152
1	I	0.45	1/846 (0.1%)	0.62	0/1145
2	C	0.71	4/2309 (0.2%)	0.77	0/3137
2	F	0.58	1/2309 (0.0%)	0.70	2/3136 (0.1%)
2	G	0.58	0/2311	0.70	2/3140 (0.1%)
2	J	0.67	6/2309 (0.3%)	0.68	2/3137 (0.1%)
3	D	0.46	0/87	0.60	0/117
3	H	0.42	0/88	0.65	0/117
3	K	0.47	0/88	0.63	0/117
3	Q	0.39	0/87	0.55	0/117
All	All	0.60	14/12974 (0.1%)	0.70	9/17601 (0.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	184	PRO	N-CD	-15.78	1.25	1.47
2	C	267	PRO	N-CD	-12.57	1.30	1.47
2	F	57	PRO	N-CD	-10.27	1.33	1.47
1	I	14	PRO	N-CD	-9.67	1.34	1.47
2	C	87	GLN	C-O	-7.41	1.14	1.23
1	B	90	PRO	N-CD	6.93	1.57	1.47
2	J	43	PRO	N-CD	6.59	1.56	1.47
2	J	82	ARG	C-O	-6.47	1.16	1.24
2	J	14	ARG	C-O	-6.44	1.17	1.24
2	J	16	GLY	C-O	-6.20	1.16	1.23
2	J	76	GLU	C-O	-5.30	1.17	1.24
2	C	76	GLU	C-O	-5.13	1.18	1.24
2	C	62	ARG	C-O	-5.01	1.18	1.24
1	A	3	ARG	C-O	-5.01	1.18	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	GLU	N-CA-C	7.60	119.35	111.14
2	J	15	PRO	N-CA-C	6.49	122.55	113.53
2	F	17	ARG	N-CA-C	-6.35	96.75	107.99
2	F	18	GLY	N-CA-C	6.06	121.18	113.24
1	A	5	PRO	N-CA-C	5.99	119.85	110.80
2	J	17	ARG	N-CA-C	5.75	119.60	112.59
2	G	180	GLU	N-CA-C	5.63	117.50	111.36
2	G	17	ARG	N-CA-C	-5.48	106.63	113.15
1	B	73	THR	CB-CA-C	-5.32	102.90	113.80

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	829	0	794	16	0
1	B	813	0	764	11	0
1	E	829	0	793	30	0
1	I	823	0	783	26	0
2	C	2247	0	2085	61	4
2	F	2248	0	2086	56	0
2	G	2249	0	2087	70	0
2	J	2247	0	2089	61	4
3	D	85	0	86	1	0
3	H	86	0	86	6	0
3	K	86	0	86	3	0
3	Q	85	0	86	3	0
4	A	4	6	6	0	0
4	E	8	12	12	0	0
4	F	4	6	6	1	0
4	H	4	6	6	0	0
4	Q	4	6	6	1	0
5	F	7	10	10	4	0
6	A	48	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	30	0	0	6	0
6	C	92	0	0	15	0
6	D	4	0	0	0	0
6	E	32	0	0	10	0
6	F	114	0	0	11	0
6	G	138	0	0	32	0
6	H	7	0	0	1	0
6	I	22	0	0	7	0
6	J	64	0	0	14	0
6	K	6	0	0	0	0
6	Q	2	0	0	0	0
All	All	13217	46	11871	325	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (325) 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:C:219:ARG:NH1	2:C:257:TYR:CE1	1.72	1.58
2:C:219:ARG:NH1	2:C:257:TYR:CZ	1.68	1.57
2:C:275:GLU:HB2	6:C:304:HOH:O	1.22	1.37
2:J:82:ARG:NH1	2:J:87:GLN:O	1.59	1.34
2:C:219:ARG:NH1	2:C:257:TYR:OH	1.58	1.32
2:G:146:LYS:HB3	6:G:302:HOH:O	1.41	1.18
2:G:146:LYS:CA	6:G:302:HOH:O	1.90	1.15
1:B:51:HIS:NE2	6:B:101:HOH:O	1.83	1.11
1:E:1:ILE:HA	6:E:202:HOH:O	1.50	1.11
2:G:146:LYS:CB	6:G:302:HOH:O	1.93	1.08
2:G:147:TRP:N	6:G:302:HOH:O	1.87	1.07
2:F:262:GLN:HB3	5:F:301:PEG:H31	1.37	1.06
2:C:146:LYS:NZ	6:C:301:HOH:O	1.84	1.04
2:C:219:ARG:NH2	2:C:253:GLU:OE1	1.93	1.01
2:J:17:ARG:NH2	6:J:304:HOH:O	1.92	1.00
