



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:00 AM UTC

PDB ID : 1RF0 / pdb_00001rf0
Title : Crystal Structure of Fragment D of gammaE132A Fibrinogen
Authors : Kostelansky, M.S.; Gorkun, O.V.; Lord, S.T.
Deposited on : 2003-11-07
Resolution : 2.81 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

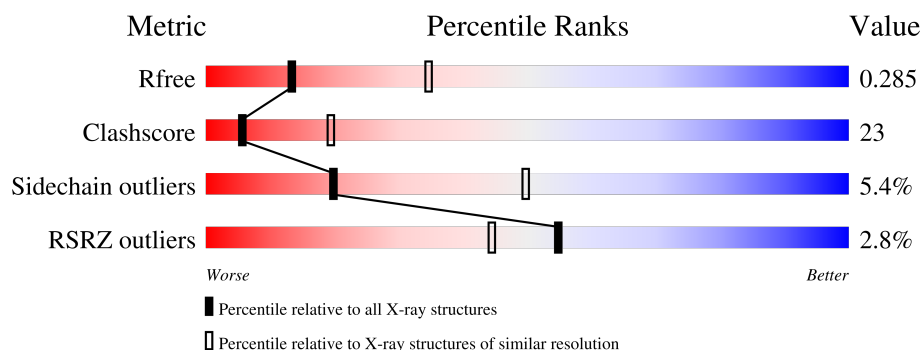
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	66	6% 59% 32% 6% .
1	D	66	6% 44% 36% 5% 15%
2	B	313	2% 55% 39% . .
2	E	313	2% 61% 30% 5% .
3	C	311	2% 57% 35% . .
3	F	311	4% 62% 31% . .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10772 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 Fibrinogen alpha/alpha-E chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	64	Total	C	N	O	S	0	0	0
			523	322	99	99	3			
1	D	56	Total	C	N	O	S	0	0	0
			458	280	87	88	3			

- Molecule 2 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	306	Total	C	N	O	S	0	0	0
			2452	1528	432	470	22			
2	E	300	Total	C	N	O	S	0	0	0
			2407	1503	425	457	22			

- Molecule 3 is a protein called Fibrinogen gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	298	Total	C	N	O	S	0	0	0
			2387	1515	402	459	11			
3	F	299	Total	C	N	O	S	0	0	0
			2395	1521	403	460	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	132	ALA	GLU	engineered mutation	UNP P02679
F	132	ALA	GLU	engineered mutation	UNP P02679

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Ca	0	0
			2	2		
5	C	1	Total	Ca	0	0
			1	1		
5	E	2	Total	Ca	0	0
			2	2		
5	F	1	Total	Ca	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	O	0	0
			2	2		
6	B	26	Total	O	0	0
			26	26		
6	C	15	Total	O	0	0
			15	15		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	3	Total 3	O 3	0	0
6	E	50	Total 50	O 50	0	0
6	F	20	Total 20	O 20	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.

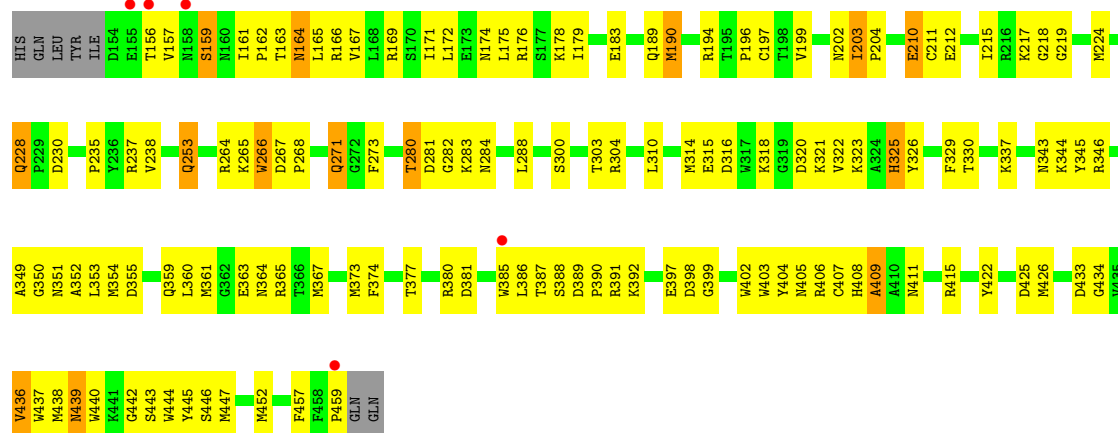
- Molecule 1: Fibrinogen alpha/alpha-E chain



