



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2017 – 08:34 PM EDT

PDB ID : 2GBI
Title : rat DPP-IV with xanthine inhibitor 4
Authors : Longenecker, K.L.; Jakob, C.G.; Fry, E.H.; Wilk, S.
Deposited on : unknown
Resolution : 3.30 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

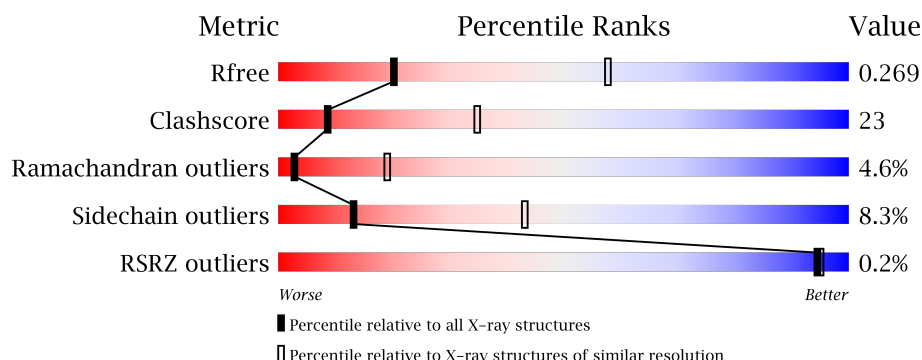
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	100719	1034 (3.36-3.24)
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	730	
1	B	730	

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	XIH	A	901	-	-	-	X

2 Entry composition [i](#)

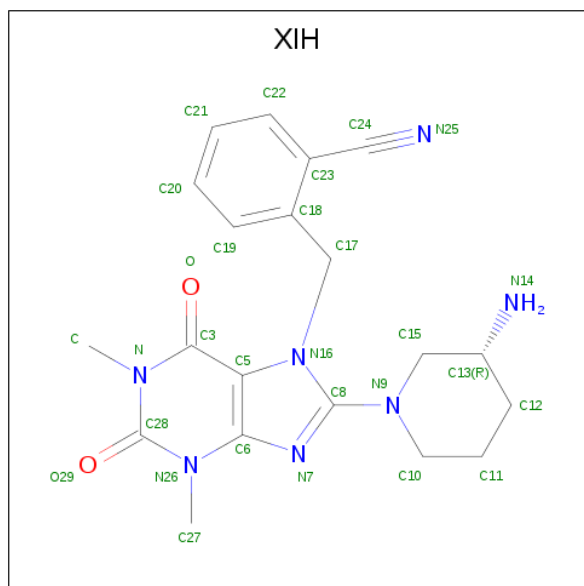
There are 2 unique types of molecules in this entry. The entry contains 11869 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	730	Total	C	N	O	S	0	0	0
			5920	3789	981	1124	26			
1	B	730	Total	C	N	O	S	0	0	0
			5920	3789	981	1124	26			

- Molecule 2 is 2-({8-[(3R)-3-AMINOPIPERIDIN-1-YL]-1,3-DIMETHYL-2,6-DIOXO-1,2,3,6-TETRAHYDRO-7H-PURIN-7-YL}METHYL)BENZONITRILE (three-letter code: XIH) (formula: C₂₀H₂₃N₇O₂).