2:G:146:LYS:N	6:G:302:HOH:O	1.90	0.98
2:G:275:GLU:OE1	6:G:301:HOH:O	1.82	0.98
1:A:1:ILE:N	6:A:202:HOH:O	1.95	0.98
1:I:31:HIS:ND1	6:I:101:HOH:O	1.96	0.97
2:J:80:ASN:O	6:J:301:HOH:O	1.81	0.97
1:E:1:ILE:CA	6:E:202:HOH:O	2.07	0.97
1:A:1:ILE:O	6:A:201:HOH:O	1.81	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:257:TYR:OH	6:F:401:HOH:O	1.82	0.96
1:E:1:ILE:N	6:E:201:HOH:O	1.96	0.96
2:G:143:THR:O	6:G:302:HOH:O	1.84	0.95
2:F:253:GLU:OE1	6:F:402:HOH:O	1.82	0.95
2:C:256:ARG:NE	6:C:306:HOH:O	1.99	0.94
1:I:29:GLY:HA3	6:I:103:HOH:O	1.68	0.93
2:J:251:SER:HA	2:J:254:GLU:OE2	1.67	0.92
2:C:128:GLU:O	6:C:302:HOH:O	1.87	0.92
2:C:219:ARG:NH1	2:C:257:TYR:HE1	1.57	0.91
2:C:232:GLU:OE2	6:C:303:HOH:O	1.89	0.91
2:C:275:GLU:O	6:C:304:HOH:O	1.89	0.91
2:G:6:ARG:CZ	6:G:308:HOH:O	2.17	0.91
1:A:1:ILE:N	6:A:203:HOH:O	2.00	0.90
2:C:275:GLU:C	6:C:304:HOH:O	2.14	0.90
1:E:49:VAL:N	6:E:204:HOH:O	2.04	0.89
2:J:119:ASP:OD1	6:J:303:HOH:O	1.89	0.89
1:E:1:ILE:N	6:E:202:HOH:O	1.99	0.89
2:G:233:THR:O	6:G:303:HOH:O	1.88	0.89
2:F:181:ARG:NH2	2:F:183:ASP:OD2	2.07	0.88
2:G:275:GLU:O	6:G:304:HOH:O	1.92	0.88
2:F:82:ARG:NH1	2:F:89:GLU:HA	1.88	0.88
1:I:79:ALA:HB2	1:I:94:LYS:HG2	1.56	0.86
1:E:48:LYS:C	6:E:204:HOH:O	2.17	0.86
2:G:105:PRO:N	6:G:307:HOH:O	2.08	0.86
2:G:20:PRO:HD3	2:G:75:ARG:HG3	1.58	0.85
2:J:154:GLU:OE2	6:J:305:HOH:O	1.93	0.85
2:J:3:HIS:NE2	2:J:180:GLU:OE2	2.08	0.85
2:G:6:ARG:NE	6:G:308:HOH:O	2.11	0.82
2:G:105:PRO:CD	6:G:307:HOH:O	2.27	0.81
1:I:29:GLY:CA	6:I:103:HOH:O	2.23	0.81
2:C:46:GLU:OE1	6:C:305:HOH:O	1.99	0.81
2:G:154:GLU:OE2	6:G:305:HOH:O	1.99	0.80
2:J:106:ASP:OD2	2:J:108:ARG:NE	2.15	0.80
2:C:114:ASP:OD1	6:C:307:HOH:O	2.01	0.79
2:J:6:ARG:HG2	2:J:6:ARG:HH11	1.48	0.79
2:G:105:PRO:HD2	6:G:307:HOH:O	1.84	0.78
2:G:6:ARG:NH2	6:G:308:HOH:O	2.14	0.78
2:G:255:GLN:NE2	2:G:273:ARG:HD2	1.99	0.77
2:F:212:GLU:OE2	6:F:404:HOH:O	2.04	0.76
1:E:76:ASP:O	6:E:203:HOH:O	2.03	0.76
2:G:82:ARG:NH2	2:G:89:GLU:HG3	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:275:GLU:CA	6:C:304:HOH:O	2.24	0.75
1:I:73:THR:CG2	1:I:75:LYS:HG2	2.16	0.75
2:C:45:GLU:O	6:C:308:HOH:O	2.04	0.74
2:C:258:THR:HG23	2:C:273:ARG:HD3	1.69	0.74
2:J:154:GLU:CD	6:J:305:HOH:O	2.30	0.74
2:F:219:ARG:HD3	2:F:257:TYR:CZ	2.24	0.73
1:E:94:LYS:HD2	1:E:94:LYS:N	2.02	0.73
2:C:54:GLN:O	6:C:309:HOH:O	2.07	0.73
2:C:258:THR:CG2	2:C:273:ARG:HD3	2.19	0.72
2:J:82:ARG:HD3	6:J:361:HOH:O	1.89	0.72
2:F:20:PRO:HD3	2:F:75:ARG:HG3	1.71	0.71
2:J:94:THR:OG1	6:J:302:HOH:O	1.82	0.71
2:G:108:ARG:NH1	6:G:316:HOH:O	2.25	0.70
1:B:71:THR:O	6:B:102:HOH:O	2.10	0.69
2:F:262:GLN:HB3	5:F:301:PEG:C3	2.20	0.69
