



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:07 AM UTC

PDB ID : 3F65 / pdb_00003f65
Title : The F4 fimbrial chaperone FaeE does not self-cap its interactive surfaces
Authors : Van Molle, I.; Moonens, K.; Buts, L.; Garcia-Pino, A.; Wyns, L.; De Greve, H.; Bouckaert, J.
Deposited on : 2008-11-05
Resolution : 2.29 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:

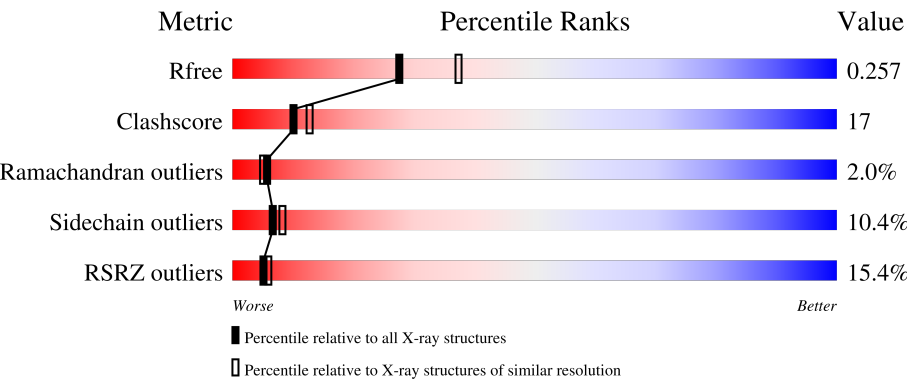
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.29 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	224	4% 66% 24% • 8%
1	B	224	3% 68% 20% • 8%
1	C	224	% 69% 17% • • 8%
1	D	224	13% 50% 17% 5% 28%
1	E	224	16% 55% 25% 5% 13%

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Mol	Chain	Length	Quality of chain
1	F	224	
1	G	224	
1	H	224	

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
2	MPD	A	225	-	-	X	-
2	MPD	C	225	X	-	-	-
2	MPD	G	225	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11425 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 Chaperone protein faeE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1587	1006	272	305	4			
1	B	205	Total	C	N	O	S	0	0	0
			1567	993	269	301	4			
1	C	206	Total	C	N	O	S	0	0	0
			1569	996	271	298	4			
1	D	161	Total	C	N	O	S	0	0	0
			1215	778	202	232	3			
1	E	194	Total	C	N	O	S	0	0	0
			1418	895	242	277	4			
1	F	166	Total	C	N	O	S	0	0	0
			1232	790	205	233	4			
1	G	193	Total	C	N	O	S	0	0	0
			1371	865	234	268	4			
1	H	153	Total	C	N	O	S	0	0	0
			1138	726	193	216	3			

There are 8 discrepancies between the modelled and reference sequences:

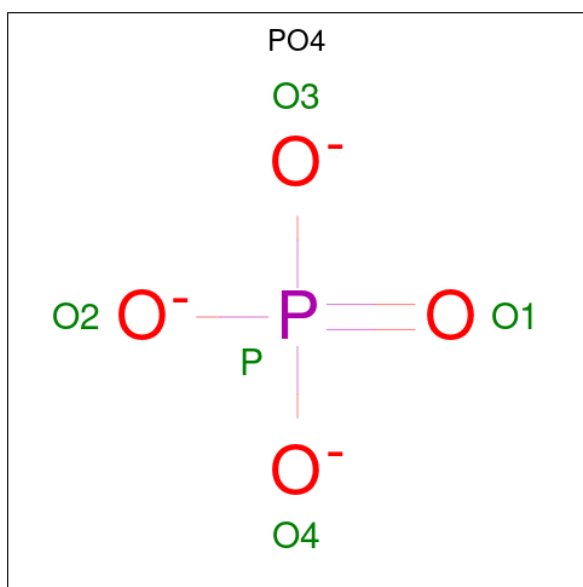
Chain	Residue	Modelled	Actual	Comment	Reference
A	15	GLU	LYS	engineered mutation	UNP P25401
B	15	GLU	LYS	engineered mutation	UNP P25401
C	15	GLU	LYS	engineered mutation	UNP P25401
D	15	GLU	LYS	engineered mutation	UNP P25401
E	15	GLU	LYS	engineered mutation	UNP P25401
F	15	GLU	LYS	engineered mutation	UNP P25401
G	15	GLU	LYS	engineered mutation	UNP P25401
H	15	GLU	LYS	engineered mutation	UNP P25401

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		
2	C	1	Total	C	O	0	0
			8	6	2		
2	G	1	Total	C	O	0	0
			8	6	2		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		

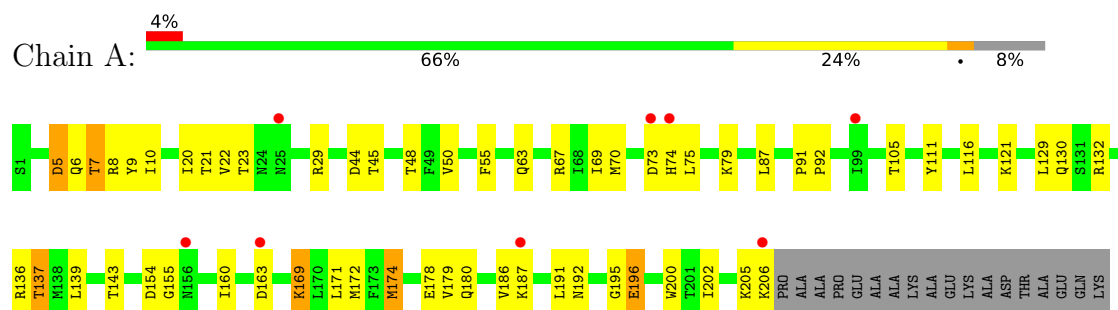
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	89	Total 89	O 89	0	0
4	B	58	Total 58	O 58	0	0
4	C	85	Total 85	O 85	0	0
4	D	32	Total 32	O 32	0	0
4	E	18	Total 18	O 18	0	0
4	F	5	Total 5	O 5	0	0
4	G	1	Total 1	O 1	0	0
4	H	11	Total 11	O 11	0	0

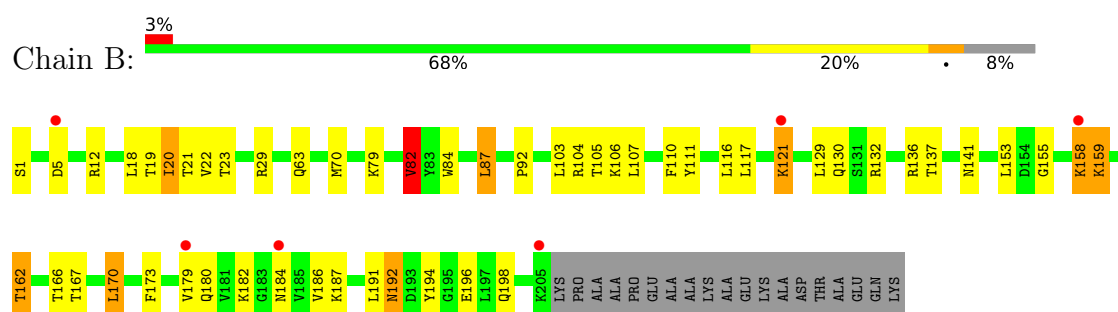
3 Residue-property plots [i](#)