- Molecule 1: Fibrinogen alpha/alpha-E chain

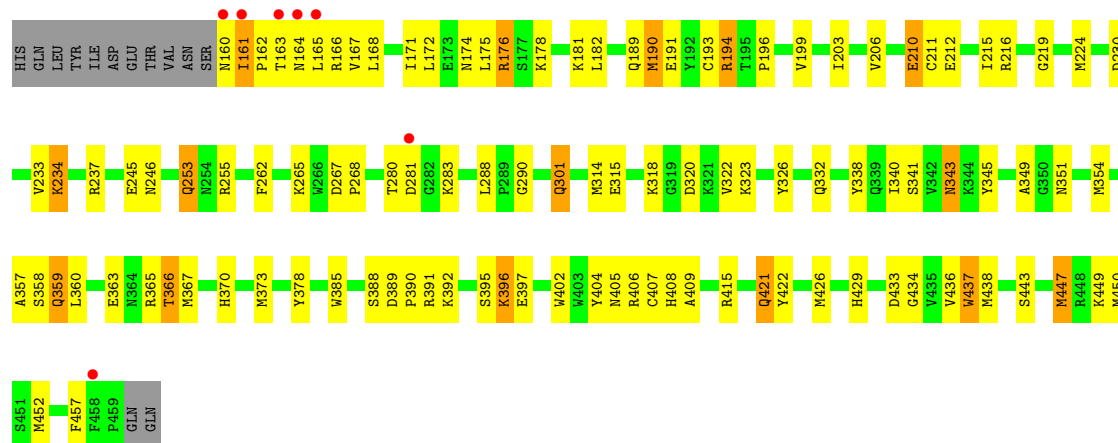


- Molecule 2: Fibrinogen beta chain

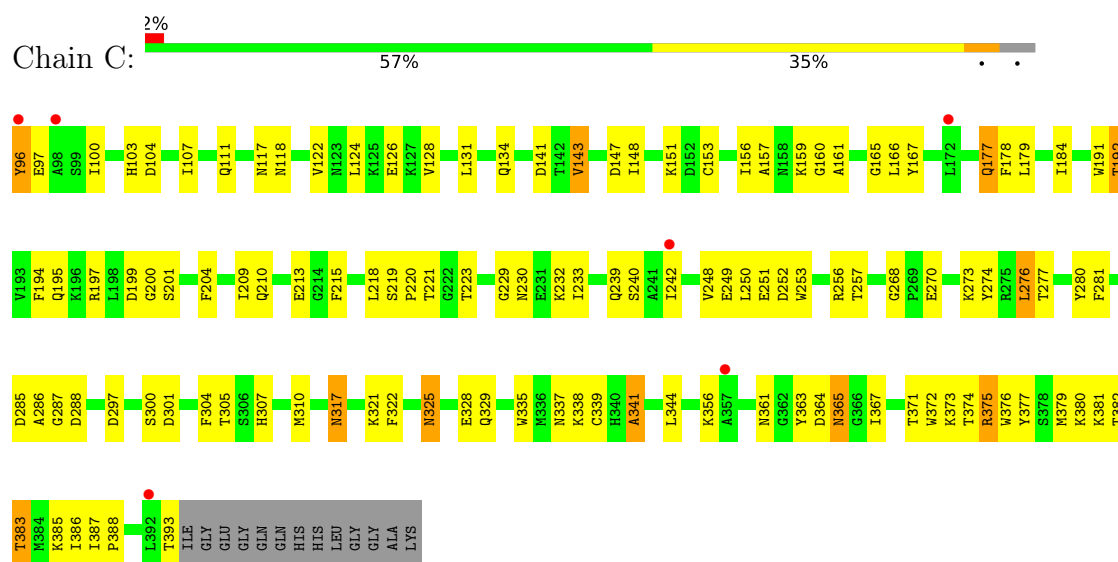


- Molecule 2: Fibrinogen beta chain

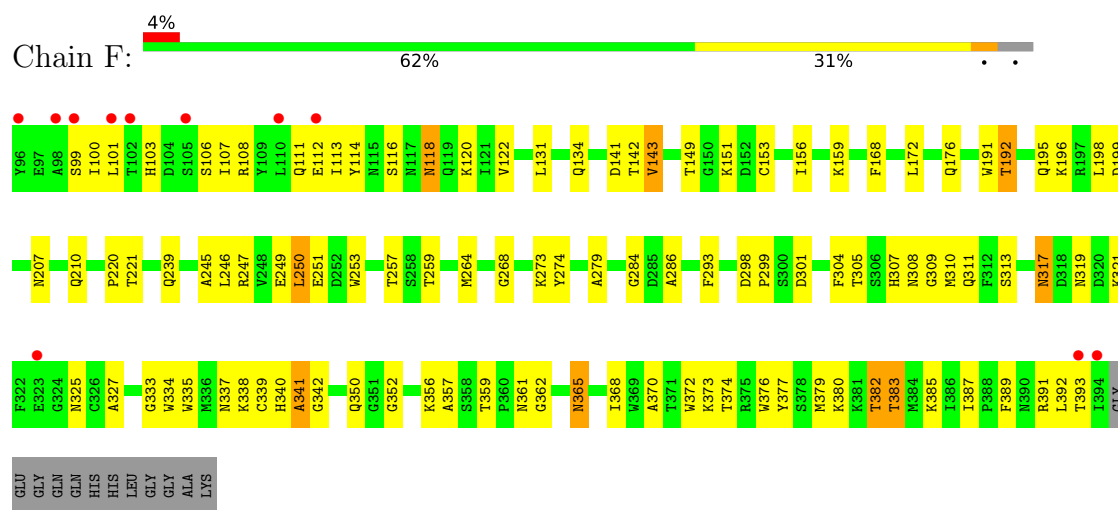




• Molecule 3: Fibrinogen gamma chain



• Molecule 3: Fibrinogen gamma chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.41Å 94.95Å 227.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.97 – 2.81 17.97 – 2.82	Depositor EDS
% Data completeness (in resolution range)	98.8 (17.97-2.81) 98.4 (17.97-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.86 (at 2.84Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.233 , 0.286 0.233 , 0.285	Depositor DCC
R_{free} test set	2345 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10772	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 19.17% 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: NAG, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.39	0/524	0.91	2/699 (0.3%)
1	D	0.43	0/458	0.88	0/610
2	B	0.44	0/2514	0.97	13/3397 (0.4%)
2	E	0.50	1/2469 (0.0%)	0.98	12/3335 (0.4%)
3	C	0.41	0/2453	0.88	2/3319 (0.1%)
3	F	0.44	0/2461	0.90	3/3330 (0.1%)
All	All	0.44	1/10879 (0.0%)	0.93	32/14690 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	161	ILE	CA-CB	5.52	1.56	1.54

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	203	ILE	N-CA-C	9.91	117.15	108.63
2	B	409	ALA	N-CA-C	-9.54	102.20	114.04
2	E	203	ILE	N-CA-C	8.79	116.19	108.63
2	E	409	ALA	N-CA-C	-8.21	103.86	114.04
2	B	159	SER	N-CA-C	-6.79	105.62	114.04
3	F	340	HIS	N-CA-C	6.37	118.99	108.99
2	E	408	HIS	N-CA-C	6.27	118.38	108.79
1	A	128	GLU	N-CA-C	-6.10	107.67	114.62
1	A	129	LYS	N-CA-C	-5.99	105.23	112.54
2	B	197	CYS	N-CA-C	-5.89	102.60	110.55
2	B	211	CYS	N-CA-C	5.83	119.21	111.75
3	F	368	ILE	N-CA-C	5.72	117.66	108.85
3	C	341	ALA	N-CA-C	-5.66	106.04	114.64
2	E	211	CYS	N-CA-C	5.63	118.96	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	436	VAL	N-CA-C	5.61	117.42	108.89
3	F	341	ALA	N-CA-C	-5.61	106.98	113.88
2	E	318	LYS	N-CA-C	-5.49	106.94	113.97
2	E	234	LYS	CA-C-N	5.48	125.75	119.83
2	E	234	LYS	C-N-CA	5.48	125.75	119.83
2	E	426	MET	N-CA-C	-5.47	107.26	114.04
2	B	194	ARG	N-CA-C	-5.37	106.56	113.01
3	C	280	TYR	N-CA-C	5.37	116.68	108.52
2	B	426	MET	N-CA-C	-5.36	106.80	113.55
2	E	194	ARG	N-CA-C	-5.28	106.79	113.18
2	E	437	TRP	N-CA-C	-5.25	99.61	110.80
2	B	411	ASN	CA-C-N	5.24	124.90	119.56
2	B	411	ASN	C-N-CA	5.24	124.90	119.56
2	B	228	GLN	CA-C-N	5.19	124.99	119.28
2	B	228	GLN	C-N-CA	5.19	124.99	119.28
2	B	266	TRP	N-CA-C	5.14	117.28	111.11
2	E	290	GLY	N-CA-C	-5.11	105.76	112.81
2	E	457	PHE	N-CA-C	5.11	117.48	108.24

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	523	0	547	33	0
1	D	458	0	477	40	0
2	B	2452	0	2312	133	0
2	E	2407	0	2275	114	0
3	C	2387	0	2234	110	0
3	F	2395	0	2245	105	0
4	B	14	0	13	2	0
4	E	14	0	13	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	E	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	1	0	0	0	0
6	A	2	0	0	0	0
6	B	26	0	0	1	0
6	C	15	0	0	3	0
6	D	3	0	0	0	0
6	E	50	0	0	2	0
6	F	20	0	0	0	0
All	All	10772	0	10116	485	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 23.