1:B:6:LYS:O	6:B:103:HOH:O	2.10	0.69
2:G:255:GLN:HE22	2:G:273:ARG:HD2	1.57	0.69
1:E:19:LYS:C	1:E:71:THR:HG23	2.18	0.68
2:J:53:GLU:O	6:J:307:HOH:O	2.11	0.67
1:B:1:ILE:HG23	1:B:2:GLN:H	1.58	0.67
2:C:50:PRO:O	2:C:53:GLU:HG3	1.95	0.67
2:G:108:ARG:NH2	6:G:317:HOH:O	2.27	0.67
2:F:123:TYR:CE2	3:Q:11:LEU:HD23	2.29	0.67
1:E:58:LYS:NZ	2:G:98:MET:HE2	2.09	0.67
2:J:274:TRP:CE2	2:J:275:GLU:HG2	2.29	0.67
2:J:130:LEU:O	6:J:308:HOH:O	2.12	0.67
1:E:94:LYS:N	1:E:94:LYS:CD	2.57	0.67
1:A:3:ARG:NH1	6:A:205:HOH:O	2.10	0.67
2:G:179:LEU:O	6:G:309:HOH:O	2.12	0.67
2:J:203:CYS:HB2	2:J:217:TRP:CZ2	2.30	0.66
2:C:258:THR:HG22	2:C:273:ARG:HG3	1.77	0.66
2:J:169:ARG:NE	6:J:306:HOH:O	2.00	0.66
2:J:201:LEU:HD12	2:J:249:VAL:HG11	1.76	0.66
2:J:187:THR:HB	2:J:272:LEU:HD11	1.78	0.66
2:J:85:TYR:OH	2:J:137:ASP:OD2	2.10	0.65
1:A:17:ASN:HD21	1:A:97:ARG:HH12	1.43	0.65
2:F:30:ASP:O	6:F:405:HOH:O	2.15	0.65
2:J:152:GLU:OE2	6:J:309:HOH:O	2.14	0.65
2:J:215:LEU:HD23	2:J:261:VAL:HG13	1.79	0.65
1:I:73:THR:HG22	1:I:75:LYS:HG2	1.78	0.65
2:J:3:HIS:HE2	2:J:180:GLU:CD	2.05	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:6:ARG:HD2	2:F:98[A]:MET:SD	2.36	0.65
2:G:275:GLU:CD	6:G:301:HOH:O	2.31	0.64
2:F:253:GLU:CD	6:F:402:HOH:O	2.35	0.64
2:J:215:LEU:CD2	2:J:261:VAL:HG13	2.27	0.64
2:C:115:GLN:NE2	6:C:311:HOH:O	2.30	0.64
2:G:194:ILE:HD11	2:G:200:THR:HG23	1.78	0.63
1:I:73:THR:HG22	1:I:75:LYS:H	1.64	0.63
2:F:219:ARG:HB2	2:F:224:GLN:NE2	2.12	0.63
1:I:59:ASP:OD2	6:I:102:HOH:O	2.15	0.63
1:I:73:THR:HG21	1:I:75:LYS:HG2	1.78	0.63
2:C:258:THR:HG22	2:C:273:ARG:CG	2.29	0.63
2:C:274:TRP:CE2	2:C:275:GLU:HG2	2.34	0.62
2:F:157:ARG:NH1	6:F:408:HOH:O	2.21	0.62
1:I:39:LEU:CB	1:I:46:ILE:HD12	2.29	0.62
2:F:20:PRO:CD	2:F:75:ARG:HG3	2.29	0.62
2:C:258:THR:CG2	2:C:273:ARG:HH11	2.12	0.62
2:C:238:ASP:OD1	2:C:240:THR:OG1	2.18	0.61
1:E:58:LYS:HZ2	2:G:98:MET:HE2	1.64	0.61
2:G:106:ASP:N	6:G:307:HOH:O	2.13	0.61
2:C:194:ILE:HD11	2:C:248:VAL:HG22	1.81	0.61
1:A:17:ASN:ND2	1:A:97:ARG:HH12	1.98	0.61
1:E:16:GLU:HB2	1:E:19:LYS:HE3	1.83	0.61
1:E:97:ARG:HG2	6:E:212:HOH:O	2.00	0.60
1:A:24:ASN:HB3	1:A:65:LEU:HD11	1.83	0.60
3:Q:4:GLY:H	4:Q:101:EDO:C2	2.15	0.60
2:F:194:ILE:HD12	2:F:198:GLU:HB3	1.84	0.59
2:C:6:ARG:HG2	2:C:6:ARG:HH11	1.67	0.59
2:G:275:GLU:C	6:G:304:HOH:O	2.40	0.59
1:E:28:SER:OG	6:E:205:HOH:O	2.17	0.59
1:B:20:SER:HA	1:B:71:THR:HG22	1.85	0.59
2:G:76:GLU:O	2:G:76:GLU:HG3	2.04	0.58
2:C:275:GLU:CB	6:C:304:HOH:O	1.95	0.58
1:I:6:LYS:NZ	6:I:104:HOH:O	2.36	0.57
1:B:6:LYS:C	6:B:103:HOH:O	2.46	0.57
2:G:14:ARG:HB3	2:G:17:ARG:HB2	1.87	0.57
2:J:201:LEU:HD12	2:J:249:VAL:CG1	2.33	0.57
