



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:55 PM UTC

PDB ID : 8F88 / pdb_00008f88
Title : Crystal structure of PTP1B D181A/Q262A/C215A phosphatase domain with monophosphorylated JAK2 activation loop phosphopeptide
Authors : Morris, R.; Kershaw, N.J.; Babon, J.J.
Deposited on : 2022-11-21
Resolution : 3.10 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:

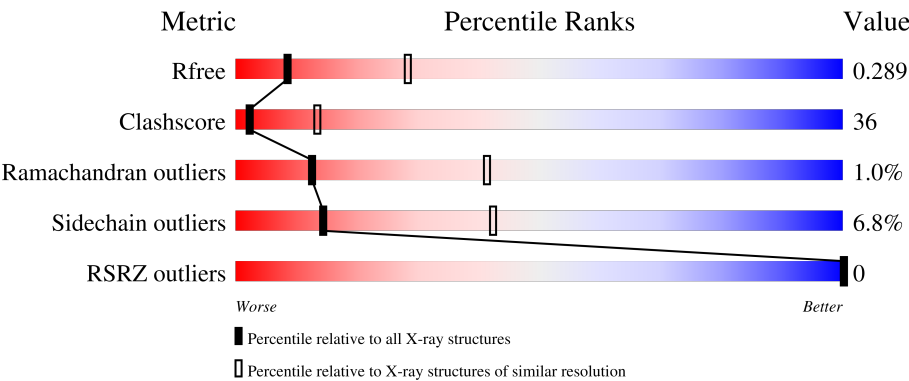
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	321	56% 32% • 8%
1	B	321	53% 36% • 8%
1	C	321	42% 43% 6% 9%
2	E	16	31% 6% 62%
2	F	16	38% 6% 6% 50%

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Mol	Chain	Length	Quality of chain
2	G	16	 12% 6% 81%

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
3	TRS	A	401	-	X	-	-
3	TRS	A	402	-	X	-	-
3	TRS	C	401	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7020 atoms, of which 36 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 Tyrosine-protein phosphatase non-receptor type 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2280	1446	396	423	15			
1	B	296	Total	C	N	O	S	0	0	0
			2313	1475	400	424	14			
1	C	293	Total	C	N	O	S	0	0	0
			2185	1391	373	410	11			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	ALA	ASP	engineered mutation	UNP P18031
A	215	ALA	CYS	engineered mutation	UNP P18031
A	262	ALA	GLN	engineered mutation	UNP P18031
B	181	ALA	ASP	engineered mutation	UNP P18031
B	215	ALA	CYS	engineered mutation	UNP P18031
B	262	ALA	GLN	engineered mutation	UNP P18031
C	181	ALA	ASP	engineered mutation	UNP P18031
C	215	ALA	CYS	engineered mutation	UNP P18031
C	262	ALA	GLN	engineered mutation	UNP P18031

- Molecule 2 is a protein called Tyrosine-protein kinase JAK2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	6	Total	C	N	O	P	0	0	0
			49	31	6	11	1			
2	F	8	Total	C	N	O	P	0	0	0
			63	39	8	15	1			
2	G	3	Total	C	N	O	P	0	0	0
			33	21	3	8	1			

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			20	4	12	1	3		
3	A	1	Total	C	H	N	O	0	0
			20	4	12	1	3		
3	C	1	Total	C	H	N	O	0	0
			20	4	12	1	3		

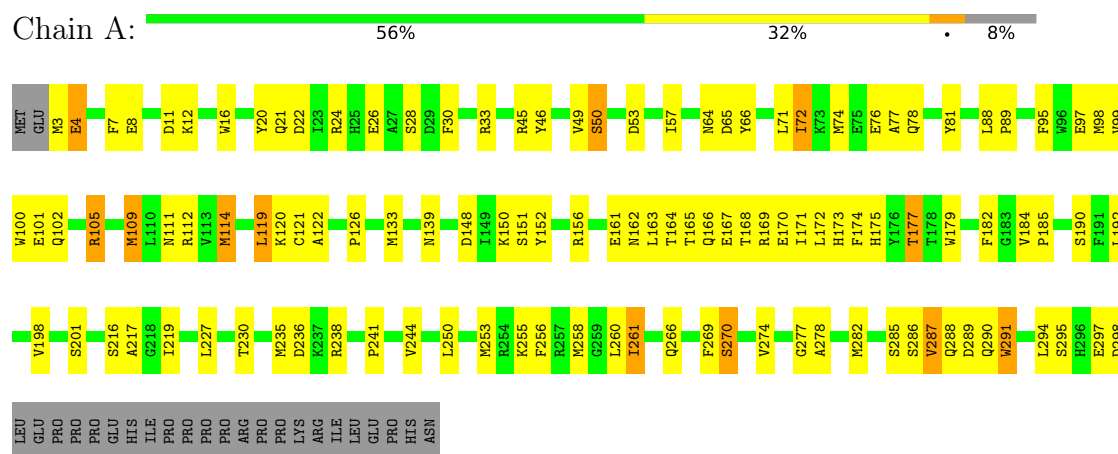
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	11	Total	O	0	0
			11	11		
4	B	16	Total	O	0	0
			16	16		
4	C	10	Total	O	0	0
			10	10		

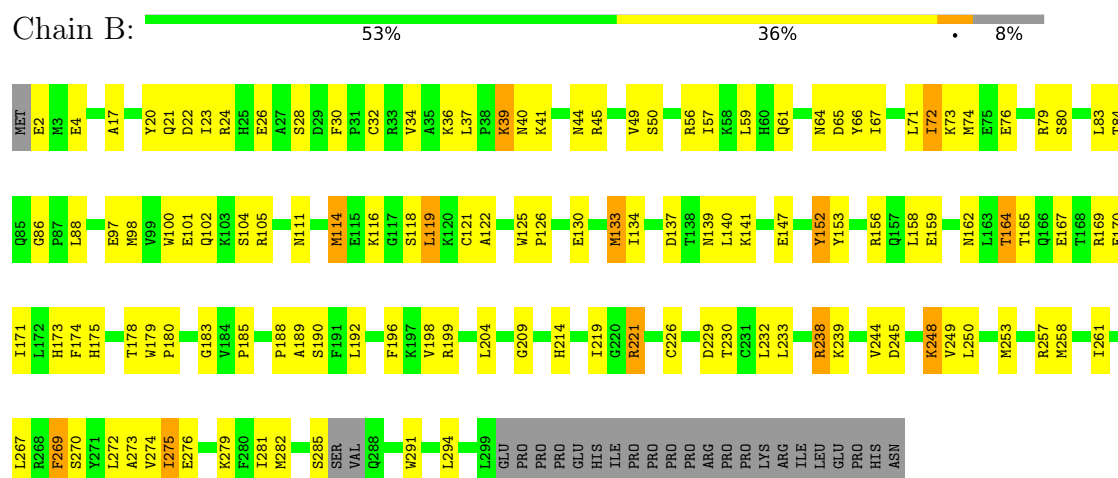
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

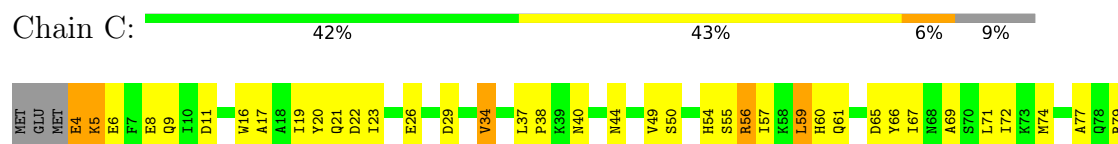
- Molecule 1: Tyrosine-protein phosphatase non-receptor type 1