All (485) 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:A:168:ALA:HA	2:B:189:GLN:HE22	1.25	0.98
1:A:150:LEU:HD21	3:C:124:LEU:HD23	1.53	0.89
3:F:307:HIS:CE1	3:F:341:ALA:H	1.90	0.89
3:F:251:GLU:HG3	3:F:257:THR:HG22	1.55	0.89
2:B:165:LEU:HD21	3:C:107:ILE:HD13	1.54	0.89
3:F:307:HIS:HE1	3:F:341:ALA:H	1.16	0.88
2:E:161:ILE:HB	2:E:162:PRO:HD3	1.55	0.88
2:E:388:SER:O	2:E:390:PRO:HD3	1.73	0.88
1:A:140:VAL:HG23	1:A:185:LEU:HD11	1.56	0.85
2:B:183:GLU:HG2	3:C:124:LEU:HD13	1.57	0.85
2:B:439:ASN:H	2:B:439:ASN:HD22	1.23	0.84
2:B:351:ASN:OD1	2:B:354:MET:HE3	1.79	0.83
3:C:325:ASN:ND2	3:C:328:GLU:H	1.78	0.81
2:B:388:SER:O	2:B:390:PRO:HD3	1.81	0.79
1:A:127:ILE:HG23	1:A:128:GLU:H	1.45	0.79
1:D:158:ILE:HG23	2:E:189:GLN:HE21	1.47	0.77
2:E:357:ALA:HB3	2:E:360:LEU:HD12	1.66	0.76
2:B:361:MET:HB2	4:B:500:NAG:H81	1.68	0.76
2:E:359:GLN:NE2	2:E:359:GLN:H	1.84	0.75
1:A:133:ILE:O	1:A:137:GLN:HG3	1.86	0.74
3:C:249:GLU:HB3	3:C:383:THR:HG23	1.67	0.74
2:B:326:TYR:CE2	2:B:353:LEU:HD12	2.22	0.74
3:F:310:MET:HA	3:F:310:MET:HE2	1.69	0.74
3:F:153:CYS:SG	3:F:192:THR:HB	2.27	0.74
3:C:338:LYS:N	3:C:339:CYS:HA	2.02	0.74
2:E:345:TYR:HB2	2:E:354:MET:CE	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:343:ASN:C	2:E:343:ASN:HD22	1.96	0.73
2:E:397:GLU:HB3	2:E:429:HIS:NE2	2.03	0.73
2:B:367:MET:HB2	2:B:406:ARG:HB2	1.72	0.72
3:F:387:ILE:HD11	3:F:391:ARG:HG2	1.71	0.72
2:B:363:GLU:HG2	2:B:367:MET:HE3	1.72	0.71
2:E:176:ARG:HB3	2:E:176:ARG:NH1	2.05	0.71
1:D:139:ASN:HB3	3:F:114:TYR:CZ	2.26	0.71
2:B:385:TRP:HE3	2:B:406:ARG:HG2	1.55	0.71
3:C:321:LYS:HB2	3:C:337:ASN:HD22	1.55	0.70
2:B:164:ASN:N	2:B:164:ASN:HD22	1.87	0.70
3:F:100:ILE:HG13	3:F:101:LEU:N	2.05	0.70
3:F:317:ASN:C	3:F:317:ASN:HD22	1.98	0.70
1:D:178:TYR:O	1:D:182:GLN:HG3	1.92	0.70
3:C:344:LEU:HB3	3:C:382:THR:HG21	1.74	0.70
3:F:321:LYS:O	3:F:338:LYS:HD3	1.93	0.69
3:F:249:GLU:HB3	3:F:383:THR:HG23	1.75	0.69
3:C:344:LEU:HD13	3:C:382:THR:HG23	1.74	0.69
2:E:326:TYR:CE1	2:E:354:MET:HE2	2.28	0.68
2:E:406:ARG:HD3	6:E:92:HOH:O	1.93	0.68
3:F:338:LYS:N	3:F:339:CYS:HA	2.08	0.68
3:C:148:ILE:H	3:C:148:ILE:HD12	1.59	0.68
3:C:307:HIS:HE1	3:C:341:ALA:H	1.41	0.68
2:E:191:GLU:HG2	2:E:194:ARG:HH11	1.58	0.68
3:C:191:TRP:CE3	3:C:385:LYS:HG3	2.28	0.68
2:E:359:GLN:HE21	2:E:359:GLN:N	1.92	0.67
3:C:305:THR:HB	3:C:341:ALA:HB2	1.77	0.67
2:B:443:SER:HG	2:B:444:TRP:CD1	2.12	0.67
2:B:439:ASN:HD22	2:B:439:ASN:N	1.93	0.67
1:D:173:VAL:HG12	1:D:175:LEU:HD22	1.76	0.66
1:D:143:GLN:HE21	3:F:118:ASN:HD22	1.43	0.66
3:F:151:LYS:HB3	3:F:239:GLN:HE22	1.61	0.65
2:E:171:ILE:HD12	2:E:172:LEU:N	2.12	0.65
2:E:165:LEU:HD21	3:F:106:SER:HB2	1.78	0.65
2:B:163:THR:HA	2:B:166:ARG:HE	1.60	0.65
3:F:99:SER:O	3:F:101:LEU:N	2.30	0.65
3:F:307:HIS:CE1	3:F:342:GLY:H	2.13	0.65
3:C:200:GLY:HA2	6:C:421:HOH:O	1.96	0.64
2:B:210:GLU:OE1	2:B:212:GLU:HB3	1.98	0.64
2:E:343:ASN:C	2:E:343:ASN:ND2	2.55	0.64
1:A:127:ILE:HG12	1:A:128:GLU:N	2.11	0.64
2:B:161:ILE:HB	2:B:162:PRO:HD3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:ASN:HD22	2:B:284:ASN:HB2	1.62	0.64
2:B:351:ASN:HD22	2:B:351:ASN:C	2.03	0.64
3:F:103:HIS:O	3:F:107:ILE:HG12	1.97	0.64
2:B:159:SER:C	2:B:162:PRO:HD2	2.22	0.64
2:B:440:TRP:HE3	2:B:447:MET:HE1	1.62	0.64
3:C:322:PHE:HE2	3:C:329:GLN:HE22	1.46	0.64
1:D:176:LYS:HB2	1:D:176:LYS:HZ3	1.62	0.63
2:E:190:MET:HE3	3:F:131:LEU:HA	1.78	0.63
2:E:176:ARG:HB3	2:E:176:ARG:HH11	1.63	0.63
1:A:140:VAL:HG12	2:B:172:LEU:HD21	1.80	0.63
3:C:192:THR:HG23	3:C:386:ILE:HG13	1.81	0.63
1:A:127:ILE:HG23	1:A:128:GLU:N	2.13	0.63
2:B:389:ASP:OD1	2:B:391:ARG:HB3	1.99	0.62
3:C:103:HIS:O	3:C:107:ILE:HG12	1.99	0.62
1:D:168:ALA:HA	2:E:189:GLN:HE22	1.64	0.62
3:C:151:LYS:HB3	3:C:239:GLN:HE22	1.64	0.62
2:E:351:ASN:OD1	2:E:354:MET:HE3	1.99	0.62
3:F:149:THR:HG22	3:F:168:PHE:O	2.00	0.62
2:E:172:LEU:HD22	3:F:113:ILE:HG13	1.82	0.61
3:F:356:LYS:O	3:F:362:GLY:HA2	1.99	0.61
2:B:169:ARG:HG2	2:B:169:ARG:HH11	1.66	0.61
2:B:176:ARG:HB2	3:C:117:ASN:HD21	1.66	0.61
1:D:134:GLN:O	1:D:138:LYS:HG3	1.99	0.61
2:B:351:ASN:ND2	2:B:354:MET:H	1.98	0.61
2:B:337:LYS:HE2	2:B:374:PHE:CG	2.35	0.61
3:C:160:GLY:O	3:C:161:ALA:C	2.42	0.61
3:C:248:VAL:HG13	3:C:344:LEU:HD11	1.82	0.61
3:C:281:PHE:HB2	3:C:288:ASP:OD2	2.00	0.61
2:B:405:ASN:C	2:B:406:ARG:HG3	2.26	0.61
3:C:321:LYS:HB2	3:C:337:ASN:ND2	2.15	0.61
2:B:326:TYR:HE1	2:B:354:MET:HE2	1.66	0.60
2:B:165:LEU:HD21	3:C:107:ILE:CD1	2.31	0.60
2:B:280:THR:CG2	2:B:288:LEU:HG	2.32	0.60
3:C:151:LYS:HB3	3:C:239:GLN:NE2	2.16	0.60
3:C:252:ASP:OD2	3:C:256:ARG:HB2	2.01	0.60
1:D:169:LEU:H	2:E:189:GLN:HE22	1.50	0.60
2:E:391:ARG:O	2:E:391:ARG:HD3	2.00	0.60
2:B:389:ASP:OD1	2:B:392:LYS:HG3	2.01	0.60
2:E:164:ASN:C	2:E:166:ARG:H	2.09	0.60
1:A:178:TYR:CZ	2:B:178:LYS:HD3	2.37	0.60
1:D:171:ARG:HG3	1:D:171:ARG:HH11	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:251:GLU:HB2	3:C:257:THR:HG22	1.85	0.59
2:B:156:THR:O	2:B:159:SER:HB3	2.01	0.59
2:B:326:TYR:CE1	2:B:354:MET:HE2	2.37	0.59
2:B:389:ASP:CG	2:B:392:LYS:HG3	2.26	0.59
2:B:343:ASN:OD1	2:B:344:LYS:HG3	2.03	0.59
2:E:199:VAL:O	3:F:142:THR:HG23	2.01	0.59
3:F:307:HIS:HE1	3:F:342:GLY:H	1.49	0.59
2:E:168:LEU:O	2:E:172:LEU:HB2	2.02	0.59
3:C:252:ASP:HB2	3:C:377:TYR:OH	2.02	0.59
3:C:325:ASN:C	3:C:325:ASN:HD22	2.10	0.59
3:C:118:ASN:O	3:C:122:VAL:HG23	2.03	0.59
3:C:307:HIS:HD2	3:C:335:TRP:O	1.86	0.59
2:B:323:LYS:NZ	2:B:325:HIS:HD2	2.00	0.58
3:F:251:GLU:CG	3:F:257:THR:HG22	2.31	0.58
2:B:217:LYS:HB3	3:C:213:GLU:HG3	1.85	0.58
3:F:250:LEU:HD12	3:F:379:MET:HG3	1.84	0.58
2:B:337:LYS:HE2	2:B:374:PHE:CD1	2.38	0.58
3:C:387:ILE:HG13	3:C:388:PRO:HD2	1.84	0.58
1:A:168:ALA:HA	2:B:189:GLN:NE2	2.08	0.58
1:D:140:VAL:HG23	1:D:141:ARG:N	2.19	0.58
2:E:165:LEU:HD21	3:F:106:SER:CB	2.33	0.58
2:B:314:MET:HE1	2:B:437:TRP:CD2	2.39	0.58
3:C:310:MET:HA	3:C:310:MET:HE2	1.85	0.58
1:A:185:LEU:O	1:A:189:ILE:HG13	2.04	0.57
1:D:169:LEU:H	2:E:189:GLN:NE2	2.01	0.57
2:B:224:MET:CE	2:B:237:ARG:HD3	2.35	0.57
2:B:385:TRP:NE1	2:B:392:LYS:HB3	2.20	0.57
3:C:195:GLN:OE1	3:C:382:THR:HG22	2.05	0.57
3:F:357:ALA:C	3:F:359:THR:H	2.12	0.57
2:E:233:VAL:HG22	2:E:234:LYS:H	1.70	0.57
2:B:408:HIS:O	2:B:438:MET:HE1	2.05	0.57
2:E:315:GLU:HB3	2:E:449:LYS:HB2	1.85	0.57
3:F:359:THR:HG22	3:F:361:ASN:H	1.69	0.56
2:B:267:ASP:O	2:B:271:GLN:HG2	2.04	0.56
2:E:340:ILE:HG12	2:E:341:SER:N	2.19	0.56
3:F:107:ILE:O	3:F:111:GLN:HG2	2.05	0.56
2:B:385:TRP:HE1	2:B:392:LYS:HB3	1.70	0.56
3:C:276:LEU:HD12	3:C:277:THR:N	2.20	0.56
2:E:363:GLU:HA	2:E:366:THR:HG23	1.87	0.56
3:F:307:HIS:HE1	3:F:341:ALA:N	1.94	0.56
3:C:156:ILE:HG22	3:C:161:ALA:CB	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:270:GLU:HG3	3:C:274:TYR:CZ	2.40	0.56
3:F:357:ALA:O	3:F:359:THR:N	2.39	0.56
3:C:338:LYS:O	3:C:338:LYS:HG2	2.04	0.56
3:C:122:VAL:O	3:C:126:GLU:HG3	2.05	0.56
3:C:248:VAL:CG1	3:C:344:LEU:HD11	2.36	0.56
2:E:210:GLU:OE1	2:E:212:GLU:HB3	2.04	0.56
3:F:365:ASN:H	3:F:365:ASN:ND2	2.04	0.56
2:B:266:TRP:HA	2:B:377:THR:HG21	1.88	0.55
2:E:215:ILE:HA	2:E:219:GLY:O	2.06	0.55
2:B:163:THR:HA	2:B:166:ARG:NE	2.20	0.55
2:E:358:SER:HA	2:E:365:ARG:HH22	1.70	0.55
1:A:130:VAL:O	1:A:134:GLN:HG3	2.06	0.55
2:B:406:ARG:N	2:B:407:CYS:HA	2.20	0.55