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

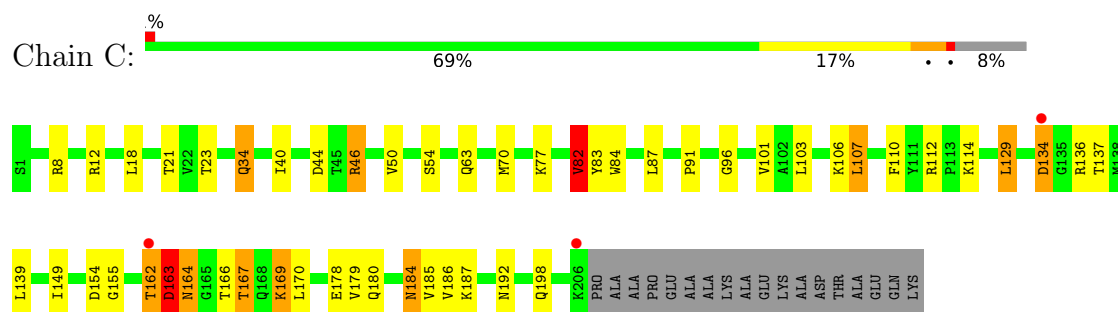
• Molecule 1: Chaperone protein faeE



• Molecule 1: Chaperone protein faeE

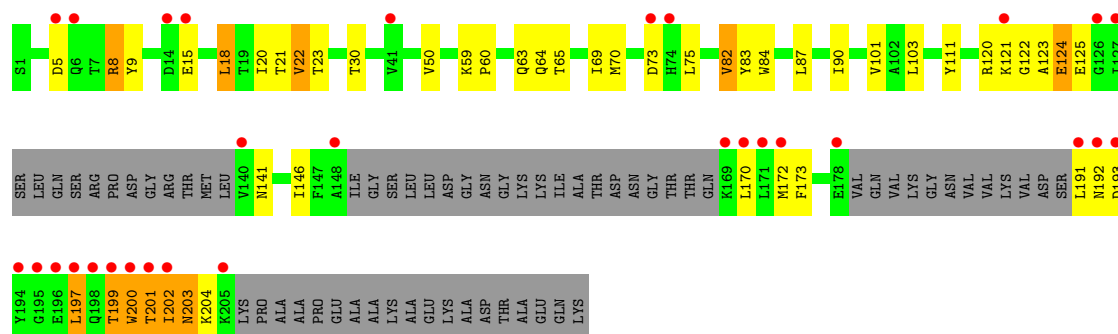


• Molecule 1: Chaperone protein faeE

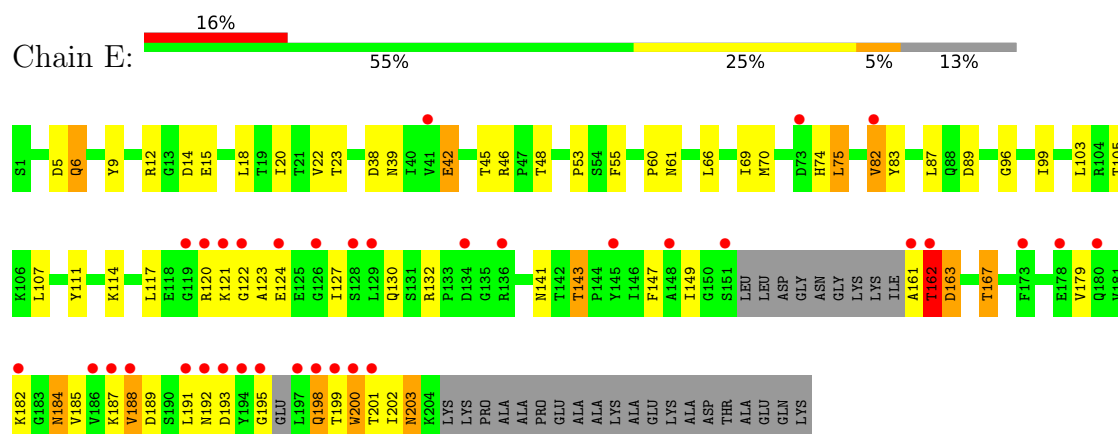


• Molecule 1: Chaperone protein faeE

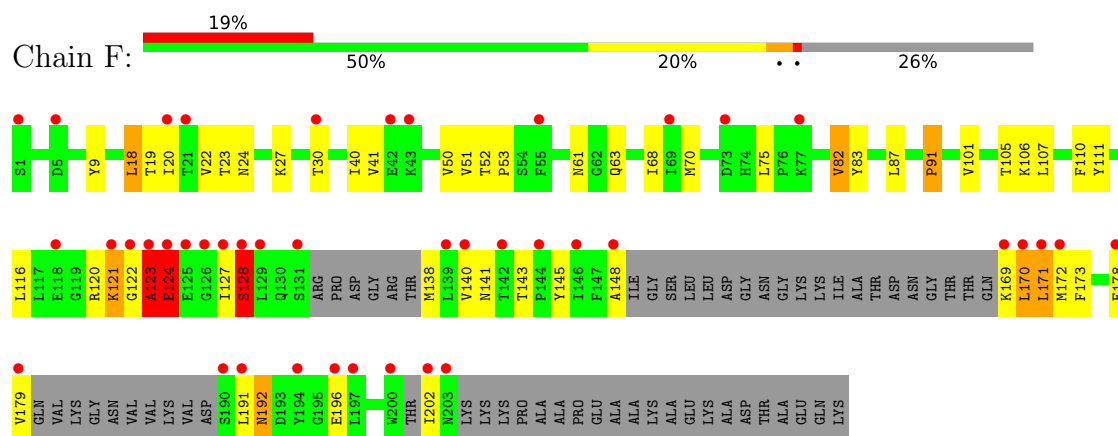




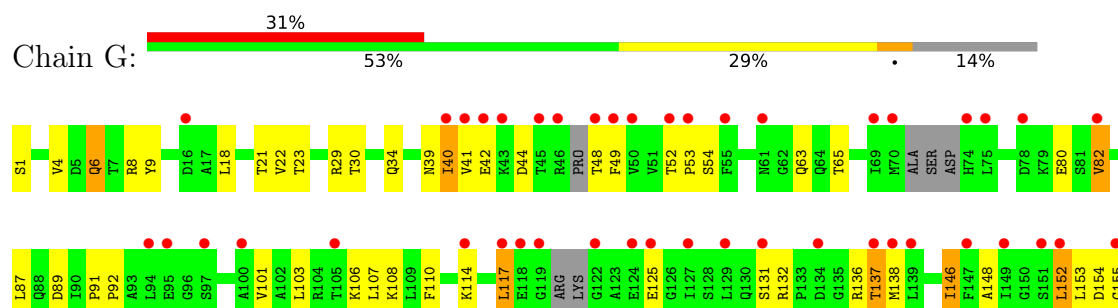
• Molecule 1: Chaperone protein faeE



• Molecule 1: Chaperone protein faeE



• Molecule 1: Chaperone protein faeE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	195.69Å 78.49Å 184.57Å 90.00° 102.15° 90.00°	Depositor
Resolution (Å)	49.85 – 2.29 49.85 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.85-2.29) 99.3 (49.85-2.29)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.29Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.224 , 0.260 0.224 , 0.257	Depositor DCC
R_{free} test set	6156 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	50.4	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11425	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.83% 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: MPD, PO4

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	0.55	0/1616	0.85	1/2195 (0.0%)
1	B	0.44	0/1595	0.84	1/2168 (0.0%)
1	C	0.51	0/1598	0.84	2/2174 (0.1%)
1	D	0.43	0/1240	0.84	3/1691 (0.2%)
1	E	0.36	0/1442	0.81	1/1970 (0.1%)
1	F	0.38	0/1255	0.85	4/1714 (0.2%)
1	G	0.29	0/1391	0.77	0/1899
1	H	0.33	0/1159	0.77	0/1579
All	All	0.43	0/11296	0.83	12/15390 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	123	ALA	N-CA-C	8.97	124.65	112.90
1	F	128	SER	CA-C-N	8.54	134.24	122.19
1	F	128	SER	C-N-CA	8.54	134.24	122.19
1	B	82	VAL	CB-CA-C	-7.98	99.41	110.90
1	C	82	VAL	CB-CA-C	-7.69	98.86	110.55
1	D	170	LEU	N-CA-C	-6.52	105.48	113.50
1	E	6	GLN	N-CA-C	5.69	115.79	108.34
1	C	149	ILE	CB-CA-C	-5.41	104.41	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	90	ILE	CA-C-N	5.36	123.52	119.66
1	D	90	ILE	C-N-CA	5.36	123.52	119.66
1	A	91	PRO	O-C-N	5.04	123.63	121.31
1	F	91	PRO	O-C-N	5.00	123.61	121.31