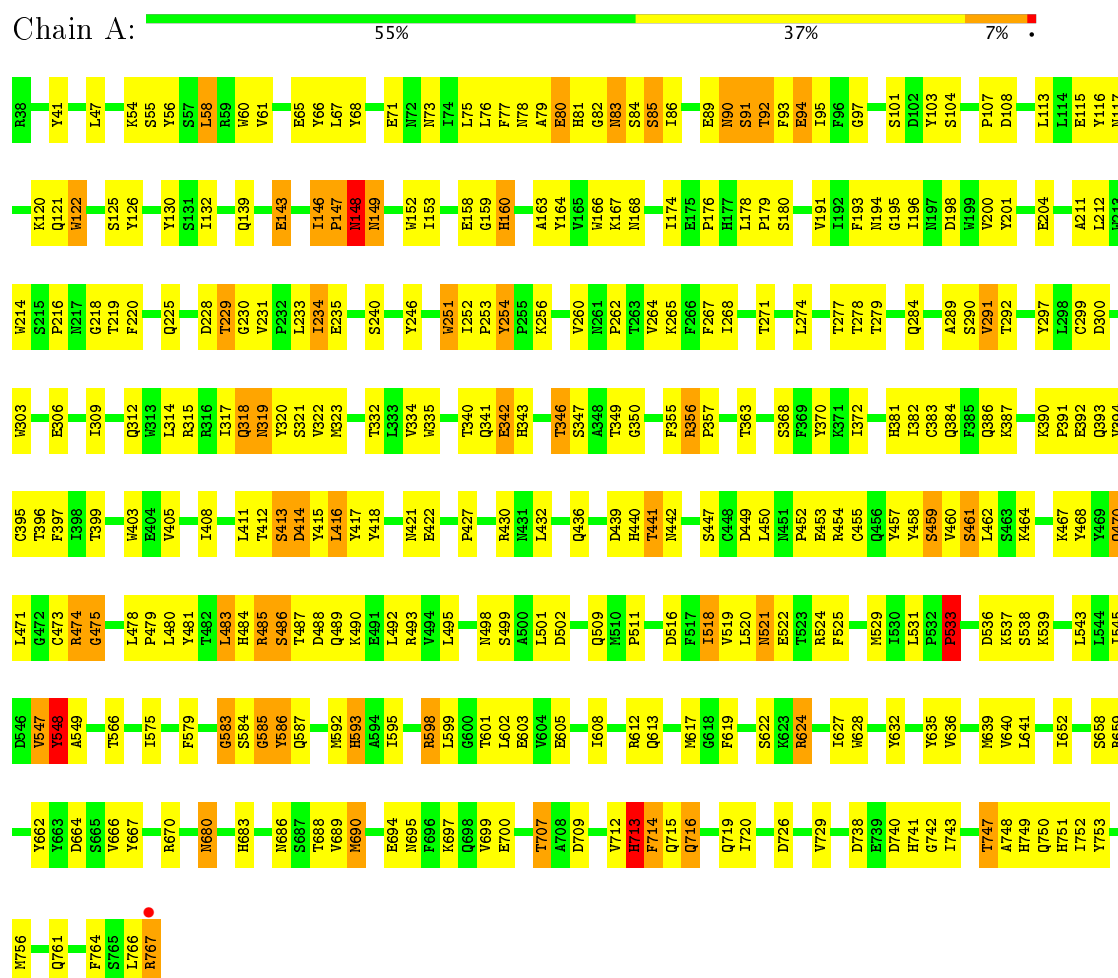


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			29	20	7	2		

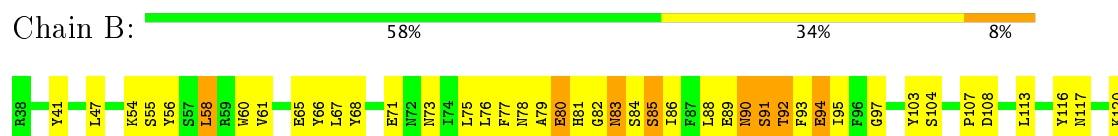
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Dipeptidyl peptidase 4