2:F:202:ARG:HG2	2:F:204:TRP:NE1	2.19	0.57
2:C:4:SER:HB2	2:C:6:ARG:HH12	1.70	0.57
2:J:98:MET:SD	2:J:98:MET:C	2.88	0.57
2:F:11:SER:OG	2:F:74:ASP:OD2	2.21	0.56
2:C:33:PHE:CD2	2:C:34:VAL:HG13	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:71:ALA:O	2:C:75:ARG:HG3	2.05	0.56
2:F:257:TYR:CZ	6:F:401:HOH:O	2.45	0.56
2:C:180:GLU:HA	2:C:180:GLU:OE1	2.04	0.56
2:F:258:THR:HG23	2:F:260:HIS:NE2	2.20	0.56
2:G:20:PRO:CD	2:G:75:ARG:HG3	2.34	0.56
2:F:139:ALA:HA	2:F:142:ILE:HD12	1.88	0.55
2:J:5:MET:HB2	2:J:168:LEU:HD13	1.89	0.55
2:C:76:GLU:HA	2:C:76:GLU:OE1	2.06	0.55
1:I:39:LEU:HB3	1:I:46:ILE:HD12	1.88	0.55
1:A:60:TRP:CE2	2:F:117:ALA:HB2	2.42	0.55
2:F:151:ARG:NH2	2:J:166:GLU:HG2	2.21	0.55
2:F:216:THR:HG23	2:F:260:HIS:HB2	1.89	0.55
2:F:269:PRO:HG3	5:F:301:PEG:H42	1.89	0.55
1:E:7:ILE:CD1	1:E:82:VAL:HG21	2.37	0.55
1:E:50:GLU:HB2	1:E:67:TYR:CZ	2.42	0.55
2:J:187:THR:CB	2:J:272:LEU:HD11	2.36	0.55
2:J:137:ASP:HB3	2:J:140:ALA:H	1.72	0.54
2:C:14:ARG:HD3	2:C:19:GLU:O	2.08	0.54
2:G:104:GLY:O	6:G:311:HOH:O	2.19	0.54
2:G:258:THR:HG22	6:G:351:HOH:O	2.08	0.54
2:J:210:PRO:O	2:J:263:HIS:HE1	1.90	0.54
2:C:146:LYS:HE2	3:D:10:THR:HG23	1.90	0.54
2:G:6:ARG:NH2	2:G:102:ASP:OD1	2.41	0.54
2:G:232:GLU:HG2	6:G:303:HOH:O	2.07	0.54
2:J:194:ILE:HD11	2:J:248:VAL:HG22	1.89	0.54
2:C:6:ARG:HD2	2:C:98:MET:SD	2.48	0.53
2:C:44:ARG:NH2	2:C:61:ASP:OD1	2.40	0.53
2:G:169:ARG:HD2	6:G:330:HOH:O	2.08	0.53
2:G:76:GLU:HG2	3:H:10:THR:CG2	2.38	0.52
1:A:58:LYS:HB2	6:A:246:HOH:O	2.10	0.52
2:F:17:ARG:N	2:F:17:ARG:CD	2.72	0.52
2:F:255:GLN:OE1	2:F:274:TRP:O	2.28	0.52
1:A:19:LYS:HE3	6:A:219:HOH:O	2.08	0.52
2:F:108:ARG:HG3	2:F:108:ARG:HH11	1.75	0.52
1:E:16:GLU:OE2	1:E:19:LYS:HE2	2.10	0.52
1:E:60:TRP:CE2	2:G:117:ALA:HB2	2.45	0.52
1:B:4:THR:CG2	1:B:5:PRO:HD2	2.39	0.51
2:G:76:GLU:CD	3:H:10:THR:HG21	2.36	0.51
2:J:250:PRO:HG2	2:J:253:GLU:OE2	2.10	0.51
2:J:267:PRO:O	2:J:268:LYS:HG3	2.10	0.51
2:F:82:ARG:CZ	2:F:89:GLU:HA	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:223:HOH:O	2:F:237:GLY:HA3	2.10	0.50
2:J:202:ARG:HG2	2:J:204:TRP:CD1	2.46	0.50
1:I:20:SER:HA	1:I:71:THR:HG22	1.93	0.50
3:H:6:LYS:HG2	3:H:6:LYS:O	2.12	0.50
1:E:7:ILE:HD13	1:E:82:VAL:HG21	1.92	0.50
2:G:106:ASP:OD2	2:G:108:ARG:HG2	2.11	0.50
2:G:146:LYS:HD3	6:H:204:HOH:O	2.11	0.50
2:J:141:GLN:HB3	2:J:145:ARG:NH2	2.27	0.50
1:A:1:ILE:HD12	1:A:2:GLN:H	1.77	0.49
1:E:20:SER:OG	1:E:69:GLU:OE2	2.31	0.49
2:C:215:LEU:HD23	2:C:261:VAL:HG13	1.94	0.49
2:G:232:GLU:CG	6:G:303:HOH:O	2.60	0.49
2:G:105:PRO:CA	6:G:307:HOH:O	2.56	0.49
2:G:255:GLN:OE1	2:G:274:TRP:O	2.30	0.49
2:F:262:GLN:HG2	2:F:269:PRO:HG3	1.93	0.49
2:F:129:ASP:O	2:F:131:ARG:HD2	2.12	0.49