2:B:439:ASN:N	2:B:439:ASN:ND2	2.53	0.55
2:E:358:SER:HA	2:E:365:ARG:NH2	2.22	0.55
3:F:264:MET:HB2	3:F:279:ALA:H	1.71	0.55
3:F:374:THR:C	3:F:376:TRP:H	2.15	0.55
3:C:96:TYR:O	3:C:97:GLU:HB2	2.07	0.55
2:B:265:LYS:O	2:B:268:PRO:HD2	2.06	0.55
2:B:351:ASN:HD21	2:B:354:MET:H	1.55	0.55
3:C:141:ASP:OD1	3:C:143:VAL:HG13	2.07	0.55
2:B:318:LYS:HD2	2:B:318:LYS:N	2.21	0.55
2:E:345:TYR:HB2	2:E:354:MET:HE3	1.89	0.55
2:B:314:MET:SD	2:B:447:MET:HE3	2.47	0.54
2:B:361:MET:HB2	4:B:500:NAG:C8	2.35	0.54
3:C:221:THR:O	3:C:223:THR:HG23	2.07	0.54
1:D:143:GLN:HE21	3:F:118:ASN:ND2	2.05	0.54
3:C:374:THR:C	3:C:376:TRP:H	2.14	0.54
2:E:332:GLN:O	2:E:338:TYR:HA	2.08	0.54
2:E:265:LYS:O	2:E:268:PRO:HD2	2.08	0.54
2:E:438:MET:HE3	2:E:443:SER:HB3	1.89	0.54
3:F:304:PHE:C	3:F:337:ASN:ND2	2.65	0.54
2:B:409:ALA:HA	2:B:438:MET:HE3	1.89	0.54
3:C:197:ARG:HB2	3:C:382:THR:HB	1.90	0.54
3:C:251:GLU:HB3	3:C:381:LYS:HB2	1.89	0.54
1:D:140:VAL:HG23	1:D:141:ARG:H	1.73	0.54
1:D:188:VAL:HB	2:E:164:ASN:OD1	2.08	0.54
2:E:233:VAL:HG22	2:E:234:LYS:N	2.22	0.54
2:B:367:MET:HE2	2:B:406:ARG:NH2	2.23	0.54
3:C:248:VAL:HG12	3:C:250:LEU:CD1	2.38	0.54
2:E:397:GLU:HB3	2:E:429:HIS:CE1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:344:LEU:HA	3:C:367:ILE:HG23	1.89	0.54
2:E:359:GLN:H	2:E:359:GLN:HE21	1.48	0.54
2:E:199:VAL:HG23	3:F:141:ASP:HA	1.89	0.53
3:F:374:THR:O	3:F:376:TRP:N	2.40	0.53
1:A:136:LEU:O	1:A:140:VAL:HG13	2.08	0.53
2:B:457:PHE:O	2:B:459:PRO:HD3	2.09	0.53
3:C:167:TYR:O	3:C:179:LEU:HD12	2.09	0.53
3:C:307:HIS:CE1	3:C:341:ALA:H	2.26	0.53
1:D:139:ASN:HB3	3:F:114:TYR:CE1	2.44	0.53
2:E:245:GLU:O	2:E:246:ASN:HB2	2.08	0.53
2:B:179:ILE:O	2:B:183:GLU:HG3	2.08	0.53
2:E:164:ASN:C	2:E:166:ARG:N	2.67	0.53
3:F:250:LEU:N	3:F:250:LEU:HD22	2.24	0.53
2:B:202:ASN:ND2	2:B:284:ASN:HB2	2.23	0.52
1:D:136:LEU:O	1:D:140:VAL:HG22	2.08	0.52
2:E:326:TYR:CD1	2:E:354:MET:HE2	2.45	0.52
2:E:326:TYR:HE1	2:E:354:MET:HE2	1.73	0.52
1:A:177:ASP:O	1:A:181:GLN:HG3	2.10	0.52
1:D:175:LEU:HD22	1:D:175:LEU:H	1.75	0.52
1:A:185:LEU:HD22	1:A:189:ILE:HD11	1.92	0.52
2:B:434:GLY:O	2:B:436:VAL:N	2.43	0.52
2:B:190:MET:HE3	3:C:131:LEU:HA	1.92	0.52
2:B:253:GLN:HB3	2:B:452:MET:HB2	1.91	0.52
3:C:156:ILE:O	3:C:159:LYS:HB2	2.10	0.52
2:E:191:GLU:HA	2:E:194:ARG:HD2	1.91	0.52
1:A:178:TYR:OH	2:B:178:LYS:HD3	2.10	0.51
2:B:360:LEU:HD13	2:B:364:ASN:O	2.10	0.51
2:E:385:TRP:CE2	2:E:392:LYS:HD2	2.44	0.51
2:E:389:ASP:C	2:E:391:ARG:H	2.18	0.51
2:B:363:GLU:HG2	2:B:367:MET:CE	2.40	0.51
3:F:207:ASN:OD1	3:F:210:GLN:HG3	2.11	0.51
1:D:176:LYS:HB2	1:D:176:LYS:NZ	2.25	0.51
3:F:246:LEU:HD12	3:F:247:ARG:N	2.25	0.51
3:C:287:GLY:HA3	3:C:371:THR:OG1	2.11	0.51
3:F:196:LYS:HD2	3:F:383:THR:HB	1.92	0.51
1:D:133:ILE:HG12	3:F:107:ILE:HD12	1.93	0.51
2:E:160:ASN:HD22	2:E:163:THR:HB	1.76	0.51
2:E:172:LEU:HD22	3:F:113:ILE:CD1	2.40	0.51
2:B:373:MET:HE2	2:B:405:ASN:HA	1.93	0.51
2:E:359:GLN:NE2	2:E:359:GLN:N	2.52	0.51
2:E:392:LYS:O	2:E:392:LYS:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:ASN:N	2:B:164:ASN:ND2	2.57	0.50
2:B:434:GLY:O	2:B:436:VAL:HG23	2.11	0.50
2:E:171:ILE:HD12	2:E:171:ILE:C	2.36	0.50
2:B:389:ASP:C	2:B:391:ARG:H	2.18	0.50
2:B:363:GLU:O	2:B:367:MET:HG2	2.11	0.50
3:F:325:ASN:HD22	3:F:325:ASN:C	2.18	0.50
2:B:351:ASN:C	2:B:351:ASN:ND2	2.67	0.50
2:E:406:ARG:N	2:E:407:CYS:HA	2.26	0.50
3:F:100:ILE:HG13	3:F:101:LEU:H	1.77	0.50
2:B:350:GLY:O	2:B:352:ALA:N	2.40	0.50
2:E:281:ASP:C	2:E:283:LYS:H	2.20	0.50
3:F:308:ASN:HD22	3:F:309:GLY:N	2.09	0.50
3:F:365:ASN:N	3:F:365:ASN:HD22	2.09	0.50
3:F:273:LYS:HD2	3:F:319:ASN:OD1	2.12	0.50
2:E:391:ARG:HD3	2:E:396:LYS:NZ	2.27	0.50
3:F:374:THR:C	3:F:376:TRP:N	2.70	0.50
2:B:199:VAL:HG23	3:C:141:ASP:HA	1.94	0.49
2:B:325:HIS:HB2	2:B:346:ARG:O	2.12	0.49
3:C:153:CYS:SG	3:C:192:THR:HB	2.52	0.49
2:E:389:ASP:O	2:E:391:ARG:N	2.45	0.49
3:F:249:GLU:HG3	3:F:259:THR:HG22	1.93	0.49
3:F:268:GLY:O	3:F:274:TYR:HD1	1.95	0.49
3:F:304:PHE:HA	3:F:337:ASN:HD21	1.77	0.49
2:E:174:ASN:O	2:E:178:LYS:HG2	2.12	0.49
2:B:228:GLN:HB2	2:B:235:PRO:HG3	1.93	0.49
3:C:361:ASN:HB2	3:C:363:TYR:CE1	2.48	0.49
3:C:364:ASP:OD2	3:C:375:ARG:NH1	2.45	0.49
3:F:108:ARG:O	3:F:112:GLU:HB2	2.12	0.49
3:F:172:LEU:CD2	3:F:239:GLN:HE21	2.25	0.49
2:B:385:TRP:CD1	2:B:392:LYS:HB3	2.47	0.49
3:C:166:LEU:HB3	3:C:179:LEU:HD11	1.93	0.49
3:C:107:ILE:O	3:C:111:GLN:HG3	2.13	0.49
3:F:307:HIS:HD2	3:F:335:TRP:O	1.95	0.49
1:D:186:GLU:C	1:D:188:VAL:H	2.21	0.49
3:F:195:GLN:OE1	3:F:382:THR:HG22	2.12	0.49
1:A:169:LEU:H	2:B:189:GLN:NE2	2.11	0.49
3:C:253:TRP:CE3	3:C:380:LYS:HG3	2.48	0.49
3:C:337:ASN:HD22	3:C:337:ASN:C	2.20	0.49
2:E:314:MET:SD	2:E:447:MET:HE3	2.53	0.49
3:F:264:MET:HE1	3:F:389:PHE:CD2	2.48	0.49
1:A:127:ILE:CG2	1:A:129:LYS:HG2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:316:ASP:HB2	2:B:445:TYR:OH	2.13	0.49
3:C:165:GLY:O	3:C:167:TYR:HD1	1.96	0.49
1:D:133:ILE:HD11	3:F:107:ILE:HD11	1.95	0.49
2:E:422:TYR:OH	2:E:433:ASP:O	2.29	0.49
2:B:280:THR:O	2:B:281:ASP:C	2.56	0.48
2:B:300:SER:O	2:B:304:ARG:HG3	2.12	0.48
3:C:124:LEU:O	3:C:128:VAL:HG23	2.13	0.48
1:D:158:ILE:HG23	2:E:189:GLN:NE2	2.25	0.48
2:E:212:GLU:HG3	2:E:216:ARG:NH1	2.29	0.48
2:E:267:ASP:HB3	2:E:268:PRO:HD3	1.95	0.48
3:F:253:TRP:HA	3:F:380:LYS:HD2	1.95	0.48
2:B:386:LEU:O	2:B:387:THR:HB	2.13	0.48
2:B:385:TRP:CE3	2:B:406:ARG:HG2	2.44	0.48
3:C:300:SER:O	3:C:301:ASP:C	2.57	0.48
1:A:127:ILE:CG2	1:A:128:GLU:H	2.15	0.48
3:C:166:LEU:HD21	3:C:219:SER:N	2.29	0.48
2:E:345:TYR:HB2	2:E:354:MET:HE1	1.95	0.48
3:F:305:THR:HB	3:F:341:ALA:HB2	1.95	0.48
2:B:176:ARG:HB2	3:C:117:ASN:ND2	2.29	0.48
3:C:197:ARG:HD3	3:C:204:PHE:CZ	2.48	0.48
2:B:224:MET:HE2	2:B:237:ARG:HD3	1.94	0.48
2:E:161:ILE:CB	2:E:162:PRO:HD3	2.31	0.48
2:E:434:GLY:O	2:E:436:VAL:HG23	2.14	0.48
2:B:316:ASP:OD2	2:B:320:ASP:HB2	2.14	0.47
3:C:166:LEU:HD22	3:C:218:LEU:HB3	1.96	0.47
3:F:251:GLU:HG3	3:F:257:THR:CG2	2.35	0.47
3:F:317:ASN:C	3:F:317:ASN:ND2	2.70	0.47
3:C:100:ILE:O	3:C:100:ILE:HG22	2.14	0.47
2:B:175:LEU:O	2:B:179:ILE:HG13	2.15	0.47
2:B:352:ALA:HB2	2:B:439:ASN:ND2	2.28	0.47
3:F:313:SER:OG	3:F:319:ASN:N	2.47	0.47
3:F:338:LYS:N	3:F:339:CYS:CA	2.78	0.47
2:E:281:ASP:O	2:E:283:LYS:N	2.47	0.47
3:C:157:ALA:C	3:C:159:LYS:H	2.21	0.47
3:C:304:PHE:HB3	3:C:338:LYS:O	2.14	0.47
2:E:255:ARG:HB2	2:E:450:MET:HB3	1.96	0.47
2:B:405:ASN:O	2:B:406:ARG:HG3	2.14	0.47
3:C:229:GLY:O	3:C:233:ILE:HG13	2.14	0.47
3:C:367:ILE:O	3:C:379:MET:HG2	2.15	0.47
3:C:393:THR:O	3:C:393:THR:HG22	2.15	0.47
3:F:118:ASN:O	3:F:122:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:397:GLU:HG2	2:B:398:ASP:N	2.30	0.47
3:C:177:GLN:HE21	3:C:177:GLN:HB2	1.53	0.47
3:F:365:ASN:H	3:F:365:ASN:HD22	1.60	0.47
3:C:230:ASN:HB3	3:C:274:TYR:CG	2.50	0.47
1:D:175:LEU:HD22	1:D:175:LEU:N	2.30	0.47
2:B:169:ARG:HG2	2:B:169:ARG:NH1	2.28	0.47
2:B:373:MET:HG3	2:B:405:ASN:HB2	1.97	0.47
2:B:266:TRP:CE3	2:B:380:ARG:HG2	2.50	0.46
2:E:396:LYS:HG3	2:E:429:HIS:CD2	2.50	0.46
2:E:167:VAL:HG23	2:E:168:LEU:N	2.30	0.46
1:A:175:LEU:O	1:A:179:GLU:HG3	2.15	0.46
3:C:251:GLU:CB	3:C:257:THR:HG22	2.44	0.46
1:D:175:LEU:O	1:D:179:GLU:HG3	2.15	0.46
1:A:185:LEU:HD22	1:A:189:ILE:CG1	2.45	0.46
2:B:157:VAL:C	2:B:159:SER:H	2.23	0.46