• Molecule 1: Dipeptidyl peptidase 4



T707	I595	K490	Y418	Q318	F220	Q121
A708	R598	E491	M421	R319	Q225	M122
D709	L599	L492	E422	Y320		S125
H713	G600	R493	Y423	S321	D228	Y126
F714	T601	V494	V424	V322	T229	
Q715	L602	L495	K424	M323	G230	I132
Q716	E603	M498	P427	T332	V231	
		L501	R430	L333	P232	Q139
Q719	R612	Q509	M431	V334	L233	
I720	F619	M510	L432	M335	I234	E143
V725	S622	P511	Q436	T339	E235	
D726	R623	D516	D439	T340	M251	I146
V729	R624	F517	H440	Q341	I252	P147
		I518	T441	E342	P253	M148
D738	I627	V519	M442	R343	Y254	M149
F739	M628	L520	K443	T346	P255	
H740	Y632	M521	S447	S347	K256	Y152
I741	Y635	E522	T349	A348	A257	I153
G742	I743	T523	C448	G350	V260	E158
I743	V636	R524	D449	G350	G159	H160
A744		F525	L450	F355	P262	
S745		F525	L450	R356	T263	A163
S746	M639	M529	M451	P357	V264	Y164
I747	V640	I530	P452		K265	V165
A748	L641	L531	E453	I372	F266	W166
H749		P453	R454		I268	
Q750	I652	P453	C455	H381	Y171	
Q751	H511	P453	D456	I382		
I752	S658	D536	Y457	I382	T271	I174
Y753	R659	R537	Y458	C383	E175	
		S538	S459		P176	
M756	Y662	K539	V460	Q386	H177	
	D664	L543	S461	K387	T277	L178
Q761	S665	L544	L462	K390	T278	P179
F764	V666	I545	S463	P391	T279	S180
S765	R670	D546	K464	E392		
L766		V547	K467	Q393	Q284	Y191
R767	D679	R548	Q470	V394	A289	I192
	M680	A549	L471	C395	S290	F193
	H683	T566	G472	T396	M194	N194
	M686	I575	C473	F397	G195	G195
	S687		R474	I398	I197	I197
	T688	F579	Q475	T399	Y297	D198
V689	M690		P479	M403	L298	M199
	E694	G583	L480	E404	C299	V200
		S584	Y481	V405	D300	Y201
		G585	T482		M303	
		Y586	L483	I408	E306	L212
		Q587	H484	T412	I309	M213
		M592	R485	S413	I309	W214
		H593	S486	D414	I314	S215
			T487	Y415	I317	P216
			D488	L416		M217
			Q489	Y417		G218
						T219

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	208.55Å 208.55Å 208.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 29.79 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-3.30) 99.9 (29.79-3.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 3.18Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.237 , 0.277 0.234 , 0.269	Depositor DCC
R_{free} test set	2293 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	58.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	11869	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 1.82% 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: XIH

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	0.45	0/6088	0.71	2/8278 (0.0%)
1	B	0.43	0/6088	0.71	3/8278 (0.0%)
All	All	0.44	0/12176	0.71	5/16556 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	713	HIS	N-CA-C	6.95	129.77	111.00
1	B	713	HIS	N-CA-C	6.87	129.54	111.00
1	B	548	TYR	N-CA-C	-5.90	95.06	111.00
1	A	548	TYR	N-CA-C	-5.87	95.14	111.00
1	B	383	CYS	CA-CB-SG	5.29	123.53	114.00