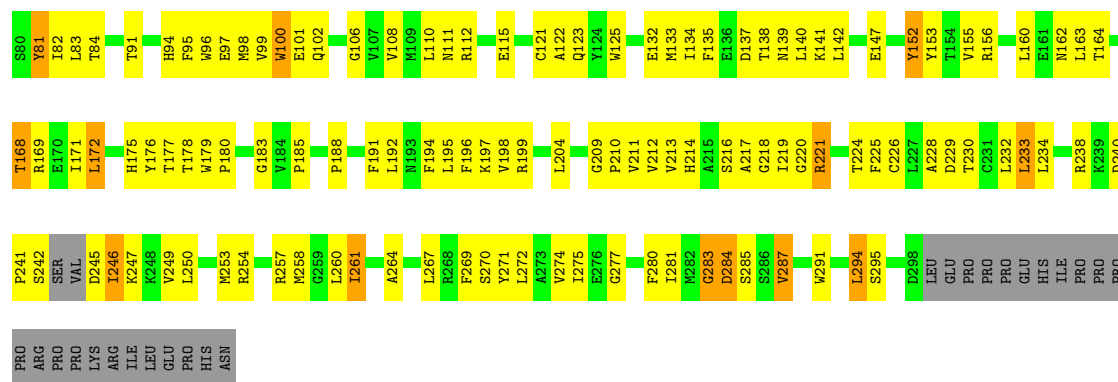


- Molecule 1: Tyrosine-protein phosphatase non-receptor type 1

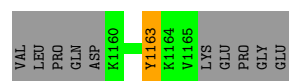


- Molecule 1: Tyrosine-protein phosphatase non-receptor type 1

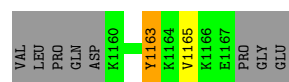
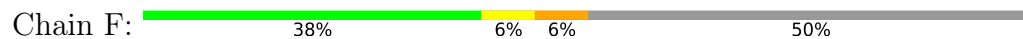




- Molecule 2: Tyrosine-protein kinase JAK2



- Molecule 2: Tyrosine-protein kinase JAK2



- Molecule 2: Tyrosine-protein kinase JAK2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.23Å 176.23Å 43.80Å 90.00° 90.29° 90.00°	Depositor
Resolution (Å)	42.79 – 3.10 42.79 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (42.79-3.10) 93.2 (42.79-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.262 , 0.291 0.258 , 0.289	Depositor DCC
R_{free} test set	2013 reflections (8.26%)	wwPDB-VP
Wilson B-factor (Å ²)	78.5	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 96.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.439 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7020	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.35	0/2333	0.58	0/3168
1	B	0.34	0/2367	0.58	0/3205
1	C	0.38	0/2236	0.66	0/3052
2	E	0.31	0/32	0.27	0/41
2	F	0.44	0/46	0.47	0/60
2	G	0.42	0/17	0.46	0/22
All	All	0.35	0/7031	0.61	0/9548

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	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	8	GLU	Peptide

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	2280	0	2134	119	0
1	B	2313	0	2210	129	0
1	C	2185	0	1979	228	0
2	E	49	0	25	4	0
2	F	63	0	33	2	0
2	G	33	0	17	1	0
3	A	16	24	24	3	0
3	C	8	12	12	2	0
4	A	11	0	0	2	0
4	B	16	0	0	2	0
4	C	10	0	0	0	0
All	All	6984	36	6434	478	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 36.