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	123	ALA	Peptide

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	1587	0	1576	42	0
1	B	1567	0	1552	43	0
1	C	1569	0	1548	41	0
1	D	1215	0	1123	44	0
1	E	1418	0	1327	60	0
1	F	1232	0	1146	59	0
1	G	1371	0	1234	65	0
1	H	1138	0	1060	32	0
2	A	8	0	14	6	0
2	C	8	0	14	3	0
2	G	8	0	14	3	0
3	A	5	0	0	0	0
4	A	89	0	0	3	0
4	B	58	0	0	2	0
4	C	85	0	0	8	0
4	D	32	0	0	0	0
4	E	18	0	0	0	0
4	F	5	0	0	0	0
4	G	1	0	0	0	0
4	H	11	0	0	0	0
All	All	11425	0	10608	375	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (375) 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:F:123:ALA:N	1:F:124:GLU:HB2	1.11	1.41
1:F:123:ALA:N	1:F:124:GLU:CB	1.99	1.25
1:F:123:ALA:CA	1:F:124:GLU:HB2	1.85	1.05
1:D:199:THR:O	1:D:200:TRP:HB2	1.47	1.05
1:D:121:LYS:CB	1:D:122:GLY:HA3	1.92	1.00
1:D:8:ARG:HH11	1:D:8:ARG:HG2	1.27	0.96
1:H:30:THR:HG22	1:H:60:PRO:HD3	1.44	0.96
1:F:124:GLU:OE2	1:F:124:GLU:HA	1.61	0.96
1:G:40:ILE:HD13	1:G:40:ILE:H	1.32	0.94
1:E:200:TRP:HA	1:E:201:THR:HB	1.50	0.94
1:H:123:ALA:HB3	1:H:124:GLU:HA	1.50	0.93
1:A:172:MET:HG2	1:A:174:MET:HE1	1.51	0.93
1:D:199:THR:HG22	1:D:200:TRP:H	1.32	0.93
1:D:70:MET:HE1	1:D:111:TYR:CE1	2.06	0.90
1:D:199:THR:HG22	1:D:200:TRP:N	1.84	0.90
1:E:39:ASN:HB3	1:E:42:GLU:HG2	1.55	0.88
1:F:122:GLY:C	1:F:124:GLU:CB	2.46	0.88
1:H:23:THR:HG22	1:H:63:GLN:HG2	1.54	0.88
1:F:127:ILE:HD12	1:F:202:ILE:CG2	2.04	0.87
1:C:166:THR:HG23	1:C:179:VAL:HG11	1.56	0.87
1:F:123:ALA:H	1:F:124:GLU:HB2	1.10	0.87
1:F:122:GLY:C	1:F:124:GLU:HB2	2.00	0.87
1:D:199:THR:O	1:D:200:TRP:CB	2.22	0.86
1:F:23:THR:HG22	1:F:63:GLN:HG2	1.58	0.86
1:B:186:VAL:HG23	1:B:187:LYS:HG3	1.59	0.85
1:A:23:THR:HG22	1:A:63:GLN:HG2	1.60	0.83
1:E:189:ASP:HA	1:E:198:GLN:HA	1.61	0.82
1:C:186:VAL:HG23	1:C:187:LYS:HG3	1.62	0.82
1:F:40:ILE:HD11	1:F:82:VAL:HB	1.62	0.82
1:G:6:GLN:HG3	1:G:9:TYR:CE2	2.14	0.82
1:D:199:THR:CG2	1:D:200:TRP:H	1.92	0.82
1:B:23:THR:HG22	1:B:63:GLN:HG2	1.60	0.81
1:G:21:THR:HG22	1:G:65:THR:HG22	1.63	0.80
1:F:124:GLU:OE2	1:F:124:GLU:CA	2.30	0.80
1:A:205:LYS:O	1:A:206:LYS:CB	2.30	0.80
1:D:201:THR:O	1:D:202:ILE:CB	2.30	0.78
1:G:52:THR:OG1	1:G:53:PRO:HD3	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:LYS:CB	1:D:122:GLY:CA	2.61	0.78
1:F:70:MET:HE2	1:F:75:LEU:HD12	1.65	0.78
2:C:225:MPD:H12	2:C:225:MPD:H52	1.65	0.78
1:G:165:GLY:N	1:G:166:THR:HA	1.99	0.77
1:E:127:ILE:HB	1:E:202:ILE:HG23	1.65	0.77
1:F:127:ILE:O	1:F:140:VAL:O	2.02	0.77
1:F:122:GLY:C	1:F:124:GLU:HB3	2.10	0.76
1:C:23:THR:HG22	1:C:63:GLN:HG2	1.66	0.75
1:F:192:ASN:ND2	1:F:196:GLU:H	1.83	0.75
1:F:51:VAL:HG22	1:F:68:ILE:HD13	1.70	0.74
1:H:123:ALA:HB2	1:H:190:SER:OG	1.87	0.74
1:D:70:MET:HE2	1:D:75:LEU:HD12	1.71	0.73
1:E:163:ASP:O	1:E:167:THR:HG22	1.88	0.72
1:G:184:ASN:C	1:G:184:ASN:HD22	1.97	0.72
1:A:8:ARG:HH21	1:A:10:ILE:HG12	1.53	0.72
1:G:91:PRO:HG3	1:G:101:VAL:O	1.88	0.71
1:H:123:ALA:CB	1:H:124:GLU:HA	2.20	0.71
1:C:70:MET:HE1	4:C:237:HOH:O	1.89	0.71
1:C:112:ARG:HH21	2:C:225:MPD:H4	1.56	0.71
1:D:82:VAL:HG21	1:D:172:MET:HE1	1.71	0.71
1:F:70:MET:HE1	1:F:111:TYR:CZ	2.26	0.71
1:B:87:LEU:HB3	1:B:105:THR:CG2	2.21	0.71
1:E:200:TRP:HA	1:E:201:THR:CB	2.22	0.70
1:F:170:LEU:HD11	1:F:173:PHE:HB2	1.71	0.70
1:G:146:ILE:HG13	1:G:175:PRO:HD3	1.71	0.70
1:F:18:LEU:HD13	1:F:20:ILE:HD11	1.74	0.70
1:F:127:ILE:HD12	1:F:202:ILE:HG22	1.74	0.70
1:A:7:THR:OG1	2:A:225:MPD:H11	1.92	0.70
1:D:8:ARG:HH11	1:D:8:ARG:CG	2.03	0.70
1:B:192:ASN:ND2	1:B:196:GLU:H	1.89	0.70
1:F:192:ASN:HD21	1:F:196:GLU:H	1.38	0.69
1:B:70:MET:HE1	1:B:111:TYR:CE1	2.28	0.69
1:G:23:THR:HG22	1:G:63:GLN:HG2	1.73	0.69
1:C:23:THR:HG23	4:C:230:HOH:O	1.94	0.68
1:D:21:THR:HG22	1:D:65:THR:HG22	1.75	0.68
1:B:12:ARG:NH1	1:B:117:LEU:HD22	2.08	0.68
1:A:29:ARG:HG2	1:A:92:PRO:HG2	1.76	0.67
1:C:112:ARG:NH2	2:C:225:MPD:H4	2.10	0.67
1:G:106:LYS:O	1:G:107:LEU:HD23	1.94	0.67
1:A:23:THR:HG23	4:A:310:HOH:O	1.94	0.67
1:C:155:GLY:HA2	1:C:186:VAL:HG21	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLN:HG2	2:A:225:MPD:H4	1.77	0.66
1:B:155:GLY:HA2	1:B:186:VAL:HG21	1.75	0.66
1:H:123:ALA:HB3	1:H:124:GLU:CA	2.24	0.65
1:B:130:GLN:HE21	1:B:132:ARG:HH12	1.43	0.65
1:G:114:LYS:HA	1:G:117:LEU:CD2	2.27	0.65
1:C:184:ASN:H	1:C:184:ASN:HD22	1.44	0.65
1:C:44:ASP:OD1	1:C:46:ARG:HD3	1.97	0.64