1:E:73:THR:OG1	1:E:76:ASP:HB2	2.13	0.49
2:G:197:HIS:C	2:G:251:SER:OG	2.56	0.49
2:J:6:ARG:HG2	2:J:6:ARG:NH1	2.18	0.49
2:F:156:ARG:CZ	3:Q:6:LYS:HD3	2.42	0.49
2:C:250:PRO:HB2	2:C:253:GLU:HG3	1.94	0.49
1:E:51:HIS:HD2	1:E:52:SER:O	1.96	0.49
2:C:131:ARG:NH2	6:C:313:HOH:O	2.37	0.48
2:G:268:LYS:HB3	2:G:268:LYS:HE3	1.59	0.48
2:C:163:GLU:OE1	2:C:163:GLU:HA	2.14	0.48
1:E:94:LYS:CD	1:E:94:LYS:H	2.25	0.48
1:I:79:ALA:CB	1:I:94:LYS:HA	2.43	0.48
2:F:111:ARG:NH1	2:F:128:GLU:HA	2.27	0.48
1:A:40:LEU:HD23	1:A:45:ARG:HA	1.94	0.47
2:C:9:TYR:CE2	2:C:70:GLN:HG2	2.48	0.47
2:F:189:VAL:HG23	2:F:272:LEU:HD13	1.96	0.47
2:J:201:LEU:CD1	2:J:249:VAL:HG11	2.43	0.47
2:F:33:PHE:CD2	2:F:34:VAL:HG13	2.48	0.47
6:B:128:HOH:O	2:C:98:MET:HG3	2.15	0.47
2:G:76:GLU:HG2	3:H:10:THR:HG21	1.95	0.47
2:C:141:GLN:HB3	2:C:145:ARG:NH2	2.29	0.47
2:C:187:THR:HB	2:C:272:LEU:HD11	1.96	0.47
1:B:4:THR:HG22	1:B:5:PRO:HD2	1.97	0.47
2:C:6:ARG:HG2	2:C:6:ARG:NH1	2.29	0.47
1:E:21:ASN:HB3	1:E:70:PHE:CE1	2.49	0.47
2:G:243:LYS:HE2	6:G:345:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:109:LEU:HB2	2:J:165:VAL:HG21	1.97	0.47
2:J:231:VAL:HG11	2:J:244:TRP:CZ2	2.49	0.47
2:C:4:SER:HB2	2:C:6:ARG:NH1	2.28	0.47
1:I:39:LEU:C	1:I:46:ILE:HD12	2.40	0.47
2:G:85:TYR:OH	2:G:137:ASP:OD2	2.22	0.47
2:J:3:HIS:NE2	2:J:180:GLU:CD	2.69	0.47
2:J:121:LYS:HB3	2:J:121:LYS:HE3	1.34	0.46
2:J:256:ARG:NE	6:J:321:HOH:O	2.47	0.46
2:F:220:ASP:N	6:F:417:HOH:O	2.48	0.46
1:A:56:PHE:CE2	2:F:8:PHE:HB3	2.50	0.46
1:B:51:HIS:CE1	6:B:101:HOH:O	2.51	0.46
2:C:260:HIS:ND1	2:C:260:HIS:N	2.63	0.46
2:G:34:VAL:HG23	6:G:362:HOH:O	2.16	0.46
2:J:202:ARG:HG2	2:J:204:TRP:NE1	2.31	0.46
2:J:44:ARG:NH1	2:J:44:ARG:HG2	2.31	0.45
2:F:219:ARG:HD3	2:F:257:TYR:OH	2.17	0.45
1:E:1:ILE:HG22	2:G:119:ASP:O	2.17	0.45
2:G:44:ARG:HH11	2:G:44:ARG:HG2	1.81	0.45
2:J:83:GLY:HA3	6:J:301:HOH:O	2.15	0.45
2:G:62:ARG:O	2:G:66:ILE:HG13	2.17	0.45
2:C:137:ASP:HB3	2:C:140:ALA:H	1.82	0.45
1:B:60:TRP:CE2	2:C:117:ALA:HB2	2.53	0.44
2:G:9:TYR:CE2	2:G:70:GLN:HG2	2.52	0.44
1:B:33:SER:HB3	1:B:62:PHE:CE2	2.51	0.44
2:G:274:TRP:CE2	2:G:275:GLU:HG2	2.51	0.44
1:I:54:LEU:HD11	1:I:62:PHE:CD1	2.52	0.44
1:A:41:LYS:HB2	1:A:46:ILE:HD11	1.99	0.44
2:F:19:GLU:OE2	2:F:75:ARG:NH1	2.50	0.44
2:F:35:ARG:NE	2:F:46:GLU:OE1	2.47	0.44
2:C:255:GLN:OE1	2:C:274:TRP:O	2.35	0.44
2:F:17:ARG:N	2:F:17:ARG:HD2	2.32	0.44
2:J:209:TYR:CD1	2:J:210:PRO:HA	2.52	0.44
1:I:99:MET:HE2	1:I:99:MET:HB2	1.83	0.44
2:J:3:HIS:CE1	2:J:180:GLU:OE2	2.69	0.44
1:I:31:HIS:CE1	6:I:101:HOH:O	2.56	0.44
2:C:258:THR:HG21	2:C:273:ARG:HH11	1.81	0.44
2:G:258:THR:OG1	2:G:271:THR:HG23	2.18	0.43