All (478) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:ILE:HD11	1:C:141:LYS:HG3	1.25	1.14
1:C:242:SER:HG	1:C:245:ASP:N	1.45	1.14
1:C:160:LEU:HD22	1:C:171:ILE:HG13	1.26	1.10
1:B:282:MET:HA	1:B:282:MET:HE2	1.40	1.03
1:C:112:ARG:NE	1:C:177:THR:O	1.93	1.01
1:A:282:MET:HE2	1:A:282:MET:HA	1.40	1.00
1:C:134:ILE:HG13	1:C:141:LYS:HA	1.44	0.99
1:C:57:ILE:HG13	1:C:98:MET:HE3	1.47	0.96
1:C:160:LEU:CD2	1:C:171:ILE:HG13	1.97	0.93
1:C:4:GLU:O	1:C:6:GLU:N	2.03	0.90
1:A:4:GLU:OE1	1:A:4:GLU:N	2.03	0.90
1:C:69:ALA:HA	1:C:84:THR:HG22	1.55	0.88
1:A:126:PRO:HA	1:A:133:MET:HE3	1.55	0.88
1:C:246:ILE:HD13	1:C:246:ILE:H	1.39	0.87
1:C:284:ASP:O	1:C:287:VAL:HG12	1.75	0.86
1:C:108:VAL:HG13	1:C:213:VAL:HA	1.57	0.86
1:B:139:ASN:HD22	1:B:164:THR:HG23	1.42	0.84
1:B:185:PRO:HG2	1:B:269:PHE:CZ	2.13	0.84
1:C:60:HIS:HB2	1:C:101:GLU:CD	2.03	0.84
1:B:270:SER:O	1:B:274:VAL:HG23	1.78	0.83
1:A:289:ASP:H	1:A:291:TRP:HZ3	1.26	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:ASP:O	1:C:26:GLU:HG3	1.78	0.82
1:C:56:ARG:NH1	1:C:65:ASP:OD2	2.11	0.82
1:C:108:VAL:CG1	1:C:213:VAL:HG22	2.09	0.82
1:C:254:ARG:NH1	1:C:260:LEU:O	2.12	0.82
1:B:56:ARG:NH1	1:B:65:ASP:OD1	2.13	0.81
1:A:50:SER:O	1:A:258:MET:HE3	1.81	0.81
1:C:97:GLU:HB2	1:C:138:THR:HG21	1.61	0.80
1:C:69:ALA:HB1	1:C:98:MET:HE1	1.61	0.80
1:C:250:LEU:O	1:C:254:ARG:HG3	1.81	0.80
1:C:271:TYR:O	1:C:275:ILE:HG13	1.81	0.80
1:A:112:ARG:NE	1:A:177:THR:O	2.12	0.80
1:A:114:MET:HE3	1:A:119:LEU:HD23	1.65	0.79
1:C:246:ILE:HG13	1:C:271:TYR:CZ	2.17	0.79
1:C:141:LYS:HB2	1:C:163:LEU:HD21	1.63	0.78
1:C:291:TRP:O	1:C:295:SER:OG	2.00	0.78
1:C:241:PRO:O	1:C:242:SER:OG	2.01	0.78
1:C:83:LEU:HD11	1:C:226:CYS:SG	2.24	0.77
1:C:123:GLN:NE2	1:C:125:TRP:O	2.17	0.77
1:C:82:ILE:HG21	1:C:98:MET:HE2	1.67	0.77
1:A:139:ASN:OD1	1:A:163:LEU:HB2	1.85	0.77
1:C:81:TYR:CE2	1:C:226:CYS:HB3	2.19	0.77
1:C:228:ALA:O	1:C:232:LEU:HD12	1.85	0.76
1:B:114:MET:HE3	1:B:114:MET:HA	1.68	0.76
1:C:139:ASN:OD1	1:C:164:THR:HG23	1.85	0.75
1:C:152:TYR:OH	1:C:295:SER:HB3	1.86	0.75
1:C:134:ILE:CD1	1:C:141:LYS:HG3	2.14	0.75
1:C:81:TYR:OH	1:C:230:THR:OG1	1.75	0.74
1:B:50:SER:O	1:B:258:MET:HE3	1.87	0.74
1:C:79:ARG:NH1	1:C:229:ASP:OD2	2.20	0.74
1:C:4:GLU:HG3	1:C:275:ILE:HG21	1.68	0.74
1:B:152:TYR:H	1:B:152:TYR:HD2	1.35	0.73
1:C:180:PRO:HG2	1:C:183:GLY:HA3	1.71	0.73
1:C:20:TYR:HA	1:C:23:ILE:HG22	1.71	0.73
1:B:165:THR:OG1	1:B:167:GLU:HG2	1.89	0.73
1:C:185:PRO:HG2	1:C:269:PHE:CE1	2.24	0.73
1:C:194:PHE:O	1:C:198:VAL:HG23	1.88	0.73
1:C:277:GLY:HA2	1:C:291:TRP:HH2	1.53	0.73
1:B:57:ILE:HD11	1:B:71:LEU:HB2	1.69	0.72
1:A:151:SER:N	1:A:297:GLU:O	2.15	0.72
1:C:250:LEU:HD21	1:C:261:ILE:HG13	1.71	0.72
1:C:108:VAL:HG11	1:C:213:VAL:HG22	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:ASN:HD21	1:B:121:CYS:HB2	1.55	0.72
1:C:140:LEU:HD23	1:C:141:LYS:N	2.04	0.72
1:A:286:SER:O	1:A:287:VAL:HG13	1.90	0.72
1:B:269:PHE:CE2	1:B:273:ALA:HB2	2.24	0.72
1:A:22:ASP:O	1:A:26:GLU:HG3	1.90	0.71
1:C:121:CYS:SG	1:C:122:ALA:N	2.63	0.71
1:B:45:ARG:NH1	1:B:88:LEU:HD23	2.05	0.71
1:C:250:LEU:CD2	1:C:261:ILE:HG13	2.21	0.71
1:B:139:ASN:ND2	1:B:164:THR:HG23	2.06	0.71
1:A:111:ASN:HD21	1:A:121:CYS:HB2	1.56	0.70
1:C:23:ILE:HD11	1:C:250:LEU:HG	1.73	0.70
1:C:97:GLU:HB2	1:C:138:THR:CG2	2.21	0.70
1:A:109:MET:HG2	1:A:175:HIS:CD2	2.26	0.70
1:C:57:ILE:HG13	1:C:98:MET:CE	2.19	0.70
1:C:20:TYR:HA	1:C:23:ILE:CG2	2.22	0.70
1:C:72:ILE:HD12	1:C:83:LEU:HD13	1.74	0.69
1:A:126:PRO:HB3	1:A:133:MET:HG3	1.72	0.69
1:C:79:ARG:HG2	1:C:81:TYR:CE1	2.28	0.69
1:C:160:LEU:HG	1:C:169:ARG:NH2	2.08	0.69
1:B:185:PRO:HG2	1:B:269:PHE:CE1	2.28	0.68
1:C:152:TYR:HA	1:C:178:THR:HG23	1.74	0.68
1:C:152:TYR:CE2	1:C:153:TYR:HD2	2.11	0.68
1:C:133:MET:C	1:C:134:ILE:HD12	2.18	0.68
1:A:28:SER:HB3	1:A:30:PHE:CE2	2.29	0.68
1:B:238:ARG:HH21	1:B:244:VAL:HA	1.59	0.68
1:A:139:ASN:OD1	1:A:163:LEU:HD12	1.94	0.68
1:B:282:MET:HA	1:B:282:MET:CE	2.21	0.67
1:C:5:LYS:O	1:C:9:GLN:N	2.27	0.67
1:B:152:TYR:CE1	1:B:190:SER:HB3	2.30	0.67
1:C:60:HIS:HB2	1:C:101:GLU:OE2	1.94	0.67
1:C:245:ASP:O	1:C:249:VAL:HG23	1.93	0.67
1:A:282:MET:HA	1:A:282:MET:CE	2.22	0.67
1:C:72:ILE:CD1	1:C:83:LEU:HD13	2.25	0.67
1:C:249:VAL:O	1:C:253:MET:HG3	1.94	0.67