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	5920	0	5632	267	0
1	B	5920	0	5632	266	0
2	A	29	0	23	3	0
All	All	11869	0	11287	527	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 (527) 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:174:ILE:H	1:A:174:ILE:HD12	1.20	1.03
1:B:174:ILE:HD12	1:B:174:ILE:H	1.22	1.01
1:A:595:ILE:HD11	1:A:603:GLU:HB3	1.47	0.96
1:B:595:ILE:HD11	1:B:603:GLU:HB3	1.47	0.94
1:A:412:THR:HG22	1:A:414:ASP:H	1.28	0.93
1:B:54:LYS:H	1:B:498:ASN:HD21	1.17	0.92
1:B:412:THR:HG22	1:B:414:ASP:H	1.33	0.91
1:A:349:THR:HB	1:A:593:HIS:HD2	1.37	0.90
1:A:54:LYS:H	1:A:498:ASN:HD21	1.18	0.90
1:A:449:ASP:O	1:A:452:PRO:HD3	1.72	0.89
1:B:449:ASP:O	1:B:452:PRO:HD3	1.73	0.89
1:B:349:THR:HB	1:B:593:HIS:HD2	1.38	0.88
1:A:747:THR:HG21	1:B:726:ASP:HA	1.58	0.83
1:B:54:LYS:H	1:B:498:ASN:ND2	1.75	0.83
1:A:54:LYS:H	1:A:498:ASN:ND2	1.76	0.83
1:A:383:CYS:HB3	1:A:397:PHE:HA	1.59	0.83
1:A:460:VAL:HG22	1:A:461:SER:H	1.44	0.82
1:B:383:CYS:HB3	1:B:397:PHE:HA	1.61	0.82
1:B:639:MET:CE	1:B:689:VAL:HA	2.11	0.81
1:A:79:ALA:O	1:A:80:GLU:HB2	1.82	0.80
1:B:460:VAL:HG22	1:B:461:SER:H	1.45	0.79
1:B:707:THR:CG2	1:B:738:ASP:H	1.95	0.79
1:A:639:MET:CE	1:A:689:VAL:HA	2.13	0.79
1:A:121:GLN:O	1:A:125:SER:HB2	1.82	0.78
1:A:658:SER:H	1:A:716:GLN:NE2	1.81	0.78
1:B:79:ALA:O	1:B:80:GLU:HB2	1.81	0.78
1:A:690:MET:HE3	1:A:720:ILE:HA	1.66	0.78
1:A:234:ILE:HD13	1:A:713:HIS:CE1	2.19	0.77
1:A:707:THR:CG2	1:A:738:ASP:H	1.97	0.76
1:B:690:MET:HE3	1:B:720:ILE:HA	1.66	0.76
1:B:121:GLN:O	1:B:125:SER:HB2	1.85	0.76
1:A:56:TYR:CE2	1:A:495:LEU:HD22	2.20	0.75
1:B:91:SER:O	1:B:93:PHE:N	2.20	0.75
1:A:91:SER:O	1:A:93:PHE:N	2.20	0.74
1:A:726:ASP:HA	1:B:747:THR:HG21	1.68	0.74
1:B:54:LYS:N	1:B:498:ASN:HD21	1.85	0.74
1:A:586:TYR:CD1	1:A:586:TYR:N	2.55	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:VAL:HG22	1:B:461:SER:N	2.02	0.74
1:A:460:VAL:HG22	1:A:461:SER:N	2.01	0.73
1:A:761:GLN:HB3	1:A:767:ARG:HB3	1.70	0.73
1:B:234:ILE:HD13	1:B:713:HIS:CE1	2.23	0.73
1:B:56:TYR:CE2	1:B:495:LEU:HD22	2.24	0.72
1:A:54:LYS:N	1:A:498:ASN:HD21	1.85	0.72
1:B:235:GLU:HG2	1:B:251:TRP:HB3	1.71	0.72
1:B:658:SER:H	1:B:716:GLN:NE2	1.86	0.72