2:F:258:THR:CG2	2:F:260:HIS:NE2	2.81	0.43
1:E:13:HIS:HB3	1:E:14:PRO:HD2	2.01	0.43
2:C:218:GLN:HB2	2:C:260:HIS:CE1	2.53	0.43
2:F:44:ARG:NH1	6:F:420:HOH:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:85:TYR:OH	2:F:137:ASP:OD2	2.28	0.43
1:I:33:SER:HB3	1:I:62:PHE:CE2	2.54	0.43
2:G:72:GLN:HG3	6:G:424:HOH:O	2.19	0.43
2:G:102:ASP:OD2	2:G:113:HIS:HE1	2.02	0.43
1:E:7:ILE:HD12	1:E:91:LYS:HD2	2.01	0.43
2:F:91:GLY:HA3	6:F:432:HOH:O	2.19	0.42
1:I:29:GLY:O	6:I:103:HOH:O	2.20	0.42
2:G:91:GLY:HA3	6:G:348:HOH:O	2.19	0.42
2:G:262:GLN:HG2	2:G:269:PRO:HG3	2.01	0.42
2:C:202:ARG:HG2	2:C:204:TRP:NE1	2.34	0.42
2:F:249:VAL:HG21	2:F:254:GLU:HG3	2.01	0.42
2:J:81:LEU:HD13	2:J:118:TYR:CD1	2.54	0.42
2:F:274:TRP:HA	2:F:275:GLU:HA	1.85	0.42
2:G:70:GLN:OE1	3:H:7:SER:HA	2.19	0.42
2:C:219:ARG:CZ	2:C:257:TYR:OH	2.51	0.42
1:I:30:PHE:CD2	1:I:35:ILE:HD12	2.55	0.42
2:C:258:THR:HG22	2:C:273:ARG:HD3	2.00	0.42
2:G:44:ARG:HG2	2:G:44:ARG:NH1	2.35	0.42
1:I:21:ASN:HB3	1:I:70:PHE:CE1	2.55	0.42
2:J:79:ARG:HG2	6:J:362:HOH:O	2.19	0.42
1:A:33:SER:HB3	1:A:62:PHE:CE2	2.55	0.42
2:G:274:TRP:HA	2:G:275:GLU:HA	1.79	0.41
1:A:2:GLN:HE21	1:A:86:THR:HG22	1.86	0.41
2:F:62:ARG:O	2:F:66:ILE:HG13	2.20	0.41
2:C:123:TYR:CZ	2:C:140:ALA:HA	2.55	0.41
1:I:30:PHE:CE2	1:I:35:ILE:HD12	2.54	0.41
2:J:82:ARG:NH1	2:J:82:ARG:HG2	2.34	0.41
1:I:54:LEU:HA	1:I:64:LEU:HD21	2.02	0.41
2:C:215:LEU:CD2	2:C:261:VAL:HG13	2.51	0.41
6:E:209:HOH:O	2:G:237:GLY:HA3	2.19	0.41
2:F:202:ARG:HG2	2:F:204:TRP:CD1	2.55	0.41
2:F:262:GLN:HG2	5:F:301:PEG:H42	2.03	0.41
2:G:5:MET:HB2	2:G:168:LEU:HD13	2.02	0.41
2:J:4:SER:HB2	2:J:6:ARG:HH12	1.86	0.41
2:J:20:PRO:HG2	2:J:75:ARG:HG2	2.01	0.41
2:J:147:TRP:HZ2	3:K:11:LEU:HD12	1.84	0.41
4:F:302:EDO:O2	2:G:262:GLN:HB3	2.21	0.41
2:J:9:TYR:CE2	2:J:70:GLN:HG2	2.55	0.41
2:F:6:ARG:HG2	2:F:6:ARG:HH11	1.86	0.41
2:C:106:ASP:OD2	2:C:108:ARG:HG3	2.21	0.41
2:C:258:THR:HG22	2:C:273:ARG:CD	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:ILE:HD13	1:E:82:VAL:CG2	2.51	0.41
1:E:16:GLU:CD	1:E:19:LYS:HE2	2.46	0.41
1:I:45:ARG:NH1	1:I:47:GLU:OE1	2.54	0.41
2:J:202:ARG:CZ	2:J:202:ARG:HB2	2.49	0.41
2:F:181:ARG:HH21	2:F:183:ASP:CG	2.25	0.41
2:F:239:ARG:NE	6:F:406:HOH:O	2.17	0.41
2:G:76:GLU:CG	3:H:10:THR:HG21	2.51	0.41
2:G:202:ARG:HD2	2:G:244:TRP:CD2	2.56	0.41
2:J:147:TRP:CZ2	3:K:11:LEU:HD12	2.56	0.40
2:J:201:LEU:CD1	2:J:249:VAL:HG21	2.52	0.40
2:J:260:HIS:CD2	2:J:262:GLN:HE21	2.39	0.40
2:J:6:ARG:NH1	2:J:6:ARG:CG	2.83	0.40
2:F:138:THR:CG2	2:F:139:ALA:N	2.85	0.40
2:J:146:LYS:HE2	3:K:10:THR:HG23	2.04	0.40
2:G:192:HIS:HB2	2:G:200:THR:OG1	2.21	0.40