1:B:114:MET:HA	1:B:114:MET:CE	2.25	0.67
1:A:126:PRO:CA	1:A:133:MET:HE3	2.23	0.66
1:C:108:VAL:HG13	1:C:213:VAL:HG13	1.77	0.66
1:C:100:TRP:HE1	1:C:162:ASN:HB2	1.60	0.66
1:C:192:LEU:HD13	1:C:291:TRP:CZ2	2.31	0.66
1:B:282:MET:HE2	1:B:282:MET:CA	2.24	0.66
1:C:59:LEU:HD12	1:C:65:ASP:C	2.21	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ILE:HD11	1:A:71:LEU:HB2	1.77	0.65
1:C:91:THR:HA	1:C:94:HIS:ND1	2.11	0.65
1:C:111:ASN:HB2	1:C:115:GLU:OE2	1.96	0.65
1:C:160:LEU:HD23	1:C:160:LEU:H	1.61	0.65
1:C:185:PRO:HG2	1:C:269:PHE:CZ	2.32	0.65
1:C:110:LEU:HD13	1:C:179:TRP:CZ3	2.32	0.65
1:A:76:GLU:OE2	1:A:238:ARG:HD3	1.97	0.64
1:B:20:TYR:HB2	1:B:267:LEU:HD23	1.78	0.64
1:C:155:VAL:HG21	1:C:197:LYS:HE3	1.80	0.64
1:A:46:TYR:CE2	1:A:217:ALA:HB2	2.32	0.64
1:C:160:LEU:HD13	1:C:171:ILE:HD11	1.79	0.64
1:C:152:TYR:HA	1:C:178:THR:CG2	2.28	0.64
1:B:114:MET:HE2	1:B:118:SER:C	2.23	0.63
1:B:188:PRO:O	1:B:192:LEU:HD12	1.97	0.63
1:C:20:TYR:O	1:C:23:ILE:HG22	1.98	0.63
1:A:165:THR:OG1	1:A:167:GLU:HB2	1.99	0.63
1:C:20:TYR:CA	1:C:23:ILE:HG22	2.28	0.63
1:C:247:LYS:HE3	1:C:271:TYR:OH	1.97	0.63
1:A:98:MET:O	1:A:102:GLN:HG2	1.98	0.63
1:C:242:SER:OG	1:C:245:ASP:N	2.23	0.63
1:C:40:ASN:HB3	1:C:66:TYR:CD2	2.33	0.63
1:C:79:ARG:HG2	1:C:81:TYR:CD1	2.33	0.63
1:C:99:VAL:HG11	1:C:171:ILE:CD1	2.28	0.63
1:B:74:MET:HE2	1:B:230:THR:HG21	1.81	0.62
1:C:147:GLU:CB	1:C:156:ARG:HG2	2.30	0.62
1:C:172:LEU:N	1:C:172:LEU:HD22	2.13	0.62
1:C:20:TYR:C	1:C:23:ILE:HG22	2.24	0.62
1:C:133:MET:O	1:C:134:ILE:HD12	2.00	0.62
3:A:402:TRS:O1	3:A:402:TRS:O3	2.18	0.61
1:C:59:LEU:HD12	1:C:65:ASP:O	1.99	0.61
3:C:401:TRS:O1	3:C:401:TRS:O2	2.12	0.61
1:C:99:VAL:HG11	1:C:171:ILE:HD13	1.80	0.61
1:A:227:LEU:HD22	1:A:250:LEU:HD13	1.83	0.61
1:B:23:ILE:HD13	1:B:250:LEU:HD23	1.82	0.61
1:C:17:ALA:HA	1:C:264:ALA:HB2	1.83	0.61
1:A:45:ARG:CZ	1:A:120:LYS:O	2.49	0.61
1:B:114:MET:HE2	1:B:118:SER:O	2.00	0.61
1:B:245:ASP:HB3	1:B:248:LYS:HB2	1.83	0.61
1:A:45:ARG:HH21	1:A:121:CYS:HA	1.66	0.60
1:C:20:TYR:O	1:C:23:ILE:CG2	2.50	0.60
1:C:246:ILE:H	1:C:246:ILE:CD1	2.13	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:ARG:NH2	1:B:229:ASP:OD1	2.35	0.60
1:A:20:TYR:CE2	1:A:24:ARG:HD2	2.36	0.60
1:C:176:TYR:CD2	1:C:179:TRP:HB2	2.37	0.60
1:B:232:LEU:HB3	1:B:281:ILE:HD11	1.84	0.59
1:B:28:SER:HB3	1:B:30:PHE:CE2	2.37	0.59
1:C:79:ARG:NH1	1:C:204:LEU:HD13	2.17	0.59
1:C:84:THR:O	1:C:218:GLY:HA3	2.02	0.59
1:A:46:TYR:CD2	2:E:1163:PTR:HB3	2.37	0.59
1:A:45:ARG:HG3	1:A:45:ARG:HH11	1.68	0.59
1:C:17:ALA:O	1:C:21:GLN:HG2	2.02	0.59
1:A:185:PRO:HD2	1:A:269:PHE:CE1	2.37	0.59
1:C:34:VAL:HA	1:C:37:LEU:HG	1.84	0.59
1:B:72:ILE:HD12	1:B:72:ILE:N	2.18	0.58
1:B:114:MET:CE	1:B:119:LEU:HA	2.33	0.58
1:C:240:ASP:CG	1:C:241:PRO:HD2	2.28	0.58
1:A:289:ASP:N	1:A:291:TRP:HZ3	1.98	0.58
1:C:100:TRP:CZ3	1:C:169:ARG:HD3	2.38	0.58
1:C:72:ILE:HD11	1:C:83:LEU:HD22	1.86	0.58
1:A:46:TYR:CE2	2:E:1163:PTR:HD2	2.39	0.58
1:C:192:LEU:HD22	1:C:291:TRP:CH2	2.39	0.58
1:C:139:ASN:CG	1:C:164:THR:HG23	2.29	0.57
3:A:402:TRS:O1	3:A:402:TRS:O2	2.09	0.57
1:A:282:MET:HE2	1:A:282:MET:CA	2.26	0.57
1:C:74:MET:HE1	1:C:253:MET:HG2	1.87	0.57
1:C:280:PHE:CD2	1:C:281:ILE:HD13	2.39	0.57
1:C:246:ILE:HD13	1:C:246:ILE:N	2.15	0.57
1:A:179:TRP:CE2	1:A:185:PRO:HD3	2.40	0.57
1:A:185:PRO:HD2	1:A:269:PHE:CD1	2.40	0.57
1:C:81:TYR:HE2	1:C:226:CYS:HB3	1.68	0.57
1:B:114:MET:CE	1:B:118:SER:C	2.79	0.56
1:C:23:ILE:CD1	1:C:250:LEU:HD23	2.35	0.56
1:B:22:ASP:O	1:B:26:GLU:HG3	2.05	0.56
1:C:169:ARG:HG3	1:C:169:ARG:HH11	1.70	0.56
1:A:20:TYR:O	1:A:24:ARG:HG3	2.06	0.56
1:C:19:ILE:HG22	1:C:267:LEU:HD21	1.88	0.56
1:C:23:ILE:HD12	1:C:250:LEU:HD23	1.87	0.56
1:A:49:VAL:CG2	1:A:219:ILE:HD13	2.35	0.56
1:B:40:ASN:O	1:B:44:ASN:ND2	2.36	0.56
1:A:45:ARG:NE	1:A:120:LYS:O	2.38	0.56
1:A:238:ARG:NH1	1:A:244:VAL:HA	2.20	0.56
1:C:152:TYR:HE2	1:C:153:TYR:CD2	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:HIS:H	1:C:101:GLU:CD	2.14	0.56
1:C:84:THR:O	1:C:214:HIS:HB2	2.06	0.56
1:C:283:GLY:O	1:C:285:SER:N	2.35	0.56
1:A:89:PRO:HD3	4:A:508:HOH:O	2.06	0.56
1:A:253:MET:HB2	1:A:260:LEU:HD12	1.86	0.56
1:B:269:PHE:HE2	1:B:273:ALA:HB2	1.68	0.56
1:C:160:LEU:HD13	1:C:171:ILE:CD1	2.36	0.56
1:A:7:PHE:CE2	1:A:16:TRP:CZ2	2.94	0.55