3:C:273:LYS:NZ	3:C:317:ASN:HD21	2.13	0.46
1:D:181:GLN:OE1	2:E:171:ILE:HA	2.15	0.46
1:A:127:ILE:HG12	1:A:128:GLU:H	1.80	0.46
2:B:237:ARG:HG3	6:B:62:HOH:O	2.14	0.46
2:B:409:ALA:CA	2:B:438:MET:HE3	2.45	0.46
3:C:209:ILE:HG13	6:C:409:HOH:O	2.15	0.46
1:D:135:LEU:HD13	1:D:139:ASN:OD1	2.16	0.46
2:E:322:VAL:HG23	2:E:349:ALA:HB2	1.98	0.46
2:E:436:VAL:HG13	6:E:51:HOH:O	2.14	0.46
3:C:184:ILE:HD12	3:C:184:ILE:N	2.31	0.46
2:B:264:ARG:HD2	2:B:273:PHE:CD2	2.51	0.46
2:E:340:ILE:CG1	2:E:341:SER:N	2.78	0.46
2:E:181:LYS:HG2	2:E:182:LEU:N	2.30	0.46
1:A:127:ILE:HG22	1:A:130:VAL:HG23	1.98	0.46
2:B:345:TYR:HB2	2:B:354:MET:CE	2.45	0.46
3:C:156:ILE:HG22	3:C:161:ALA:HB2	1.97	0.46
2:E:167:VAL:O	2:E:171:ILE:HG13	2.16	0.46
3:F:393:THR:HG22	3:F:393:THR:O	2.16	0.46
2:B:385:TRP:CZ3	2:B:406:ARG:HB3	2.50	0.45
3:F:143:VAL:HA	3:F:220:PRO:HG2	1.98	0.45
1:D:143:GLN:NE2	3:F:118:ASN:HD22	2.13	0.45
2:E:280:THR:HB	2:E:288:LEU:HG	1.99	0.45
1:A:175:LEU:O	1:A:178:TYR:HB2	2.16	0.45
3:C:387:ILE:HG13	3:C:388:PRO:CD	2.46	0.45
3:F:249:GLU:HB3	3:F:383:THR:CG2	2.44	0.45
1:A:185:LEU:HD22	1:A:189:ILE:HG13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:323:LYS:NZ	2:B:325:HIS:CD2	2.82	0.45
3:C:165:GLY:O	3:C:167:TYR:CD1	2.70	0.45
2:E:301:GLN:NE2	2:E:301:GLN:C	2.74	0.45
2:B:190:MET:HE2	2:B:190:MET:HA	1.98	0.45
2:B:215:ILE:HA	2:B:219:GLY:O	2.16	0.45
2:B:315:GLU:OE1	2:B:321:LYS:HE2	2.17	0.45
1:D:165:CYS:HB3	2:E:193:CYS:HA	1.99	0.45
2:E:351:ASN:C	2:E:351:ASN:HD22	2.23	0.45
3:C:96:TYR:O	3:C:97:GLU:CB	2.64	0.45
3:C:177:GLN:H	3:C:177:GLN:HG3	1.44	0.45
1:D:136:LEU:HD21	3:F:111:GLN:HB3	1.97	0.45
2:E:281:ASP:C	2:E:283:LYS:N	2.75	0.45
2:E:436:VAL:HG12	2:E:437:TRP:N	2.31	0.45
2:B:212:GLU:O	2:B:215:ILE:HG22	2.17	0.45
2:B:440:TRP:CE3	2:B:447:MET:HE1	2.47	0.45
2:E:206:VAL:O	2:E:206:VAL:HG13	2.17	0.45
2:E:373:MET:HE2	2:E:405:ASN:HA	1.99	0.45
2:B:159:SER:CA	2:B:162:PRO:HD2	2.47	0.44
3:F:172:LEU:HD23	3:F:239:GLN:HE21	1.82	0.44
3:F:198:LEU:HD12	3:F:199:ASP:N	2.32	0.44
1:D:181:GLN:HG2	2:E:171:ILE:HG22	2.00	0.44
2:E:253:GLN:HB3	2:E:452:MET:HB2	1.99	0.44
2:B:422:TYR:OH	2:B:433:ASP:O	2.34	0.44
2:E:351:ASN:ND2	2:E:354:MET:HB2	2.33	0.44
3:F:325:ASN:HD21	3:F:327:ALA:HB3	1.82	0.44
3:F:350:GLN:C	3:F:352:GLY:H	2.26	0.44
2:B:337:LYS:HB2	2:B:374:PHE:CD1	2.52	0.44
2:E:172:LEU:HD22	3:F:113:ILE:CG1	2.45	0.44
2:E:224:MET:CE	2:E:237:ARG:HD3	2.47	0.44
3:F:293:PHE:CG	3:F:370:ALA:HB1	2.53	0.44
3:F:333:GLY:O	3:F:334:TRP:HB2	2.17	0.44
2:B:351:ASN:ND2	2:B:351:ASN:O	2.51	0.44
1:D:188:VAL:HG12	2:E:164:ASN:HD21	1.82	0.44
2:E:421:GLN:HE21	2:E:421:GLN:HB2	1.56	0.44
3:F:359:THR:C	3:F:361:ASN:H	2.25	0.44
3:F:372:TRP:O	3:F:373:LYS:HD3	2.18	0.44
3:C:179:LEU:HD23	3:C:218:LEU:HD12	2.00	0.43
3:F:268:GLY:O	3:F:274:TYR:HA	2.17	0.43
3:F:373:LYS:HB3	3:F:377:TYR:HB3	2.00	0.43
2:E:164:ASN:O	2:E:166:ARG:N	2.51	0.43
3:F:310:MET:HE2	3:F:310:MET:CA	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:392:LEU:O	3:F:393:THR:C	2.60	0.43
3:C:199:ASP:OD1	3:C:201:SER:N	2.50	0.43
1:D:171:ARG:HG3	1:D:171:ARG:NH1	2.33	0.43
2:E:255:ARG:HD3	2:E:262:PHE:CZ	2.53	0.43
2:E:370:HIS:CE1	2:E:402:TRP:HE1	2.36	0.43
3:F:172:LEU:HD22	3:F:172:LEU:H	1.84	0.43
3:C:178:PHE:CD2	3:C:232:LYS:HD3	2.53	0.43
3:C:270:GLU:HG3	3:C:274:TYR:CE2	2.54	0.43
2:B:280:THR:HG23	2:B:288:LEU:HG	1.99	0.43
2:B:381:ASP:OD1	2:B:381:ASP:C	2.61	0.43
2:B:228:GLN:CD	2:B:235:PRO:HG3	2.43	0.43
3:C:297:ASP:OD1	3:C:375:ARG:NH2	2.51	0.43
3:C:338:LYS:N	3:C:339:CYS:CA	2.79	0.43
3:C:365:ASN:C	3:C:365:ASN:HD22	2.26	0.43
2:E:171:ILE:O	2:E:175:LEU:HG	2.19	0.43
2:B:281:ASP:O	2:B:282:GLY:C	2.62	0.43
3:C:156:ILE:CG2	3:C:161:ALA:HB2	2.49	0.43
3:C:373:LYS:HB2	3:C:379:MET:HE1	2.01	0.43
1:D:175:LEU:H	1:D:175:LEU:CD2	2.31	0.43
3:F:305:THR:O	3:F:341:ALA:HB2	2.19	0.42
1:A:127:ILE:HG21	1:A:129:LYS:HG2	2.00	0.42
2:B:438:MET:O	2:B:442:GLY:HA2	2.20	0.42
1:D:188:VAL:HB	2:E:164:ASN:CG	2.44	0.42
2:E:373:MET:SD	2:E:405:ASN:ND2	2.93	0.42
3:F:311:GLN:O	3:F:335:TRP:HA	2.19	0.42
1:A:148:LYS:HD3	2:B:425:ASP:OD2	2.19	0.42
3:C:240:SER:O	3:C:242:ILE:HG13	2.20	0.42
3:C:286:ALA:O	3:C:372:TRP:HB2	2.20	0.42
3:F:191:TRP:CE3	3:F:385:LYS:HG3	2.54	0.42
2:B:345:TYR:CG	2:B:346:ARG:N	2.86	0.42
3:F:116:SER:O	3:F:120:LYS:HG3	2.19	0.42
2:E:163:THR:HG23	2:E:166:ARG:NH2	2.35	0.42
2:E:172:LEU:HD11	3:F:114:TYR:HB2	2.02	0.42
2:E:357:ALA:HB3	2:E:360:LEU:CD1	2.44	0.42
1:D:136:LEU:O	1:D:140:VAL:HG13	2.19	0.42
2:E:391:ARG:O	2:E:391:ARG:CD	2.68	0.42
3:F:245:ALA:HB1	3:F:392:LEU:HD11	2.00	0.42
3:F:357:ALA:C	3:F:359:THR:N	2.76	0.42
2:B:310:LEU:HB2	2:B:329:PHE:CD2	2.54	0.42
2:E:160:ASN:ND2	2:E:163:THR:HB	2.34	0.42
3:C:356:LYS:HG3	3:C:376:TRP:CH2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:GLN:HE22	3:C:117:ASN:HB2	1.85	0.42
1:A:185:LEU:HD22	1:A:189:ILE:CD1	2.49	0.42
2:E:415:ARG:O	2:E:434:GLY:HA2	2.19	0.42
3:F:246:LEU:HD12	3:F:247:ARG:H	1.84	0.42
2:B:355:ASP:O	2:B:365:ARG:HD3	2.19	0.41
3:C:194:PHE:CD1	3:C:194:PHE:C	2.98	0.41
1:D:150:LEU:O	1:D:154:ILE:HG13	2.19	0.41
3:F:387:ILE:CD1	3:F:391:ARG:HG2	2.45	0.41
2:B:303:THR:HB	2:B:330:THR:HA	2.01	0.41
2:E:378:TYR:HA	2:E:395:SER:O	2.20	0.41
3:F:304:PHE:C	3:F:337:ASN:HD22	2.28	0.41
3:C:215:PHE:HA	6:C:410:HOH:O	2.20	0.41
3:C:219:SER:HA	3:C:220:PRO:HD3	1.89	0.41
2:B:373:MET:HE2	2:B:404:TYR:O	2.20	0.41
3:C:268:GLY:O	3:C:274:TYR:HA	2.20	0.41
3:C:387:ILE:CG1	3:C:388:PRO:HD2	2.48	0.41
2:E:363:GLU:HG2	2:E:367:MET:HE2	2.02	0.41
1:A:181:GLN:HE22	2:B:174:ASN:CG	2.27	0.41
3:C:304:PHE:CD1	3:C:338:LYS:HD3	2.55	0.41
1:D:175:LEU:O	1:D:178:TYR:HB2	2.21	0.41
3:F:284:GLY:C	3:F:286:ALA:H	2.28	0.41
1:A:136:LEU:HD21	3:C:111:GLN:HG2	2.01	0.41
2:B:282:GLY:O	2:B:283:LYS:HG2	2.20	0.41
2:B:397:GLU:C	2:B:399:GLY:H	2.29	0.41
2:B:322:VAL:HG23	2:B:349:ALA:HB2	2.02	0.41
2:B:359:GLN:O	2:B:360:LEU:HD23	2.20	0.41
2:E:395:SER:HB2	2:E:404:TYR:CE2	2.55	0.41
2:B:163:THR:O	2:B:167:VAL:HG23	2.21	0.41
2:B:203:ILE:HA	2:B:204:PRO:HD3	1.93	0.41
3:F:325:ASN:C	3:F:325:ASN:ND2	2.76	0.41
3:C:285:ASP:OD1	3:C:285:ASP:N	2.54	0.40
3:C:374:THR:O	3:C:376:TRP:N	2.53	0.40
1:D:188:VAL:HG12	2:E:164:ASN:ND2	2.36	0.40
2:E:436:VAL:CG1	2:E:437:TRP:N	2.84	0.40
3:F:298:ASP:HA	3:F:299:PRO:HD3	1.95	0.40
2:B:218:GLY:HA3	3:C:210:GLN:HG2	2.02	0.40
2:B:402:TRP:CG	2:B:403:TRP:N	2.89	0.40
3:C:148:ILE:HD12	3:C:148:ILE:N	2.32	0.40
3:F:149:THR:HA	3:F:156:ILE:HD11	2.03	0.40
3:F:373:LYS:HG3	3:F:377:TYR:HD2	1.86	0.40
2:B:171:ILE:O	2:B:174:ASN:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:415:ARG:O	2:B:434:GLY:HA2	2.21	0.40
1:D:141:ARG:O	1:D:145:VAL:HG23	2.22	0.40
1:A:176:LYS:O	1:A:179:GLU:N	2.55	0.40
2:E:212:GLU:O	2:E:215:ILE:HG22	2.21	0.40
1:A:158:ILE:HG23	2:B:189:GLN:HE21	1.86	0.40
2:E:163:THR:HG23	2:E:166:ARG:HH21	1.86	0.40
3:F:350:GLN:O	3:F:352:GLY:N	2.51	0.40
3:F:373:LYS:CG	3:F:377:TYR:HD2	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	59/61 (97%)	55 (93%)	4 (7%)	14	40
1	D	52/61 (85%)	48 (92%)	4 (8%)	12	34
2	B	264/271 (97%)	252 (96%)	12 (4%)	24	57
2	E	258/271 (95%)	243 (94%)	15 (6%)	18	47
3	C	250/258 (97%)	237 (95%)	13 (5%)	21	51
3	F	251/258 (97%)	238 (95%)	13 (5%)	21	51
All	All	1134/1180 (96%)	1073 (95%)	61 (5%)	20	50