1:D:202:ILE:O	1:D:203:ASN:CB	2.46	0.64
1:G:192:ASN:C	1:G:192:ASN:HD22	2.04	0.64
1:D:23:THR:HG22	1:D:63:GLN:HG2	1.79	0.64
1:A:67:ARG:NH1	1:A:69:ILE:HD11	2.13	0.63
1:C:82:VAL:HG13	1:C:110:PHE:CD2	2.34	0.63
1:B:182:LYS:C	1:B:184:ASN:H	2.06	0.63
1:G:132:ARG:HE	1:G:138:MET:HG3	1.64	0.62
1:E:192:ASN:O	1:E:193:ASP:HB2	1.99	0.62
1:E:39:ASN:HD21	1:E:48:THR:HG23	1.64	0.62
1:C:91:PRO:HG3	1:C:101:VAL:O	2.00	0.62
1:G:39:ASN:ND2	1:G:44:ASP:HB3	2.15	0.62
1:D:202:ILE:O	1:D:203:ASN:HB2	2.01	0.61
1:C:162:THR:O	1:C:166:THR:HB	2.01	0.61
1:F:120:ARG:O	1:F:120:ARG:HD3	2.00	0.61
1:D:30:THR:HG22	1:D:60:PRO:HD3	1.82	0.61
1:D:191:LEU:N	1:D:192:ASN:CB	2.64	0.60
1:H:4:VAL:HG21	1:H:107:LEU:HD11	1.81	0.60
1:B:182:LYS:HG2	1:B:184:ASN:HB2	1.84	0.60
1:B:192:ASN:HD22	1:B:192:ASN:C	2.09	0.60
1:H:88:GLN:OE1	1:H:104:ARG:HB2	2.01	0.60
1:B:23:THR:HG23	4:B:230:HOH:O	2.01	0.59
1:E:161:ALA:O	1:E:162:THR:HG23	2.02	0.59
1:G:40:ILE:H	1:G:40:ILE:CD1	2.09	0.59
1:A:186:VAL:O	1:A:202:ILE:HG12	2.02	0.58
1:G:153:LEU:O	1:G:187:LYS:N	2.36	0.58
1:A:187:LYS:HB3	1:A:200:TRP:O	2.03	0.58
1:D:197:LEU:N	1:D:197:LEU:HD12	2.16	0.58
1:H:191:LEU:O	1:H:192:ASN:HB3	2.03	0.58
1:B:87:LEU:HB3	1:B:105:THR:HG23	1.85	0.58
1:A:7:THR:H	2:A:225:MPD:H31	1.67	0.58
1:B:130:GLN:NE2	1:B:132:ARG:HH12	2.00	0.58
1:A:136:ARG:HH11	1:A:180:GLN:NE2	2.02	0.58
1:B:79:LYS:HA	1:B:116:LEU:HD11	1.84	0.58
1:C:101:VAL:HG22	1:D:103:LEU:CD2	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:ARG:HH11	1:C:180:GLN:NE2	2.01	0.57
1:B:70:MET:HE1	1:B:111:TYR:HE1	1.68	0.57
1:G:82:VAL:HG13	1:G:110:PHE:CE2	2.39	0.57
1:A:9:TYR:CE2	1:A:20:ILE:HD12	2.39	0.57
1:F:82:VAL:HG13	1:F:110:PHE:CD2	2.39	0.57
1:G:166:THR:HG23	1:G:168:GLN:O	2.04	0.57
1:B:136:ARG:HH11	1:B:180:GLN:HE22	1.52	0.57
1:D:30:THR:HG22	1:D:59:LYS:HA	1.87	0.56
1:E:99:ILE:HG12	1:F:105:THR:HG22	1.86	0.56
1:A:79:LYS:HA	1:A:116:LEU:HD11	1.88	0.56
1:F:141:ASN:HB2	1:F:173:PHE:CE2	2.40	0.56
1:H:82:VAL:HG22	1:H:146:ILE:HD13	1.85	0.56
1:C:164:ASN:H	1:C:164:ASN:ND2	2.02	0.56
1:A:137:THR:HG22	4:A:251:HOH:O	2.06	0.56
1:G:168:GLN:C	1:G:170:LEU:H	2.14	0.56
1:F:116:LEU:HB3	1:F:145:TYR:CE2	2.41	0.56
1:B:82:VAL:HG13	1:B:110:PHE:CE2	2.40	0.55
1:F:120:ARG:HH12	1:F:124:GLU:HG2	1.71	0.55
1:D:141:ASN:HB2	1:D:173:PHE:CE2	2.42	0.55
1:G:154:ASP:CG	1:G:155:GLY:H	2.13	0.55
1:B:70:MET:CE	1:B:111:TYR:CE1	2.90	0.54
1:C:136:ARG:HH11	1:C:180:GLN:HE22	1.55	0.54
1:E:187:LYS:HA	1:E:201:THR:H	1.71	0.54
1:E:191:LEU:HA	1:E:195:GLY:O	2.07	0.54
1:D:191:LEU:CB	1:D:192:ASN:HA	2.38	0.54
1:G:154:ASP:CG	1:G:155:GLY:N	2.66	0.54
1:E:184:ASN:ND2	1:E:184:ASN:H	2.04	0.54
1:B:82:VAL:HG13	1:B:110:PHE:CD2	2.43	0.54
1:C:162:THR:HG21	4:C:282:HOH:O	2.07	0.53
1:G:1:SER:HB3	1:G:103:LEU:HD12	1.90	0.53
1:G:110:PHE:CD2	2:G:225:MPD:HM2	2.43	0.53
1:H:122:GLY:O	1:H:123:ALA:C	2.51	0.53
1:H:9:TYR:CE2	1:H:20:ILE:HG13	2.44	0.53
1:G:114:LYS:HA	1:G:117:LEU:HD22	1.89	0.53
1:G:192:ASN:ND2	1:G:196:GLU:H	2.06	0.53
1:E:75:LEU:HD12	1:E:111:TYR:CD2	2.44	0.52
1:H:123:ALA:CB	1:H:124:GLU:CA	2.85	0.52
1:B:136:ARG:HH11	1:B:180:GLN:NE2	2.08	0.52
1:F:123:ALA:H	1:F:124:GLU:CB	1.91	0.52
1:A:172:MET:CG	1:A:174:MET:HE1	2.32	0.52
1:H:72:SER:OG	1:H:74:HIS:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ASN:HD21	1:A:196:GLU:HG3	1.73	0.52
1:F:170:LEU:HD11	1:F:173:PHE:CB	2.40	0.52
1:G:82:VAL:HG13	1:G:110:PHE:CD2	2.45	0.52
1:E:48:THR:CG2	1:E:74:HIS:HE1	2.23	0.51
1:F:148:ALA:HB3	1:F:191:LEU:H	1.74	0.51
1:A:130:GLN:HE21	1:A:132:ARG:HH12	1.58	0.51
1:A:195:GLY:HA3	2:A:225:MPD:HM3	1.93	0.51
1:H:126:GLY:O	1:H:127:ILE:O	2.28	0.51
1:A:44:ASP:OD1	1:A:45:THR:N	2.44	0.51
1:E:202:ILE:HG22	1:E:203:ASN:N	2.25	0.51
1:G:152:LEU:HD12	1:G:188:VAL:HG12	1.93	0.51
1:C:34:GLN:HG3	1:C:54:SER:O	2.11	0.50
1:A:136:ARG:HH11	1:A:180:GLN:HE22	1.59	0.50
1:C:184:ASN:HD22	1:C:184:ASN:N	2.05	0.50
1:D:70:MET:HE1	1:D:111:TYR:CZ	2.45	0.50
1:E:120:ARG:O	1:E:122:GLY:N	2.44	0.50
1:G:82:VAL:HG11	1:G:172:MET:HE1	1.92	0.50
1:B:192:ASN:HB3	1:B:198:GLN:HE21	1.76	0.50
1:F:91:PRO:HG3	1:F:101:VAL:O	2.11	0.50
1:G:41:VAL:HG22	1:G:41:VAL:O	2.12	0.50
1:E:12:ARG:HB2	1:E:15:GLU:HG3	1.94	0.50
1:A:169:LYS:HD3	1:A:179:VAL:CG1	2.41	0.50
1:B:158:LYS:O	1:B:159:LYS:CB	2.60	0.50
1:C:163:ASP:O	1:C:167:THR:HG22	2.11	0.50
1:A:8:ARG:HG3	2:A:225:MPD:C1	2.42	0.49