1:A:46:TYR:HE2	1:A:217:ALA:HB2	1.72	0.55
1:C:108:VAL:CG1	1:C:213:VAL:HA	2.31	0.55
1:A:8:GLU:O	1:A:12:LYS:N	2.33	0.55
1:C:98:MET:O	1:C:102:GLN:HG2	2.07	0.55
1:B:45:ARG:HH12	1:B:88:LEU:HD23	1.71	0.55
1:C:4:GLU:HG3	1:C:275:ILE:CG2	2.35	0.55
1:C:50:SER:O	1:C:258:MET:HE3	2.07	0.55
1:B:147:GLU:HB2	1:B:156:ARG:HG2	1.89	0.55
1:B:257:ARG:HH11	1:B:257:ARG:HG3	1.70	0.55
1:C:56:ARG:HA	1:C:69:ALA:O	2.06	0.55
1:C:188:PRO:O	1:C:192:LEU:HD12	2.06	0.55
1:A:64:ASN:OD1	1:A:65:ASP:N	2.40	0.55
1:C:198:VAL:HG11	1:C:225:PHE:HZ	1.70	0.54
1:A:290:GLN:O	1:A:294:LEU:HD13	2.07	0.54
1:A:120:LYS:HD2	1:A:120:LYS:N	2.22	0.54
1:A:114:MET:CE	1:A:119:LEU:HD23	2.36	0.54
1:B:50:SER:H	1:B:258:MET:HE3	1.72	0.54
1:A:45:ARG:NH2	1:A:121:CYS:HA	2.23	0.54
1:C:40:ASN:HB3	1:C:66:TYR:HD2	1.73	0.54
1:B:126:PRO:HD3	1:B:133:MET:HG3	1.88	0.54
1:A:162:ASN:OD1	1:A:164:THR:OG1	2.10	0.54
1:C:139:ASN:ND2	1:C:164:THR:HG23	2.23	0.53
1:A:64:ASN:OD1	1:A:66:TYR:N	2.32	0.53
1:C:17:ALA:HA	1:C:264:ALA:CB	2.37	0.53
1:C:102:GLN:O	1:C:209:GLY:HA3	2.08	0.53
1:C:138:THR:O	1:C:138:THR:HG22	2.08	0.53
1:B:49:VAL:CG2	1:B:219:ILE:HD13	2.37	0.53
1:B:67:ILE:HD13	1:B:98:MET:SD	2.49	0.53
1:C:23:ILE:CD1	1:C:250:LEU:CD2	2.86	0.53
1:C:195:LEU:O	1:C:199:ARG:N	2.36	0.53
1:B:20:TYR:CE2	1:B:24:ARG:HD2	2.44	0.53
1:A:100:TRP:CD2	1:A:169:ARG:NH1	2.77	0.53
1:C:270:SER:O	1:C:274:VAL:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:GLU:O	1:A:7:PHE:HB3	2.09	0.53
1:C:69:ALA:CA	1:C:84:THR:HG22	2.33	0.53
1:C:247:LYS:H	1:C:247:LYS:HD2	1.74	0.53
1:A:152:TYR:OH	1:A:295:SER:HB2	2.09	0.53
1:A:45:ARG:HG2	1:A:46:TYR:CE1	2.43	0.52
1:B:221:ARG:HD3	2:F:1163:PTR:O1P	2.10	0.52
1:C:152:TYR:HE2	1:C:153:TYR:HD2	1.50	0.52
1:C:153:TYR:CE1	1:C:155:VAL:HG23	2.44	0.52
1:B:114:MET:HE1	1:B:119:LEU:N	2.25	0.52
1:B:165:THR:OG1	1:B:167:GLU:CG	2.57	0.52
1:C:220:GLY:O	1:C:224:THR:HG23	2.10	0.52
1:C:95:PHE:HE2	1:C:96:TRP:CZ3	2.28	0.52
1:B:119:LEU:HD12	1:B:119:LEU:O	2.10	0.51
1:A:161:GLU:HG3	1:A:168:THR:HG22	1.92	0.51
1:A:120:LYS:HB3	1:A:216:SER:OG	2.11	0.51
1:A:156:ARG:HH12	1:A:175:HIS:HB2	1.75	0.51
1:B:158:LEU:CD1	1:B:173:HIS:HB2	2.40	0.51
1:B:249:VAL:O	1:B:253:MET:HG3	2.10	0.51
1:B:285:SER:OG	1:C:29:ASP:O	2.28	0.51
1:C:81:TYR:CD2	1:C:226:CYS:SG	3.04	0.51
1:C:199:ARG:HH21	1:C:233:LEU:HD13	1.76	0.51
1:A:172:LEU:CD1	1:A:201:SER:HB2	2.40	0.51
1:B:64:ASN:OD1	1:B:65:ASP:N	2.44	0.51
1:B:100:TRP:CE3	1:B:169:ARG:NH1	2.79	0.51
1:B:269:PHE:C	1:B:269:PHE:CD2	2.89	0.51
1:B:189:ALA:HA	1:B:291:TRP:CE3	2.46	0.50
1:C:139:ASN:HD21	1:C:164:THR:HG23	1.75	0.50
1:B:114:MET:CE	1:B:119:LEU:CA	2.89	0.50
1:C:96:TRP:CD1	1:C:135:PHE:CZ	2.99	0.50
1:C:54:HIS:O	3:C:401:TRS:H11	2.12	0.50
1:A:111:ASN:ND2	1:A:121:CYS:HB2	2.25	0.50
1:B:192:LEU:O	1:B:196:PHE:HD2	1.94	0.50
1:C:96:TRP:HD1	1:C:135:PHE:CZ	2.30	0.50
1:C:191:PHE:CB	1:C:269:PHE:HZ	2.24	0.50
1:A:184:VAL:HB	1:A:269:PHE:HD1	1.77	0.50
1:B:239:LYS:HA	1:C:38:PRO:HG2	1.93	0.50
1:C:134:ILE:HG13	1:C:141:LYS:CA	2.30	0.50
1:C:257:ARG:HB3	1:C:260:LEU:HD21	1.94	0.49
1:B:97:GLU:CG	1:B:101:GLU:OE2	2.60	0.49
1:B:174:PHE:CD1	1:B:198:VAL:HG22	2.47	0.49
1:C:61:GLN:CB	1:C:97:GLU:OE2	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:VAL:CG1	1:C:213:VAL:HG13	2.40	0.49
1:C:79:ARG:HG2	1:C:81:TYR:HE1	1.76	0.49
1:A:8:GLU:O	1:A:11:ASP:N	2.46	0.49
1:A:253:MET:CB	1:A:260:LEU:HD12	2.43	0.49
1:B:20:TYR:HB2	1:B:267:LEU:CD2	2.42	0.49
1:B:100:TRP:CZ2	1:B:162:ASN:HB2	2.47	0.49
1:B:121:CYS:SG	1:B:122:ALA:N	2.85	0.49
1:C:69:ALA:CB	1:C:98:MET:HE1	2.39	0.49
1:A:77:ALA:O	1:A:78:GLN:HB2	2.13	0.49
1:C:82:ILE:O	1:C:212:VAL:HA	2.13	0.49
1:C:152:TYR:CE2	1:C:153:TYR:CD2	2.96	0.49
1:C:283:GLY:C	1:C:285:SER:H	2.17	0.49
1:B:34:VAL:O	1:B:37:LEU:HG	2.12	0.49
1:C:168:THR:HA	1:C:169:ARG:HH12	1.78	0.49
1:B:105:ARG:HG3	1:B:105:ARG:HH11	1.78	0.48
1:C:137:ASP:OD1	1:C:137:ASP:N	2.44	0.48
1:A:235:MET:HB3	1:A:241:PRO:HB3	1.96	0.48
1:C:172:LEU:N	1:C:172:LEU:CD2	2.76	0.48
1:B:276:GLU:O	1:B:279:LYS:HB2	2.14	0.48
1:C:179:TRP:CE2	1:C:221:ARG:HG2	2.48	0.48
1:C:106:GLY:C	1:C:211:VAL:HG23	2.37	0.48
1:C:49:VAL:HG21	1:C:217:ALA:HB1	1.96	0.48
1:C:204:LEU:HD21	1:C:211:VAL:HG11	1.96	0.48
1:C:280:PHE:CE2	1:C:281:ILE:HD13	2.49	0.48