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	LEU
1	A	145	VAL
1	A	169	LEU
1	A	185	LEU
2	B	164	ASN
2	B	190	MET
2	B	196	PRO
2	B	210	GLU
2	B	230	ASP
2	B	238	VAL
2	B	253	GLN
2	B	271	GLN
2	B	280	THR
2	B	325	HIS
2	B	439	ASN
2	B	446	SER
3	C	96	TYR
3	C	104	ASP
3	C	134	GLN
3	C	143	VAL
3	C	147	ASP
3	C	177	GLN
3	C	192	THR
3	C	276	LEU
3	C	317	ASN
3	C	325	ASN
3	C	365	ASN
3	C	375	ARG
3	C	383	THR
1	D	135	LEU
1	D	176	LYS
1	D	181	GLN
1	D	185	LEU
2	E	176	ARG
2	E	190	MET
2	E	196	PRO
2	E	210	GLU
2	E	230	ASP
2	E	253	GLN
2	E	301	GLN
2	E	320	ASP
2	E	323	LYS
2	E	343	ASN

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Mol	Chain	Res	Type
2	E	359	GLN
2	E	366	THR
2	E	396	LYS
2	E	421	GLN
2	E	447	MET
3	F	118	ASN
3	F	134	GLN
3	F	143	VAL
3	F	159	LYS
3	F	176	GLN
3	F	192	THR
3	F	221	THR
3	F	250	LEU
3	F	301	ASP
3	F	317	ASN
3	F	365	ASN
3	F	382	THR
3	F	383	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	187	GLN
2	B	158	ASN
2	B	160	ASN
2	B	164	ASN
2	B	189	GLN
2	B	228	GLN
2	B	253	GLN
2	B	271	GLN
2	B	296	ASN
2	B	301	GLN
2	B	325	HIS
2	B	339	GLN
2	B	351	ASN
2	B	405	ASN
2	B	408	HIS
2	B	421	GLN
2	B	439	ASN
3	C	103	HIS
3	C	111	GLN