1:E:48:THR:HG21	1:E:74:HIS:HE1	1.76	0.49
1:A:73:ASP:CG	1:A:73:ASP:O	2.56	0.49
1:D:8:ARG:CG	1:D:8:ARG:NH1	2.70	0.49
1:E:103:LEU:CD2	1:F:101:VAL:HG22	2.42	0.49
1:B:182:LYS:C	1:B:184:ASN:N	2.71	0.49
1:C:107:LEU:HD12	1:C:107:LEU:N	2.28	0.49
1:E:38:ASP:OD2	1:H:45:THR:HG21	2.13	0.49
1:E:127:ILE:HD11	1:E:147:PHE:CD1	2.48	0.49
1:F:82:VAL:HG13	1:F:110:PHE:CE2	2.47	0.49
1:C:44:ASP:OD1	1:C:46:ARG:CD	2.61	0.49
1:C:134:ASP:OD1	1:C:136:ARG:HG3	2.13	0.49
1:H:127:ILE:O	1:H:142:THR:HB	2.13	0.49
1:D:70:MET:CE	1:D:75:LEU:HD12	2.42	0.49
1:E:14:ASP:OD1	1:E:15:GLU:HG2	2.13	0.49
1:E:123:ALA:HA	1:E:199:THR:CB	2.43	0.49
1:E:127:ILE:HD11	1:E:147:PHE:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:9:TYR:CE2	1:F:20:ILE:HG13	2.48	0.49
1:A:154:ASP:HB3	1:A:160:ILE:HD11	1.95	0.48
1:G:103:LEU:CD2	1:H:101:VAL:HG22	2.44	0.48
1:E:123:ALA:HA	1:E:199:THR:HB	1.95	0.48
1:F:148:ALA:HB1	1:F:191:LEU:HD13	1.95	0.48
1:E:70:MET:HE1	1:E:111:TYR:CZ	2.49	0.48
1:E:75:LEU:N	1:E:75:LEU:HD23	2.27	0.48
1:F:70:MET:CE	1:F:75:LEU:HD12	2.38	0.48
1:A:70:MET:HE1	1:A:111:TYR:CZ	2.48	0.48
1:A:192:ASN:OD1	1:A:196:GLU:HG3	2.14	0.48
1:A:137:THR:CG2	4:A:251:HOH:O	2.61	0.48
1:E:189:ASP:HB3	1:E:198:GLN:HB2	1.96	0.48
1:A:55:PHE:CD1	1:D:69:ILE:HD11	2.48	0.48
1:F:169:LYS:N	1:F:170:LEU:C	2.72	0.48
1:B:84:TRP:CD2	1:B:106:LYS:HE2	2.49	0.48
1:G:40:ILE:HD13	1:G:40:ILE:N	2.15	0.47
1:E:199:THR:O	1:E:200:TRP:CB	2.62	0.47
1:G:30:THR:O	1:G:92:PRO:HG3	2.14	0.47
1:C:129:LEU:HD21	1:C:185:VAL:O	2.15	0.47
1:F:107:LEU:HD23	1:F:107:LEU:N	2.30	0.47
1:G:167:THR:O	1:G:168:GLN:CB	2.63	0.47
1:C:101:VAL:HG22	1:D:103:LEU:HD22	1.96	0.47
1:F:178:GLU:O	1:F:179:VAL:HB	2.15	0.47
1:E:141:ASN:C	1:E:141:ASN:HD22	2.22	0.47
1:F:170:LEU:O	1:F:172:MET:N	2.47	0.47
1:C:82:VAL:C	1:C:83:TYR:CD1	2.93	0.47
1:F:120:ARG:O	1:F:121:LYS:C	2.58	0.47
1:G:131:SER:C	1:G:132:ARG:HD2	2.40	0.47
1:A:169:LYS:HD3	1:A:179:VAL:HG12	1.96	0.47
1:E:120:ARG:C	1:E:122:GLY:N	2.73	0.47
1:D:82:VAL:HG22	1:D:146:ILE:HD13	1.97	0.47
1:A:75:LEU:HD12	1:A:111:TYR:CD2	2.51	0.47
1:C:82:VAL:HG13	1:C:110:PHE:CE2	2.50	0.46
1:G:80:GLU:CB	1:G:146:ILE:HD12	2.45	0.46
1:A:139:LEU:O	1:A:178:GLU:HA	2.16	0.46
1:B:12:ARG:HD3	4:B:227:HOH:O	2.15	0.46
1:E:39:ASN:CB	1:E:42:GLU:HG2	2.36	0.46
1:D:124:GLU:C	1:D:125:GLU:OE2	2.59	0.46
1:F:127:ILE:CD1	1:F:202:ILE:HG22	2.45	0.46
1:F:170:LEU:HD13	1:F:171:LEU:N	2.31	0.46
1:C:192:ASN:HB3	1:C:198:GLN:HE21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:42:GLU:O	1:G:44:ASP:N	2.39	0.46
1:G:137:THR:HG21	1:G:183:GLY:CA	2.45	0.46
1:F:27:LYS:HG2	1:F:61:ASN:OD1	2.16	0.46
1:G:125:GLU:HB3	1:G:204:LYS:HD2	1.98	0.46
1:B:1:SER:OG	1:B:103:LEU:HD12	2.16	0.45
1:F:141:ASN:ND2	1:F:143:THR:H	2.14	0.45
1:G:40:ILE:HG12	1:G:41:VAL:N	2.32	0.45
1:A:192:ASN:ND2	1:A:196:GLU:HG3	2.31	0.45
1:F:141:ASN:C	1:F:141:ASN:HD22	2.23	0.45
1:E:55:PHE:CE1	1:H:69:ILE:HD11	2.51	0.45
1:B:166:THR:HG23	1:B:179:VAL:HG21	1.98	0.45
1:C:103:LEU:CD2	1:D:101:VAL:HG22	2.46	0.45
1:D:22:VAL:HG13	1:D:64:GLN:O	2.17	0.45
1:F:127:ILE:HD12	1:F:202:ILE:HG21	1.90	0.45
2:G:225:MPD:H4	2:G:225:MPD:HM1	1.70	0.45
1:C:114:LYS:HG3	4:C:236:HOH:O	2.15	0.45
1:B:170:LEU:HD12	1:B:170:LEU:HA	1.88	0.45
1:F:192:ASN:C	1:F:192:ASN:HD22	2.24	0.45
1:G:137:THR:HG23	1:G:181:VAL:O	2.17	0.45
1:C:84:TRP:CD2	1:C:106:LYS:HE3	2.51	0.45
1:C:164:ASN:H	1:C:164:ASN:HD22	1.64	0.45
1:F:24:ASN:O	1:F:61:ASN:HA	2.17	0.45
1:E:60:PRO:O	1:E:61:ASN:HB2	2.16	0.45
1:E:141:ASN:HD22	1:E:143:THR:H	1.64	0.45
1:A:5:ASP:HB2	1:A:6:GLN:HG3	1.99	0.44
1:F:169:LYS:N	1:F:170:LEU:O	2.49	0.44
1:E:130:GLN:HE21	1:E:132:ARG:NH1	2.15	0.44
1:E:162:THR:O	1:E:163:ASP:HB3	2.17	0.44
1:F:124:GLU:O	1:F:127:ILE:HD11	2.17	0.44
1:G:146:ILE:HG12	1:G:174:MET:SD	2.56	0.44
1:H:120:ARG:O	1:H:121:LYS:C	2.60	0.44
1:E:114:LYS:HA	1:E:117:LEU:HG	1.99	0.44
1:G:184:ASN:ND2	1:G:185:VAL:HG23	2.33	0.44
1:G:4:VAL:HB	1:G:9:TYR:OH	2.18	0.44
1:H:190:SER:C	1:H:191:LEU:HD12	2.42	0.44
1:B:141:ASN:HB2	1:B:173:PHE:CE2	2.53	0.44
1:D:9:TYR:CE2	1:D:20:ILE:HG12	2.52	0.44
1:E:184:ASN:N	1:E:184:ASN:HD22	2.16	0.44
1:D:69:ILE:C	1:D:69:ILE:HD12	2.42	0.44
1:G:137:THR:HG21	1:G:183:GLY:HA2	2.00	0.44
1:F:127:ILE:HD12	1:F:202:ILE:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:90:ILE:HA	1:H:91:PRO:HD2	1.89	0.44
1:A:75:LEU:N	1:A:75:LEU:HD23	2.31	0.43