1:C:57:ILE:HG21	1:C:98:MET:HE3	1.95	0.48
1:A:46:TYR:CD2	1:A:217:ALA:HB2	2.49	0.48
1:A:74:MET:HE2	1:A:230:THR:HG21	1.95	0.48
1:C:96:TRP:CE2	1:C:142:LEU:CD2	2.97	0.48
1:A:235:MET:O	1:A:241:PRO:HG3	2.14	0.47
1:C:204:LEU:CD2	1:C:211:VAL:HG11	2.43	0.47
1:A:150:LYS:HG2	1:A:297:GLU:HB3	1.96	0.47
1:B:100:TRP:CD2	1:B:169:ARG:NH1	2.79	0.47
1:C:195:LEU:O	1:C:198:VAL:HB	2.14	0.47
1:B:98:MET:O	1:B:102:GLN:HG2	2.14	0.47
1:C:246:ILE:HG12	1:C:247:LYS:HD2	1.94	0.47
1:A:49:VAL:HG21	1:A:219:ILE:HD13	1.96	0.47
1:B:158:LEU:HD12	1:B:173:HIS:HB2	1.97	0.47
1:B:178:THR:O	1:B:180:PRO:HD3	2.15	0.47
1:C:50:SER:H	1:C:258:MET:HE3	1.79	0.47
1:C:57:ILE:HB	1:C:69:ALA:HB3	1.97	0.47
1:C:110:LEU:HD13	1:C:179:TRP:CE3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:VAL:HG22	1:A:219:ILE:HD13	1.96	0.47
1:A:3:MET:N	1:A:4:GLU:OE1	2.48	0.47
1:A:97:GLU:CG	1:A:101:GLU:OE2	2.63	0.47
1:B:34:VAL:HA	1:B:37:LEU:HG	1.96	0.47
1:B:152:TYR:N	1:B:152:TYR:CD2	2.79	0.47
1:B:59:LEU:HD12	1:B:61:GLN:OE1	2.15	0.47
1:B:294:LEU:HD12	1:B:294:LEU:N	2.28	0.47
1:C:108:VAL:HG12	1:C:212:VAL:O	2.15	0.47
1:B:49:VAL:HG22	1:B:219:ILE:HD13	1.97	0.46
1:A:182:PHE:HZ	2:E:1163:PTR:O	1.97	0.46
1:A:185:PRO:HB2	1:A:269:PHE:HE1	1.80	0.46
1:C:160:LEU:CD1	1:C:171:ILE:HD11	2.45	0.46
1:A:269:PHE:HD2	1:A:269:PHE:O	1.97	0.46
1:C:11:ASP:CB	1:C:16:TRP:HE1	2.28	0.46
1:A:45:ARG:HG3	1:A:45:ARG:NH1	2.30	0.46
1:A:278:ALA:O	1:A:282:MET:HG2	2.14	0.46
1:B:17:ALA:O	1:B:21:GLN:HB2	2.15	0.46
1:B:97:GLU:OE2	1:B:101:GLU:OE2	2.34	0.46
1:B:114:MET:HE3	1:B:119:LEU:HA	1.96	0.46
1:C:171:ILE:C	1:C:172:LEU:HD22	2.40	0.46
1:C:260:LEU:O	1:C:261:ILE:HB	2.16	0.46
1:A:298:ASP:OD1	1:A:298:ASP:N	2.49	0.46
1:B:21:GLN:HA	1:B:21:GLN:OE1	2.16	0.46
1:C:57:ILE:HD11	1:C:71:LEU:CB	2.46	0.46
1:C:198:VAL:HG11	1:C:225:PHE:CZ	2.49	0.46
1:A:170:GLU:C	1:A:171:ILE:HD13	2.41	0.46
1:B:45:ARG:NH1	1:B:86:GLY:O	2.49	0.46
1:B:57:ILE:HG21	1:B:98:MET:HG3	1.98	0.46
1:B:83:LEU:HD11	1:B:226:CYS:SG	2.55	0.46
1:B:72:ILE:HD12	1:B:72:ILE:H	1.79	0.46
1:B:275:ILE:HG22	1:B:276:GLU:N	2.31	0.46
1:C:108:VAL:HG13	1:C:213:VAL:CA	2.37	0.46
1:C:160:LEU:HD23	1:C:169:ARG:O	2.16	0.46
1:A:185:PRO:CD	1:A:269:PHE:CE1	2.99	0.45
1:C:152:TYR:CD2	1:C:153:TYR:HD2	2.34	0.45
1:A:28:SER:CB	1:A:30:PHE:CE2	3.00	0.45
1:A:165:THR:O	1:A:166:GLN:HB2	2.15	0.45
1:C:60:HIS:CG	1:C:101:GLU:HG2	2.51	0.45
1:A:192:LEU:HD21	1:A:277:GLY:HA3	1.98	0.45
1:A:288:GLN:O	1:A:289:ASP:CB	2.65	0.45
1:B:111:ASN:O	1:B:175:HIS:NE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:ASN:OD1	1:B:164:THR:OG1	2.17	0.45
1:C:132:GLU:O	1:C:132:GLU:HG3	2.15	0.45
1:B:2:GLU:C	1:B:4:GLU:H	2.23	0.45
1:A:72:ILE:N	1:A:72:ILE:HD12	2.32	0.45
1:B:114:MET:CE	1:B:119:LEU:N	2.80	0.45
1:C:11:ASP:HA	1:C:16:TRP:NE1	2.31	0.45
1:C:139:ASN:HD21	1:C:164:THR:CG2	2.30	0.45
1:C:221:ARG:HB2	2:G:1163:PTR:O2P	2.17	0.45
1:A:7:PHE:CE2	1:A:16:TRP:HZ2	2.33	0.45
1:A:174:PHE:CD1	1:A:198:VAL:HG22	2.51	0.45
1:C:74:MET:CE	1:C:253:MET:HG2	2.46	0.45
1:A:95:PHE:O	1:A:99:VAL:HG23	2.17	0.45
1:A:184:VAL:HB	1:A:269:PHE:CD1	2.52	0.45
1:A:270:SER:O	1:A:274:VAL:HG23	2.16	0.45
1:B:125:TRP:HE1	1:B:156:ARG:NE	2.15	0.45
1:A:121:CYS:SG	1:A:122:ALA:N	2.90	0.44
1:A:185:PRO:CD	1:A:269:PHE:HE1	2.30	0.44
1:C:216:SER:HB2	1:C:221:ARG:HH22	1.82	0.44
1:C:254:ARG:HH11	1:C:261:ILE:HB	1.81	0.44
1:C:277:GLY:HA2	1:C:291:TRP:CH2	2.43	0.44
1:A:148:ASP:OD1	1:A:150:LYS:HD2	2.17	0.44
1:C:153:TYR:CE1	1:C:155:VAL:CG2	3.00	0.44
1:A:88:LEU:HB3	1:A:89:PRO:HD2	2.00	0.44
1:A:290:GLN:O	1:A:294:LEU:CD1	2.66	0.44
1:B:175:HIS:HE1	4:B:408:HOH:O	2.01	0.44
1:A:156:ARG:HB2	1:A:173:HIS:HB3	1.99	0.44
1:A:269:PHE:C	1:A:269:PHE:CD2	2.94	0.44
1:B:76:GLU:OE1	1:B:238:ARG:NH1	2.51	0.44
1:C:23:ILE:HD11	1:C:250:LEU:CG	2.45	0.44
1:C:280:PHE:CD2	1:C:280:PHE:C	2.95	0.44
1:A:105:ARG:HD3	1:A:105:ARG:O	2.18	0.44
1:B:73:LYS:HG3	1:B:80:SER:OG	2.18	0.44
1:B:100:TRP:HZ2	1:B:167:GLU:CD	2.25	0.44
1:C:153:TYR:CD1	1:C:155:VAL:HG23	2.53	0.44
1:B:188:PRO:C	1:B:192:LEU:HD12	2.42	0.43
1:B:221:ARG:N	2:F:1163:PTR:O1P	2.42	0.43
1:C:82:ILE:HG21	1:C:98:MET:CE	2.43	0.43
1:C:125:TRP:CZ2	1:C:156:ARG:NH2	2.85	0.43
1:C:246:ILE:HG13	1:C:271:TYR:CE2	2.53	0.43
1:B:39:LYS:HE2	1:B:64:ASN:ND2	2.33	0.43