1:A:235:GLU:HG2	1:A:251:TRP:HB3	1.72	0.71
1:B:586:TYR:N	1:B:586:TYR:CD1	2.56	0.71
1:A:662:TYR:OH	1:A:719:GLN:HG2	1.91	0.70
1:A:277:THR:HG22	1:A:278:THR:H	1.57	0.70
1:B:761:GLN:HB3	1:B:767:ARG:HB3	1.74	0.70
1:A:349:THR:HB	1:A:593:HIS:CD2	2.26	0.69
1:B:55:SER:HA	1:B:481:TYR:CE1	2.28	0.69
1:A:107:PRO:HG2	1:A:158:GLU:O	1.92	0.69
1:B:277:THR:HG22	1:B:278:THR:H	1.58	0.69
1:B:91:SER:HA	1:B:94:GLU:OE1	1.93	0.69
1:A:652:ILE:HG21	1:A:756:MET:HE3	1.75	0.68
1:A:204:GLU:OE2	2:A:901:XIH:N14	2.26	0.68
1:A:747:THR:CG2	1:B:726:ASP:HA	2.24	0.68
1:B:485:ARG:HG3	1:B:485:ARG:O	1.93	0.68
1:A:91:SER:HA	1:A:94:GLU:OE1	1.94	0.68
1:A:277:THR:HG21	1:A:279:THR:O	1.93	0.68
1:A:624:ARG:HB2	1:A:624:ARG:HH11	1.58	0.67
1:B:349:THR:HB	1:B:593:HIS:CD2	2.27	0.67
1:B:485:ARG:HD2	1:B:487:THR:HB	1.77	0.67
1:B:277:THR:HG21	1:B:279:THR:O	1.95	0.67
1:A:518:ILE:CD1	1:A:519:VAL:H	2.08	0.67
1:B:107:PRO:HG2	1:B:158:GLU:O	1.94	0.67
1:A:473:CYS:O	1:A:479:PRO:HA	1.95	0.67
1:A:219:THR:O	1:A:271:THR:HB	1.94	0.66
1:B:473:CYS:O	1:B:479:PRO:HA	1.95	0.66
1:B:219:THR:O	1:B:271:THR:HB	1.94	0.66
1:A:412:THR:CG2	1:A:413:SER:N	2.58	0.66
1:B:767:ARG:HH11	1:B:767:ARG:HG3	1.61	0.66
1:B:662:TYR:OH	1:B:719:GLN:HG2	1.96	0.66
1:A:323:MET:O	1:A:342:GLU:O	2.14	0.65
1:A:65:GLU:HB3	1:A:76:LEU:HD11	1.78	0.65
1:A:55:SER:HA	1:A:481:TYR:CE1	2.31	0.65
1:A:688:THR:CG2	1:A:690:MET:HG2	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:ARG:HD2	1:A:487:THR:HB	1.78	0.65
1:B:412:THR:CG2	1:B:413:SER:N	2.59	0.65
1:A:518:ILE:HD12	1:A:519:VAL:H	1.62	0.65
1:A:641:LEU:HD22	1:A:699:VAL:HG11	1.77	0.65
1:A:767:ARG:HG3	1:A:767:ARG:HH11	1.62	0.64
1:B:688:THR:CG2	1:B:690:MET:HG2	2.27	0.64
1:A:485:ARG:HG3	1:A:485:ARG:O	1.97	0.64
1:A:195:GLY:C	1:A:211:ALA:HB3	2.18	0.64
1:B:65:GLU:HB3	1:B:76:LEU:HD11	1.78	0.64
1:A:439:ASP:OD1	1:A:441:THR:HB	1.98	0.64
1:B:697:LYS:HG2	1:B:729:VAL:HG22	1.79	0.64
1:B:195:GLY:C	1:B:211:ALA:HB3	2.18	0.64
1:A:612:ARG:HH11	1:A:612:ARG:HG3	1.64	0.63
1:B:518:ILE:CD1	1:B:519:VAL:H	2.11	0.63
1:A:697:LYS:HG2	1:A:729:VAL:HG22	1.80	0.63
1:B:256:LYS:NZ	1:B:713:HIS:HD2	1.96	0.63
1:B:612:ARG:HH11	1:B:612:ARG:HG3	1.63	0.63