1:I:37:VAL:HG21	1:I:66:TYR:CE1	2.56	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:177:ASP:CA	2:J:255:GLN:NE2[1_656]	1.54	0.66
2:C:183:ASP:OD1	2:J:273:ARG:NH1[1_656]	2.01	0.19
2:C:177:ASP:OD1	2:J:255:GLN:NE2[1_656]	2.13	0.07
2:C:183:ASP:OD1	2:J:273:ARG:NH2[1_656]	2.17	0.03

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	97/99 (98%)	96 (99%)	1 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	97/99 (98%)	96 (99%)	1 (1%)	0	100	100
1	E	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
1	I	97/99 (98%)	96 (99%)	1 (1%)	0	100	100
2	C	273/275 (99%)	264 (97%)	9 (3%)	0	100	100
2	F	274/275 (100%)	267 (97%)	7 (3%)	0	100	100
2	G	273/275 (99%)	265 (97%)	8 (3%)	0	100	100
2	J	273/275 (99%)	266 (97%)	7 (3%)	0	100	100
3	D	9/11 (82%)	9 (100%)	0	0	100	100
3	H	9/11 (82%)	9 (100%)	0	0	100	100
3	K	9/11 (82%)	9 (100%)	0	0	100	100
3	Q	9/11 (82%)	9 (100%)	0	0	100	100
All	All	1517/1540 (98%)	1481 (98%)	36 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	94/94 (100%)	93 (99%)	1 (1%)	65	82
1	B	90/94 (96%)	90 (100%)	0	100	100
1	E	94/94 (100%)	93 (99%)	1 (1%)	65	82
1	I	93/94 (99%)	92 (99%)	1 (1%)	65	82
2	C	231/233 (99%)	230 (100%)	1 (0%)	84	92
2	F	230/233 (99%)	230 (100%)	0	100	100
2	G	232/233 (100%)	231 (100%)	1 (0%)	84	92
2	J	231/233 (99%)	231 (100%)	0	100	100
3	D	10/10 (100%)	10 (100%)	0	100	100
3	H	10/10 (100%)	9 (90%)	1 (10%)	7	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	K	10/10 (100%)	10 (100%)	0	100	100
3	Q	10/10 (100%)	10 (100%)	0	100	100
All	All	1335/1348 (99%)	1329 (100%)	6 (0%)	84	92

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ILE
2	C	14	ARG
1	E	70	PHE
2	G	14	ARG
3	H	6	LYS
1	I	9	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	13	HIS
1	A	17	ASN
2	F	72	GLN
2	F	191	HIS
2	F	224	GLN
2	F	255	GLN
1	B	13	HIS
2	C	86	ASN
2	C	87	GLN
2	C	188	HIS
2	C	255	GLN
1	E	51	HIS
2	G	65	GLN
2	G	72	GLN
2	G	141	GLN
2	G	144	GLN
2	G	224	GLN
2	G	255	GLN
1	I	51	HIS
2	J	191	HIS
2	J	192	HIS
2	J	197	HIS

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Mol	Chain	Res	Type
2	J	224	GLN
2	J	255	GLN
2	J	262	GLN
2	J	263	HIS

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](#)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	EDO	H	101	-	3,3,3	0.40	0	2,2,2	0.22	0
4	EDO	E	101	-	3,3,3	0.26	0	2,2,2	0.44	0
4	EDO	A	101	-	3,3,3	0.50	0	2,2,2	0.98	0
4	EDO	E	102	-	3,3,3	0.42	0	2,2,2	0.77	0
4	EDO	F	302	-	3,3,3	0.48	0	2,2,2	0.41	0
5	PEG	F	301	-	6,6,6	0.50	0	5,5,5	0.65	0
4	EDO	Q	101	-	3,3,3	0.34	0	2,2,2	0.20	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	H	101	-	-	1/1/1/1	-
4	EDO	E	101	-	-	1/1/1/1	-