1:B:116:LYS:HA	4:B:404:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:ARG:HA	1:C:175:HIS:HE2	1.83	0.43
1:C:160:LEU:HD21	1:C:169:ARG:HB2	1.99	0.43
1:A:46:TYR:CE2	2:E:1163:PTR:CD2	3.01	0.43
1:B:269:PHE:C	1:B:269:PHE:HD2	2.26	0.43
1:C:176:TYR:HD1	1:C:194:PHE:CD1	2.36	0.43
1:A:185:PRO:CB	1:A:269:PHE:HE1	2.31	0.43
1:B:84:THR:O	1:B:214:HIS:HB2	2.18	0.43
1:B:102:GLN:O	1:B:209:GLY:HA3	2.19	0.43
1:C:153:TYR:HA	1:C:175:HIS:O	2.18	0.43
3:A:401:TRS:O3	3:A:401:TRS:O1	2.10	0.43
1:B:45:ARG:NH2	1:B:121:CYS:HA	2.34	0.43
1:B:125:TRP:HE1	1:B:156:ARG:CD	2.31	0.43
1:B:133:MET:HE2	1:B:133:MET:HB3	1.74	0.43
1:C:245:ASP:OD1	1:C:247:LYS:N	2.52	0.43
1:C:283:GLY:C	1:C:285:SER:N	2.77	0.43
1:A:266:GLN:O	1:A:270:SER:OG	2.34	0.43
1:B:170:GLU:C	1:B:171:ILE:HD13	2.43	0.43
1:C:82:ILE:HG13	1:C:210:PRO:HB2	2.01	0.43
1:C:108:VAL:CG1	1:C:213:VAL:CG2	2.91	0.43
1:C:140:LEU:HD23	1:C:141:LYS:C	2.43	0.43
1:A:77:ALA:O	1:A:78:GLN:CB	2.67	0.43
1:C:246:ILE:HG12	1:C:247:LYS:N	2.33	0.43
1:B:257:ARG:HG3	1:B:257:ARG:NH1	2.33	0.42
1:C:81:TYR:CD1	1:C:81:TYR:N	2.87	0.42
1:C:168:THR:HA	1:C:169:ARG:NH1	2.34	0.42
1:A:260:LEU:O	1:A:261:ILE:HB	2.19	0.42
1:A:294:LEU:HD12	1:A:294:LEU:N	2.34	0.42
1:B:76:GLU:CD	1:B:238:ARG:HH11	2.23	0.42
1:B:105:ARG:HG3	1:B:105:ARG:NH1	2.34	0.42
1:B:294:LEU:HD12	1:B:294:LEU:H	1.84	0.42
1:C:257:ARG:HG3	1:C:257:ARG:HH11	1.84	0.42
1:A:72:ILE:HG13	1:A:256:PHE:HB2	2.00	0.42
1:B:180:PRO:O	1:B:183:GLY:N	2.47	0.42
1:C:196:PHE:HA	1:C:199:ARG:HB2	2.01	0.42
1:C:245:ASP:OD1	1:C:245:ASP:C	2.63	0.42
1:C:44:ASN:ND2	1:C:66:TYR:HE2	2.18	0.42
1:C:280:PHE:HD2	1:C:281:ILE:HD13	1.81	0.42
1:B:79:ARG:NH1	1:B:233:LEU:HD22	2.34	0.42
1:B:153:TYR:HA	1:B:175:HIS:O	2.19	0.42
1:C:152:TYR:CA	1:C:178:THR:HG23	2.45	0.42
1:A:238:ARG:HH11	1:A:244:VAL:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:TRP:HB3	1:C:140:LEU:HD13	2.01	0.42
1:C:111:ASN:CB	1:C:115:GLU:OE2	2.67	0.42
1:A:162:ASN:OD1	1:A:164:THR:N	2.50	0.42
1:A:169:ARG:HD3	4:A:509:HOH:O	2.19	0.42
1:C:19:ILE:CG2	1:C:267:LEU:HD21	2.50	0.42
1:C:153:TYR:HE1	1:C:155:VAL:CG2	2.33	0.42
1:C:219:ILE:HG13	1:C:220:GLY:N	2.34	0.42
1:C:250:LEU:HD22	1:C:261:ILE:HG13	2.00	0.42
1:A:179:TRP:CD1	1:A:179:TRP:C	2.98	0.41
1:A:286:SER:O	1:A:287:VAL:CG1	2.65	0.41
1:C:19:ILE:O	1:C:23:ILE:HG22	2.20	0.41
1:C:57:ILE:CG1	1:C:98:MET:HE3	2.32	0.41
1:A:28:SER:CB	1:A:30:PHE:HE2	2.34	0.41
1:B:134:ILE:HG12	1:B:141:LYS:HB2	2.01	0.41
1:C:11:ASP:HA	1:C:16:TRP:HE1	1.85	0.41
1:C:160:LEU:HG	1:C:169:ARG:CZ	2.49	0.41
1:C:240:ASP:OD1	1:C:241:PRO:HD2	2.19	0.41
1:B:49:VAL:HG21	1:B:219:ILE:HD13	2.01	0.41
1:B:76:GLU:OE2	1:B:238:ARG:NH1	2.40	0.41
1:B:192:LEU:O	1:B:196:PHE:CD2	2.72	0.41
1:A:7:PHE:HE2	1:A:16:TRP:CZ2	2.39	0.41
1:A:100:TRP:CE3	1:A:169:ARG:NH1	2.88	0.41
1:A:33:ARG:N	1:A:53:ASP:OD2	2.45	0.41
1:A:253:MET:C	1:A:255:LYS:N	2.78	0.41
1:A:289:ASP:N	1:A:291:TRP:CZ3	2.84	0.41
1:C:96:TRP:CZ2	1:C:142:LEU:HD21	2.55	0.41
1:A:172:LEU:HD12	1:A:201:SER:HB2	2.02	0.41
1:B:72:ILE:N	1:B:72:ILE:CD1	2.84	0.41
1:B:72:ILE:HD13	1:B:83:LEU:HD13	2.03	0.41
1:B:76:GLU:OE2	1:B:238:ARG:HD3	2.21	0.41
1:B:134:ILE:HD11	1:B:141:LYS:HD3	2.02	0.41
1:C:55:SER:OG	1:C:71:LEU:O	2.36	0.41
1:C:50:SER:HB3	1:C:258:MET:CE	2.51	0.41
1:B:137:ASP:OD1	1:B:137:ASP:N	2.55	0.40
1:B:179:TRP:CD1	1:B:221:ARG:HG2	2.56	0.40
1:C:77:ALA:HB2	1:C:234:LEU:HD21	2.03	0.40
1:A:156:ARG:HH12	1:A:175:HIS:CB	2.33	0.40
1:B:76:GLU:CD	1:B:238:ARG:NH1	2.79	0.40
1:B:199:ARG:HG2	1:B:204:LEU:HD12	2.02	0.40
1:C:294:LEU:O	1:C:294:LEU:HG	2.22	0.40
1:B:40:ASN:HB3	1:B:66:TYR:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:GLU:OE1	1:B:130:GLU:N	2.55	0.40
1:B:140:LEU:HD23	1:B:162:ASN:HA	2.03	0.40
1:B:2:GLU:HG2	1:B:2:GLU:O	2.20	0.40
1:B:171:ILE:HD13	1:B:171:ILE:N	2.36	0.40
1:B:32:CYS:O	1:B:36:LYS:HG2	2.22	0.40
1:C:108:VAL:HG13	1:C:213:VAL:CG1	2.48	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	294/321 (92%)	274 (93%)	17 (6%)	3 (1%)	12	41
1	B	292/321 (91%)	274 (94%)	17 (6%)	1 (0%)	36	67
1	C	289/321 (90%)	273 (94%)	12 (4%)	4 (1%)	9	34
2	E	3/16 (19%)	3 (100%)	0	0	100	100
2	F	5/16 (31%)	3 (60%)	1 (20%)	1 (20%)	0	0
2	G	1/16 (6%)	1 (100%)	0	0	100	100
All	All	884/1011 (87%)	828 (94%)	47 (5%)	9 (1%)	12	41