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Mol	Chain	Res	Type
3	C	117	ASN
3	C	119	GLN
3	C	144	GLN
3	C	163	GLN
3	C	176	GLN
3	C	177	GLN
3	C	217	HIS
3	C	230	ASN
3	C	239	GLN
3	C	307	HIS
3	C	317	ASN
3	C	325	ASN
3	C	329	GLN
3	C	337	ASN
3	C	365	ASN
1	D	134	GLN
1	D	184	GLN
1	D	187	GLN
2	E	160	ASN
2	E	164	ASN
2	E	174	ASN
2	E	189	GLN
2	E	202	ASN
2	E	243	ASN
2	E	254	ASN
2	E	296	ASN
2	E	301	GLN
2	E	325	HIS
2	E	339	GLN
2	E	343	ASN
2	E	351	ASN
2	E	359	GLN
2	E	421	GLN
2	E	429	HIS
3	F	115	ASN
3	F	118	ASN
3	F	176	GLN
3	F	230	ASN
3	F	239	GLN
3	F	307	HIS
3	F	308	ASN
3	F	317	ASN

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Mol	Chain	Res	Type
3	F	325	ASN
3	F	337	ASN
3	F	365	ASN
3	F	390	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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	NAG	B	500	2	14,14,15	0.58	0	17,19,21	0.80	1 (5%)
4	NAG	E	500	2	14,14,15	0.59	0	17,19,21	0.75	1 (5%)