1:E:149:ILE:HG23	1:E:188:VAL:HG13	1.99	0.43
1:G:184:ASN:C	1:G:184:ASN:ND2	2.68	0.43
1:G:201:THR:O	1:G:204:LYS:HE3	2.17	0.43
1:C:136:ARG:NH1	1:C:180:GLN:HE22	2.17	0.43
1:D:123:ALA:O	1:D:125:GLU:N	2.50	0.43
1:G:191:LEU:HD22	1:G:195:GLY:C	2.43	0.43
1:D:202:ILE:O	1:D:203:ASN:ND2	2.51	0.43
1:C:169:LYS:CD	4:C:285:HOH:O	2.65	0.43
1:E:141:ASN:ND2	1:E:143:THR:H	2.15	0.43
1:A:155:GLY:CA	1:A:186:VAL:HG21	2.48	0.43
1:G:29:ARG:CB	1:G:92:PRO:HG2	2.49	0.43
1:G:154:ASP:C	1:G:156:ASN:N	2.77	0.43
1:E:6:GLN:HG2	1:E:9:TYR:CZ	2.54	0.43
1:E:141:ASN:C	1:E:141:ASN:ND2	2.76	0.43
1:B:130:GLN:HE21	1:B:132:ARG:NH1	2.14	0.43
1:B:192:ASN:HD21	1:B:196:GLU:H	1.61	0.43
1:E:184:ASN:HD22	1:E:185:VAL:N	2.17	0.43
1:F:52:THR:HA	1:F:53:PRO:C	2.43	0.43
1:G:52:THR:CB	1:G:53:PRO:HD3	2.49	0.43
1:H:75:LEU:HA	1:H:76:PRO:HD3	1.84	0.43
1:B:162:THR:CG2	1:B:167:THR:OG1	2.67	0.43
1:E:184:ASN:ND2	1:E:184:ASN:N	2.65	0.43
1:E:202:ILE:N	1:E:202:ILE:HD12	2.34	0.43
1:F:120:ARG:NH1	1:F:124:GLU:HG2	2.32	0.43
1:G:148:ALA:HB2	2:G:225:MPD:H51	2.01	0.43
1:H:82:VAL:C	1:H:83:TYR:CD1	2.97	0.43
1:H:144:PRO:HD2	1:H:145:TYR:CD1	2.54	0.43
1:B:18:LEU:HG	1:B:20:ILE:CD1	2.50	0.42
1:D:202:ILE:O	1:D:203:ASN:CG	2.62	0.42
1:E:53:PRO:HD2	1:E:66:LEU:HD23	2.02	0.42
1:H:72:SER:C	1:H:74:HIS:H	2.27	0.42
1:H:82:VAL:HG13	1:H:110:PHE:CD2	2.54	0.42
1:B:192:ASN:ND2	1:B:194:TYR:H	2.17	0.42
1:H:123:ALA:HB1	1:H:147:PHE:CE2	2.55	0.42
1:A:8:ARG:HG3	2:A:225:MPD:H12	2.02	0.42
1:C:12:ARG:NH2	4:C:238:HOH:O	2.50	0.42
1:B:121:LYS:HA	1:B:121:LYS:HD2	1.83	0.42
1:C:96:GLY:HA2	1:D:84:TRP:CH2	2.54	0.42
1:C:154:ASP:C	1:C:186:VAL:HG22	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:168:GLN:C	1:G:170:LEU:N	2.75	0.42
1:B:19:THR:C	1:B:20:ILE:HD12	2.45	0.42
1:G:155:GLY:O	1:G:156:ASN:CB	2.68	0.42
1:G:192:ASN:C	1:G:192:ASN:ND2	2.75	0.42
1:E:82:VAL:C	1:E:83:TYR:CD1	2.98	0.42
1:G:136:ARG:HD3	1:G:180:GLN:CD	2.45	0.42
1:A:74:HIS:CD2	1:A:75:LEU:HD23	2.55	0.42
1:E:96:GLY:O	1:F:106:LYS:HE3	2.20	0.42
1:A:70:MET:HE2	1:A:75:LEU:HG	2.02	0.41
1:C:77:LYS:NZ	4:C:342:HOH:O	2.43	0.41
1:E:45:THR:O	1:E:46:ARG:C	2.61	0.41
1:E:69:ILE:C	1:E:69:ILE:HD12	2.44	0.41
1:A:48:THR:HG21	1:A:75:LEU:HD21	2.01	0.41
1:E:120:ARG:C	1:E:122:GLY:H	2.28	0.41
1:E:202:ILE:CG2	1:E:203:ASN:N	2.84	0.41
1:D:8:ARG:HG2	1:D:8:ARG:NH1	2.08	0.41
1:B:70:MET:HE3	1:B:70:MET:HB2	1.66	0.41
1:D:120:ARG:O	1:D:121:LYS:C	2.63	0.41
1:F:192:ASN:ND2	1:F:192:ASN:C	2.79	0.41
1:G:192:ASN:ND2	1:G:194:TYR:H	2.18	0.41
1:B:158:LYS:O	1:B:159:LYS:HB3	2.21	0.41
1:E:89:ASP:OD1	1:E:89:ASP:C	2.63	0.41
1:G:80:GLU:HB2	1:G:146:ILE:HD12	2.03	0.41
1:H:30:THR:O	1:H:92:PRO:HG3	2.21	0.41
1:F:19:THR:C	1:F:20:ILE:HD12	2.45	0.41
1:B:87:LEU:HB3	1:B:105:THR:HG22	1.97	0.41
1:G:89:ASP:OD1	1:G:89:ASP:C	2.62	0.41
1:E:55:PHE:CD1	1:H:69:ILE:HD11	2.56	0.41
1:A:171:LEU:HD23	1:A:171:LEU:HA	1.93	0.41
1:D:9:TYR:HB3	1:D:18:LEU:HD11	2.02	0.41
1:D:82:VAL:C	1:D:83:TYR:CD1	2.99	0.41
1:G:154:ASP:C	1:G:156:ASN:H	2.29	0.41
1:G:155:GLY:O	1:G:156:ASN:HB2	2.21	0.41
1:B:104:ARG:HH22	1:D:73:ASP:CB	2.33	0.41
1:F:70:MET:HE2	1:F:75:LEU:CD1	2.42	0.41
1:G:8:ARG:HB2	1:G:108:LYS:HB2	2.03	0.41
1:G:48:THR:HB	1:G:49:PHE:H	1.70	0.41
1:B:29:ARG:HB2	1:B:92:PRO:HG3	2.02	0.40
1:B:153:LEU:HD23	1:B:159:LYS:HA	2.03	0.40
1:C:139:LEU:O	1:C:178:GLU:HA	2.22	0.40
1:H:72:SER:CB	1:H:74:HIS:HD2	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:TYR:CE2	1:E:20:ILE:HG12	2.55	0.40
1:G:34:GLN:HA	1:G:54:SER:O	2.22	0.40
1:E:130:GLN:NE2	1:E:132:ARG:HH12	2.20	0.40
1:E:162:THR:O	1:E:163:ASP:CB	2.69	0.40
1:E:184:ASN:H	1:E:184:ASN:HD22	1.66	0.40
1:F:82:VAL:C	1:F:83:TYR:CD1	2.99	0.40
1:G:4:VAL:HG21	1:G:107:LEU:CD1	2.52	0.40
1:C:163:ASP:HB3	4:C:283:HOH:O	2.21	0.40
1:H:38:ASP:HB2	1:H:84:TRP:HB2	2.04	0.40
1:G:192:ASN:HD21	1:G:196:GLU:H	1.67	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	204/224 (91%)	198 (97%)	5 (2%)	1 (0%)	24	31
1	B	203/224 (91%)	193 (95%)	7 (3%)	3 (2%)	8	8
1	C	204/224 (91%)	195 (96%)	7 (3%)	2 (1%)	12	15
1	D	153/224 (68%)	136 (89%)	11 (7%)	6 (4%)	2	1
1	E	188/224 (84%)	166 (88%)	15 (8%)	7 (4%)	2	1
1	F	156/224 (70%)	145 (93%)	8 (5%)	3 (2%)	6	5
1	G	181/224 (81%)	163 (90%)	17 (9%)	1 (1%)	21	27
1	H	143/224 (64%)	130 (91%)	7 (5%)	6 (4%)	2	1
All	All	1432/1792 (80%)	1326 (93%)	77 (5%)	29 (2%)	6	5