4	EDO	A	101	-	-	1/1/1/1	-
4	EDO	E	102	-	-	0/1/1/1	-
4	EDO	F	302	-	-	0/1/1/1	-
5	PEG	F	301	-	-	3/4/4/4	-
4	EDO	Q	101	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	101	EDO	O1-C1-C2-O2
5	F	301	PEG	C1-C2-O2-C3
5	F	301	PEG	C4-C3-O2-C2
4	A	101	EDO	O1-C1-C2-O2
4	H	101	EDO	O1-C1-C2-O2
5	F	301	PEG	O2-C3-C4-O4

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	302	EDO	1	0
5	F	301	PEG	4	0
4	Q	101	EDO	1	0

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	99/99 (100%)	-0.00	1 (1%) 79 76	21, 39, 61, 69	0
1	B	99/99 (100%)	0.09	1 (1%) 79 76	24, 43, 69, 90	0
1	E	99/99 (100%)	-0.00	2 (2%) 65 60	20, 36, 64, 71	0
1	I	99/99 (100%)	0.65	6 (6%) 27 23	33, 54, 88, 116	0
2	C	275/275 (100%)	0.15	9 (3%) 49 45	20, 36, 69, 94	0
2	F	275/275 (100%)	-0.02	8 (2%) 53 50	13, 28, 67, 101	1 (0%)
2	G	275/275 (100%)	-0.17	4 (1%) 72 68	17, 26, 49, 92	0
2	J	275/275 (100%)	0.56	25 (9%) 15 12	22, 44, 102, 126	0
3	D	11/11 (100%)	-0.37	0 100 100	22, 24, 27, 28	0
3	H	11/11 (100%)	-0.51	0 100 100	20, 22, 24, 25	0
3	K	11/11 (100%)	0.12	0 100 100	28, 30, 35, 36	0
3	Q	11/11 (100%)	-0.38	0 100 100	21, 25, 26, 27	0
All	All	1540/1540 (100%)	0.13	56 (3%) 46 42	13, 35, 75, 126	1 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	1	ILE	5.1
2	J	255	GLN	4.8
1	B	1	ILE	4.6
2	C	177	ASP	4.5
2	C	255	GLN	4.2
2	G	17	ARG	4.0
2	J	268	LYS	3.7
2	F	181	ARG	3.5
2	J	181	ARG	3.5
2	F	15	PRO	3.4
2	J	197	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
2	C	186	LYS	3.2
2	J	273	ARG	3.1
2	J	254	GLU	3.0
2	F	226	GLN	3.0
2	C	273	ARG	3.0
2	J	274	TRP	2.9
2	G	225	THR	2.8
2	F	225	THR	2.7
2	J	225	THR	2.7
2	J	192	HIS	2.7
2	J	275	GLU	2.7
2	G	18	GLY	2.6
2	J	191	HIS	2.6
2	C	223	ASP	2.6
1	I	99	MET	2.6
2	J	250	PRO	2.6
2	F	273	ARG	2.5
2	J	204	TRP	2.5
2	F	252	GLY	2.5
2	J	249	VAL	2.5
1	I	94	LYS	2.4
2	J	221	GLY	2.4
1	A	1	ILE	2.4
1	I	74	GLU	2.4
2	J	222	GLU	2.4
2	C	225	THR	2.3
2	J	251	SER	2.3
2	C	275	GLU	2.3
2	J	267	PRO	2.3
1	E	19	LYS	2.2
1	E	1	ILE	2.2
2	F	17	ARG	2.2
1	I	75	LYS	2.2
2	C	194	ILE	2.2
2	J	180	GLU	2.2
2	J	239	ARG	2.1
2	G	226	GLN	2.1
2	C	173	GLU	2.1
2	J	256	ARG	2.1
2	J	189	VAL	2.1
2	F	274	TRP	2.1
2	J	199	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	J	1	GLY	2.0
1	I	97	ARG	2.0
2	J	206	LEU	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	E	102	4/4	0.76	0.20	33,39,43,45	0
5	PEG	F	301	7/7	0.79	0.23	26,32,38,38	0
4	EDO	F	302	4/4	0.89	0.16	31,37,41,41	0
4	EDO	Q	101	4/4	0.90	0.21	23,33,40,44	0
4	EDO	E	101	4/4	0.92	0.11	31,38,43,49	0
4	EDO	H	101	4/4	0.94	0.14	24,29,33,38	0
4	EDO	A	101	4/4	0.95	0.07	32,39,42,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.