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	NAG	B	500	2	-	2/6/23/26	0/1/1/1
4	NAG	E	500	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	500	NAG	C2-N2-C7	-2.46	119.60	122.90
4	E	500	NAG	C2-N2-C7	-2.06	120.14	122.90

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	500	NAG	C8-C7-N2-C2
4	B	500	NAG	O7-C7-N2-C2
4	E	500	NAG	C8-C7-N2-C2
4	E	500	NAG	O7-C7-N2-C2
4	E	500	NAG	C4-C5-C6-O6
4	E	500	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	500	NAG	2	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(Å²)	Q<0.9	
1	A	64/66 (96%)	0.33	4 (6%)	26	19	20, 56, 85, 91	0
1	D	56/66 (84%)	0.52	4 (7%)	22	16	24, 52, 105, 113	0
2	B	306/313 (97%)	-0.13	5 (1%)	70	61	16, 33, 73, 94	0
2	E	300/313 (95%)	-0.29	7 (2%)	61	51	11, 25, 68, 114	0
3	C	298/311 (95%)	0.10	6 (2%)	65	55	23, 43, 68, 89	0
3	F	299/311 (96%)	-0.02	11 (3%)	45	36	11, 34, 78, 101	0
All	All	1323/1380 (95%)	-0.04	37 (2%)	55	44	11, 35, 79, 114	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	190	ALA	5.2
2	E	161	ILE	4.5
3	F	98	ALA	3.7
1	D	188	VAL	3.5
3	F	394	ILE	3.3
2	E	281	ASP	3.2
3	F	101	LEU	3.1
1	D	135	LEU	2.9
3	C	96	TYR	2.8
2	B	158	ASN	2.8
3	C	98	ALA	2.8
1	D	185	LEU	2.7
2	B	385	TRP	2.7
2	E	164	ASN	2.7
2	B	155	GLU	2.5
3	C	392	LEU	2.5
2	E	163	THR	2.5
2	B	459	PRO	2.4
3	F	105	SER	2.4

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Mol	Chain	Res	Type	RSRZ
3	F	393	THR	2.4
3	F	99	SER	2.3
3	F	112	GLU	2.3
2	E	160	ASN	2.3
3	C	242	ILE	2.3
3	F	96	TYR	2.2
2	E	458	PHE	2.2
1	A	183	LYS	2.2
3	F	110	LEU	2.2
1	A	127	ILE	2.2
1	A	188	VAL	2.2
2	E	165	LEU	2.2
3	F	323	GLU	2.2
2	B	156	THR	2.1
3	F	102	THR	2.1
1	D	181	GLN	2.1
3	C	172	LEU	2.1
3	C	357	ALA	2.1

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	NAG	B	500	14/15	0.49	0.14	80,83,84,85	0
4	NAG	E	500	14/15	0.66	0.15	65,68,69,71	0
5	CA	F	407	1/1	0.91	0.07	39,39,39,39	0
5	CA	B	501	1/1	0.94	0.06	48,48,48,48	0
5	CA	C	407	1/1	0.95	0.06	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CA	B	502	1/1	0.95	0.12	40,40,40,40	0
5	CA	E	501	1/1	0.96	0.05	31,31,31,31	0
5	CA	E	502	1/1	0.97	0.08	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.