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	159	LYS
1	D	200	TRP
1	D	202	ILE
1	D	203	ASN
1	E	162	THR
1	F	124	GLU
1	G	156	ASN
1	H	121	LYS
1	H	123	ALA
1	B	158	LYS
1	C	134	ASP
1	F	121	LYS
1	H	124	GLU
1	H	141	ASN
1	B	121	LYS
1	D	124	GLU
1	D	199	THR
1	E	121	LYS
1	E	124	GLU
1	E	163	ASP
1	E	198	GLN
1	H	73	ASP
1	H	196	GLU
1	A	163	ASP
1	D	204	LYS
1	E	182	LYS
1	E	200	TRP
1	C	163	ASP
1	F	128	SER

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	170/189 (90%)	155 (91%)	15 (9%)	9	12
1	B	166/189 (88%)	153 (92%)	13 (8%)	11	16
1	C	165/189 (87%)	146 (88%)	19 (12%)	5	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	118/189 (62%)	107 (91%)	11 (9%)	8	11
1	E	141/189 (75%)	124 (88%)	17 (12%)	5	5
1	F	121/189 (64%)	108 (89%)	13 (11%)	6	8
1	G	128/189 (68%)	113 (88%)	15 (12%)	5	6
1	H	112/189 (59%)	98 (88%)	14 (12%)	4	5
All	All	1121/1512 (74%)	1004 (90%)	117 (10%)	7	8

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
1	A	7	THR
1	A	21	THR
1	A	22	VAL
1	A	50	VAL
1	A	87	LEU
1	A	105	THR
1	A	121	LYS
1	A	129	LEU
1	A	137	THR
1	A	143	THR
1	A	169	LYS
1	A	174	MET
1	A	191	LEU
1	A	196	GLU
1	B	5	ASP
1	B	20	ILE
1	B	21	THR
1	B	22	VAL
1	B	82	VAL
1	B	87	LEU
1	B	107	LEU
1	B	129	LEU
1	B	137	THR
1	B	162	THR
1	B	170	LEU
1	B	191	LEU
1	B	192	ASN
1	C	8	ARG
1	C	18	LEU

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Mol	Chain	Res	Type
1	C	21	THR
1	C	34	GLN
1	C	40	ILE
1	C	46	ARG
1	C	50	VAL
1	C	82	VAL
1	C	87	LEU
1	C	107	LEU
1	C	129	LEU
1	C	137	THR
1	C	162	THR
1	C	163	ASP
1	C	164	ASN
1	C	167	THR
1	C	169	LYS
1	C	170	LEU
1	C	184	ASN
1	D	5	ASP
1	D	8	ARG
1	D	15	GLU
1	D	18	LEU
1	D	22	VAL
1	D	50	VAL
1	D	82	VAL
1	D	87	LEU
1	D	193	ASP
1	D	197	LEU
1	D	201	THR
1	E	5	ASP
1	E	18	LEU
1	E	22	VAL
1	E	23	THR
1	E	42	GLU
1	E	75	LEU
1	E	82	VAL
1	E	87	LEU
1	E	105	THR
1	E	107	LEU
1	E	143	THR
1	E	162	THR
1	E	167	THR
1	E	179	VAL

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Mol	Chain	Res	Type
1	E	184	ASN
1	E	188	VAL
1	E	203	ASN
1	F	18	LEU
1	F	22	VAL
1	F	30	THR
1	F	41	VAL
1	F	50	VAL
1	F	82	VAL
1	F	87	LEU
1	F	124	GLU
1	F	128	SER
1	F	138	MET
1	F	170	LEU
1	F	171	LEU
1	F	192	ASN
1	G	6	GLN
1	G	18	LEU
1	G	22	VAL
1	G	40	ILE
1	G	82	VAL
1	G	87	LEU
1	G	117	LEU
1	G	137	THR
1	G	146	ILE
1	G	152	LEU
1	G	156	ASN
1	G	184	ASN
1	G	189	ASP
1	G	192	ASN
1	G	202	ILE
1	H	5	ASP
1	H	18	LEU
1	H	20	ILE
1	H	21	THR
1	H	22	VAL
1	H	25	ASN
1	H	69	ILE
1	H	82	VAL
1	H	87	LEU
1	H	105	THR
1	H	107	LEU

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Mol	Chain	Res	Type
1	H	127	ILE
1	H	142	THR
1	H	143	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	39	ASN
1	A	61	ASN
1	A	64	GLN
1	A	130	GLN
1	A	180	GLN
1	B	34	GLN
1	B	63	GLN
1	B	64	GLN
1	B	130	GLN
1	B	168	GLN
1	B	180	GLN
1	B	192	ASN
1	B	198	GLN
1	C	39	ASN
1	C	63	GLN
1	C	64	GLN
1	C	164	ASN
1	C	180	GLN
1	C	184	ASN
1	C	198	GLN
1	D	6	GLN
1	D	25	ASN
1	D	39	ASN
1	D	63	GLN
1	D	74	HIS
1	D	141	ASN
1	D	203	ASN
1	E	39	ASN
1	E	63	GLN
1	E	64	GLN
1	E	130	GLN
1	E	141	ASN
1	E	184	ASN
1	F	6	GLN

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Mol	Chain	Res	Type
1	F	64	GLN
1	F	130	GLN
1	F	141	ASN
1	F	192	ASN
1	F	203	ASN
1	G	6	GLN
1	G	34	GLN
1	G	39	ASN
1	G	63	GLN
1	G	64	GLN
1	G	130	GLN
1	G	156	ASN
1	G	180	GLN
1	G	184	ASN
1	G	192	ASN
1	G	198	GLN
1	G	203	ASN
1	H	25	ASN
1	H	61	ASN
1	H	64	GLN
1	H	74	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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MPD	A	225	-	7,7,7	0.34	0	9,10,10	0.35	0
3	PO4	A	226	-	4,4,4	0.89	0	6,6,6	0.44	0
2	MPD	C	225	-	7,7,7	0.30	0	9,10,10	0.57	0
2	MPD	G	225	-	7,7,7	0.33	0	9,10,10	0.23	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
2	MPD	A	225	-	-	3/5/5/5	-
2	MPD	C	225	-	1/1/2/2	1/5/5/5	-
2	MPD	G	225	-	1/1/2/2	0/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	225	MPD	C4
2	G	225	MPD	C4

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	225	MPD	C2-C3-C4-C5
2	A	225	MPD	C2-C3-C4-O4
2	A	225	MPD	C1-C2-C3-C4
2	A	225	MPD	CM-C2-C3-C4

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	225	MPD	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	225	MPD	3	0
2	G	225	MPD	3	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	206/224 (91%)	0.03	8 (3%) 43 45	27, 41, 66, 81	0
1	B	205/224 (91%)	0.25	6 (2%) 53 56	35, 51, 78, 95	0
1	C	206/224 (91%)	0.08	3 (1%) 72 73	29, 45, 67, 104	0
1	D	161/224 (71%)	0.90	30 (18%) 3 4	33, 55, 122, 150	0
1	E	194/224 (86%)	1.05	35 (18%) 3 4	39, 75, 127, 162	0
1	F	166/224 (74%)	1.44	42 (25%) 1 2	20, 74, 122, 146	0
1	G	193/224 (86%)	1.78	70 (36%) 1 1	68, 93, 121, 140	0
1	H	153/224 (68%)	1.24	34 (22%) 2 2	46, 71, 117, 139	0
All	All	1484/1792 (82%)	0.81	228 (15%) 5 6	20, 61, 117, 162	0