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	5	LYS
1	A	285	SER
1	A	287	VAL
1	B	261	ILE
1	C	283	GLY
1	C	284	ASP

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Mol	Chain	Res	Type
1	A	261	ILE
1	C	261	ILE
2	F	1165	VAL

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	232/291 (80%)	218 (94%)	14 (6%)	17	47
1	B	240/291 (82%)	224 (93%)	16 (7%)	15	43
1	C	213/291 (73%)	196 (92%)	17 (8%)	11	37
2	E	1/14 (7%)	1 (100%)	0	100	100
2	F	2/14 (14%)	2 (100%)	0	100	100
2	G	1/14 (7%)	1 (100%)	0	100	100
All	All	689/915 (75%)	642 (93%)	47 (7%)	14	42

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	21	GLN
1	A	50	SER
1	A	72	ILE
1	A	81	TYR
1	A	105	ARG
1	A	109	MET
1	A	114	MET
1	A	119	LEU
1	A	177	THR
1	A	190	SER
1	A	236	ASP
1	A	270	SER
1	A	291	TRP
1	B	39	LYS

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Mol	Chain	Res	Type
1	B	41	LYS
1	B	72	ILE
1	B	104	SER
1	B	114	MET
1	B	119	LEU
1	B	133	MET
1	B	152	TYR
1	B	159	GLU
1	B	164	THR
1	B	221	ARG
1	B	238	ARG
1	B	248	LYS
1	B	269	PHE
1	B	272	LEU
1	B	275	ILE
1	C	4	GLU
1	C	34	VAL
1	C	56	ARG
1	C	59	LEU
1	C	67	ILE
1	C	81	TYR
1	C	100	TRP
1	C	152	TYR
1	C	168	THR
1	C	172	LEU
1	C	221	ARG
1	C	233	LEU
1	C	238	ARG
1	C	246	ILE
1	C	272	LEU
1	C	287	VAL
1	C	294	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	B	61	GLN
1	B	111	ASN
1	B	139	ASN
1	B	157	GLN
1	C	78	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	PTR	G	1163	2	15,16,17	1.30	2 (13%)	17,22,24	0.81	1 (5%)
2	PTR	F	1163	2	15,16,17	1.51	1 (6%)	17,22,24	0.83	1 (5%)
2	PTR	E	1163	2	15,16,17	1.17	1 (6%)	17,22,24	0.54	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	PTR	G	1163	2	-	0/10/11/13	0/1/1/1
2	PTR	F	1163	2	-	1/10/11/13	0/1/1/1
2	PTR	E	1163	2	-	0/10/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1163	PTR	OH-CZ	-4.29	1.31	1.40
2	E	1163	PTR	OH-CZ	-4.18	1.31	1.40
2	G	1163	PTR	OH-CZ	-3.84	1.32	1.40
2	G	1163	PTR	P-OH	2.48	1.64	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1163	PTR	O3P-P-O2P	2.24	116.21	107.80
2	G	1163	PTR	O2P-P-O1P	-2.01	103.00	110.83

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1163	PTR	CZ-OH-P-O2P

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1163	PTR	1	0
2	F	1163	PTR	2	0
2	E	1163	PTR	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
3	TRS	C	401	-	7,7,7	1.79	2 (28%)	9,9,9	2.55	4 (44%)
3	TRS	A	402	-	7,7,7	2.33	2 (28%)	9,9,9	3.33	5 (55%)
3	TRS	A	401	-	7,7,7	2.16	1 (14%)	9,9,9	3.26	4 (44%)

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
3	TRS	C	401	-	-	9/9/9/9	-
3	TRS	A	402	-	-	7/9/9/9	-
3	TRS	A	401	-	-	7/9/9/9	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	TRS	C-N	4.92	1.65	1.49
3	A	401	TRS	C-N	4.71	1.64	1.49
3	C	401	TRS	C-N	3.80	1.61	1.49
3	A	402	TRS	C2-C	2.43	1.59	1.53
3	C	401	TRS	C3-C	2.24	1.59	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	TRS	C2-C-N	6.63	125.08	108.17
3	A	401	TRS	C3-C-N	5.87	123.15	108.17
3	A	401	TRS	C3-C-C1	-4.89	97.64	110.66
3	C	401	TRS	C3-C-N	4.85	120.55	108.17
3	A	402	TRS	C2-C-C1	-4.73	98.05	110.66
3	A	401	TRS	C2-C-N	4.20	118.89	108.17
3	A	402	TRS	C3-C-C1	-4.02	99.96	110.66
3	A	401	TRS	C3-C-C2	-3.84	100.44	110.66
3	A	402	TRS	C3-C-N	3.31	116.61	108.17
3	C	401	TRS	C2-C-C1	-3.17	102.22	110.66
3	C	401	TRS	C2-C-N	3.03	115.89	108.17
3	C	401	TRS	O3-C3-C	2.56	118.02	110.88
3	A	402	TRS	C3-C-C2	-2.49	104.02	110.66

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	TRS	C3-C-C2-O2
3	A	401	TRS	N-C-C2-O2
3	A	402	TRS	C1-C-C2-O2
3	A	402	TRS	C1-C-C3-O3
3	A	402	TRS	C2-C-C3-O3

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Mol	Chain	Res	Type	Atoms
3	A	402	TRS	N-C-C3-O3
3	C	401	TRS	N-C-C1-O1
3	C	401	TRS	C1-C-C2-O2
3	C	401	TRS	N-C-C2-O2
3	C	401	TRS	C1-C-C3-O3
3	C	401	TRS	C2-C-C3-O3
3	C	401	TRS	N-C-C3-O3
3	A	401	TRS	C2-C-C1-O1
3	A	401	TRS	C1-C-C2-O2
3	A	401	TRS	C1-C-C3-O3
3	C	401	TRS	C2-C-C1-O1
3	A	401	TRS	N-C-C1-O1
3	A	401	TRS	N-C-C3-O3
3	A	402	TRS	N-C-C1-O1
3	A	402	TRS	N-C-C2-O2
3	C	401	TRS	C3-C-C1-O1
3	C	401	TRS	C3-C-C2-O2
3	A	402	TRS	C3-C-C1-O1

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	TRS	2	0
3	A	402	TRS	2	0
3	A	401	TRS	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	296/321 (92%)	-0.83	0 100 100	44, 66, 114, 128	0
1	B	296/321 (92%)	-0.85	0 100 100	45, 65, 113, 124	0
1	C	293/321 (91%)	-0.54	0 100 100	80, 111, 157, 172	0
2	E	5/16 (31%)	-0.62	0 100 100	76, 79, 85, 99	0
2	F	7/16 (43%)	-0.83	0 100 100	80, 87, 99, 100	0
2	G	2/16 (12%)	0.36	0 100 100	103, 103, 103, 109	0
All	All	899/1011 (88%)	-0.74	0 100 100	44, 80, 135, 172	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	PTR	E	1163	16/17	0.98	0.07	55,58,73,73	0
2	PTR	F	1163	16/17	0.98	0.06	54,59,73,73	0
2	PTR	G	1163	16/17	0.99	0.05	110,114,121,124	0

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($\text{\AA}^2$)	Q<0.9
3	TRS	A	401	8/8	0.97	0.10	71,101,121,121	0
3	TRS	A	402	8/8	0.97	0.07	66,88,106,106	0
3	TRS	C	401	8/8	0.97	0.06	92,116,129,129	0

6.5 Other polymers [i](#)

There are no such residues in this entry.