All (228) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	125	GLU	8.3
1	E	161	ALA	7.6
1	F	179	VAL	7.2
1	F	126	GLY	7.1
1	G	165	GLY	7.1
1	D	169	LYS	6.8
1	G	74	HIS	6.7
1	G	160	ILE	6.6
1	D	191	LEU	6.6
1	F	127	ILE	6.4
1	F	131	SER	6.3
1	G	119	GLY	5.9
1	F	202	ILE	5.8
1	H	127	ILE	5.8
1	F	200	TRP	5.5
1	E	151	SER	5.4

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Mol	Chain	Res	Type	RSRZ
1	G	178	GLU	5.3
1	D	201	THR	5.3
1	F	128	SER	5.2
1	H	195	GLY	5.2
1	H	168	GLN	5.0
1	H	140	VAL	5.0
1	D	200	TRP	5.0
1	H	123	ALA	4.8
1	D	178	GLU	4.8
1	F	142	THR	4.7
1	H	192	ASN	4.7
1	D	170	LEU	4.7
1	G	45	THR	4.7
1	D	199	THR	4.7
1	F	170	LEU	4.7
1	F	148	ALA	4.7
1	H	148	ALA	4.6
1	G	124	GLU	4.6
1	F	123	ALA	4.5
1	D	194	TYR	4.5
1	H	125	GLU	4.5
1	E	197	LEU	4.5
1	E	195	GLY	4.4
1	G	181	VAL	4.4
1	E	122	GLY	4.3
1	G	122	GLY	4.3
1	G	187	LYS	4.3
1	F	144	PRO	4.3
1	H	198	GLN	4.3
1	G	190	SER	4.3
1	H	190	SER	4.3
1	G	46	ARG	4.2
1	D	127	ILE	4.2
1	D	148	ALA	4.1
1	G	139	LEU	4.1
1	F	140	VAL	4.0
1	G	179	VAL	3.9
1	D	192	ASN	3.9
1	C	206	LYS	3.9
1	G	159	LYS	3.8
1	D	140	VAL	3.8
1	F	172	MET	3.8

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Mol	Chain	Res	Type	RSRZ
1	F	171	LEU	3.8
1	D	171	LEU	3.7
1	G	137	THR	3.7
1	E	120	ARG	3.7
1	D	73	ASP	3.6
1	B	205	LYS	3.6
1	G	185	VAL	3.6
1	F	190	SER	3.5
1	G	78	ASP	3.5
1	G	129	LEU	3.5
1	F	169	LYS	3.5
1	G	169	LYS	3.5
1	F	73	ASP	3.5
1	H	126	GLY	3.4
1	G	127	ILE	3.4
1	E	194	TYR	3.4
1	F	197	LEU	3.4
1	G	49	PHE	3.4
1	E	199	THR	3.4
1	D	121	LYS	3.4
1	D	126	GLY	3.4
1	B	5	ASP	3.4
1	H	94	LEU	3.3
1	D	172	MET	3.3
1	G	168	GLN	3.3
1	G	166	THR	3.3
1	H	122	GLY	3.3
1	H	124	GLU	3.2
1	G	75	LEU	3.2
1	E	201	THR	3.2
1	E	192	ASN	3.2
1	F	42	GLU	3.2
1	F	178	GLU	3.2
1	A	73	ASP	3.2
1	C	134	ASP	3.2
1	F	191	LEU	3.1
1	G	50	VAL	3.1
1	A	206	LYS	3.1
1	F	77	LYS	3.1
1	E	186	VAL	3.1
1	G	170	LEU	3.1
1	C	162	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	138	MET	3.0
1	G	151	SER	3.0
1	H	169	LYS	3.0
1	G	125	GLU	3.0
1	G	53	PRO	3.0
1	G	55	PHE	2.9
1	H	197	LEU	2.9
1	F	139	LEU	2.9
1	G	94	LEU	2.9
1	E	128	SER	2.9
1	G	131	SER	2.9
1	B	121	LYS	2.9
1	G	191	LEU	2.9
1	H	191	LEU	2.9
1	F	124	GLU	2.9
1	G	167	THR	2.9
1	H	73	ASP	2.9
1	G	188	VAL	2.9
1	F	122	GLY	2.8
1	E	129	LEU	2.8
1	G	69	ILE	2.8
1	G	177	ASP	2.8
1	D	193	ASP	2.8
1	G	95	GLU	2.8
1	F	20	ILE	2.8
1	G	16	ASP	2.7
1	D	15	GLU	2.7
1	H	196	GLU	2.7
1	D	197	LEU	2.7
1	G	171	LEU	2.7
1	A	163	ASP	2.7
1	F	118	GLU	2.7
1	F	194	TYR	2.7
1	E	126	GLY	2.7
1	E	182	LYS	2.7
1	E	187	LYS	2.7
1	G	41	VAL	2.7
1	G	82	VAL	2.7
1	G	40	ILE	2.7
1	F	129	LEU	2.7
1	H	31	PHE	2.6
1	G	202	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	152	LEU	2.6
1	H	170	LEU	2.6
1	E	134	ASP	2.6
1	D	205	LYS	2.6
1	G	201	THR	2.6
1	H	74	HIS	2.6
1	H	23	THR	2.5
1	G	158	LYS	2.5
1	H	72	SER	2.5
1	G	118	GLU	2.5
1	H	105	THR	2.5
1	E	82	VAL	2.5
1	E	73	ASP	2.5
1	E	173	PHE	2.4
1	F	43	LYS	2.4
1	A	74	HIS	2.4
1	E	124	GLU	2.4
1	F	196	GLU	2.4
1	G	42	GLU	2.4
1	G	155	GLY	2.4
1	G	70	MET	2.4
1	A	25	ASN	2.4
1	F	203	ASN	2.4
1	G	134	ASP	2.4
1	E	41	VAL	2.4
1	A	156	ASN	2.3
1	G	203	ASN	2.3
1	D	74	HIS	2.3
1	G	189	ASP	2.3
1	G	48	THR	2.3
1	H	95	GLU	2.3
1	B	158	LYS	2.3
1	E	121	LYS	2.3
1	E	193	ASP	2.3
1	G	204	LYS	2.3
1	G	197	LEU	2.3
1	H	27	LYS	2.3
1	B	184	ASN	2.3
1	E	162	THR	2.3
1	D	202	ILE	2.3
1	E	188	VAL	2.3
1	E	191	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	148	ALA	2.2
1	D	198	GLN	2.2
1	G	52	THR	2.2
1	A	187	LYS	2.2
1	G	173	PHE	2.2
1	H	173	PHE	2.2
1	E	119	GLY	2.2
1	D	196	GLU	2.2
1	E	178	GLU	2.2
1	G	97	SER	2.2
1	G	147	PHE	2.2
1	E	198	GLN	2.2
1	G	43	LYS	2.2
1	F	21	THR	2.2
1	H	171	LEU	2.2
1	B	179	VAL	2.2
1	E	180	GLN	2.2
1	F	30	THR	2.1
1	E	145	TYR	2.1
1	H	99	ILE	2.1
1	D	5	ASP	2.1
1	F	5	ASP	2.1
1	H	101	VAL	2.1
1	E	136	ARG	2.1
1	F	1	SER	2.1
1	H	1	SER	2.1
1	H	30	THR	2.1
1	H	115	ALA	2.1
1	A	99	ILE	2.1
1	G	61	ASN	2.1
1	E	200	TRP	2.1
1	F	121	LYS	2.1
1	G	100	ALA	2.1
1	F	69	ILE	2.1
1	G	149	ILE	2.1
1	D	195	GLY	2.1
1	G	114	LYS	2.0
1	G	105	THR	2.0
1	D	6	GLN	2.0
1	D	41	VAL	2.0
1	F	55	PHE	2.0
1	D	14	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	117	LEU	2.0
1	F	146	ILE	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
3	PO4	A	226	5/5	0.81	0.17	135,136,137,138	0
2	MPD	A	225	8/8	0.82	0.22	72,86,90,94	0
2	MPD	G	225	8/8	0.89	0.23	78,86,90,98	0
2	MPD	C	225	8/8	0.91	0.21	42,59,78,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.