1:B:624:ARG:HB2	1:B:624:ARG:HH11	1.61	0.63
1:B:84:SER:O	1:B:85:SER:HB2	1.98	0.62
1:B:439:ASP:OD1	1:B:441:THR:HB	1.99	0.62
1:A:73:ASN:OD1	1:A:90:ASN:N	2.32	0.62
1:B:595:ILE:HG21	1:B:599:LEU:HD23	1.82	0.62
1:B:78:ASN:HB3	1:B:83:ASN:HB3	1.82	0.62
1:A:595:ILE:CG2	1:A:599:LEU:HD23	2.29	0.62
1:A:595:ILE:HG21	1:A:599:LEU:HD23	1.80	0.62
1:B:595:ILE:CG2	1:B:599:LEU:HD23	2.30	0.62
1:B:652:ILE:HG21	1:B:756:MET:HE3	1.81	0.62
1:A:256:LYS:NZ	1:A:713:HIS:HD2	1.98	0.61
1:A:174:ILE:H	1:A:174:ILE:CD1	2.00	0.61
1:B:639:MET:HE3	1:B:689:VAL:HA	1.80	0.61
1:B:707:THR:HG22	1:B:738:ASP:H	1.66	0.61
1:A:639:MET:HE3	1:A:689:VAL:HA	1.83	0.61
1:B:518:ILE:HD12	1:B:519:VAL:H	1.66	0.61
1:B:73:ASN:OD1	1:B:90:ASN:N	2.33	0.60
1:A:712:VAL:HG22	2:A:901:XIH:H21	1.83	0.60
1:A:483:LEU:HB3	1:A:495:LEU:HD11	1.83	0.60
1:B:641:LEU:HD22	1:B:699:VAL:HG11	1.82	0.60
1:B:767:ARG:C	1:B:767:ARG:HD2	2.20	0.60
1:A:713:HIS:O	1:A:714:PHE:CB	2.49	0.60
1:B:323:MET:O	1:B:342:GLU:O	2.20	0.60
1:B:713:HIS:O	1:B:714:PHE:CB	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ASN:HB3	1:A:83:ASN:HB3	1.82	0.60
1:B:79:ALA:O	1:B:80:GLU:CB	2.49	0.60
1:A:79:ALA:O	1:A:80:GLU:CB	2.50	0.59
1:A:84:SER:O	1:A:85:SER:HB2	2.01	0.59
1:B:483:LEU:HB3	1:B:495:LEU:HD11	1.83	0.59
1:A:713:HIS:O	1:A:714:PHE:HB3	2.02	0.59
1:A:460:VAL:CG2	1:A:461:SER:H	2.15	0.59
1:A:412:THR:HG22	1:A:413:SER:N	2.17	0.59
1:B:713:HIS:O	1:B:714:PHE:HB3	2.03	0.59
1:A:58:LEU:HD12	1:A:58:LEU:H	1.68	0.58
1:B:583:GLY:O	1:B:584:SER:HB3	2.04	0.58
1:B:412:THR:HG22	1:B:413:SER:N	2.16	0.58
1:A:583:GLY:O	1:A:584:SER:HB3	2.02	0.58
1:A:636:VAL:O	1:A:640:VAL:HG23	2.03	0.58
1:B:408:ILE:HG23	1:B:416:LEU:HD11	1.85	0.58
1:A:233:LEU:HD23	1:A:253:PRO:HA	1.86	0.58
1:B:383:CYS:CB	1:B:397:PHE:HA	2.33	0.58
1:A:383:CYS:CB	1:A:397:PHE:HA	2.33	0.58
1:A:408:ILE:HG23	1:A:416:LEU:HD11	1.85	0.58
1:B:470:GLN:HG2	1:B:471:LEU:N	2.20	0.57
1:B:460:VAL:CG2	1:B:461:SER:H	2.16	0.57
1:B:636:VAL:O	1:B:640:VAL:HG23	2.04	0.57
1:A:470:GLN:HG2	1:A:471:LEU:N	2.18	0.57
1:B:264:VAL:HG12	1:B:265:LYS:N	2.20	0.57
1:A:277:THR:HG22	1:A:278:THR:N	2.20	0.57
1:B:178:LEU:HB3	1:B:179:PRO:HD2	1.87	0.57
1:B:233:LEU:HD23	1:B:253:PRO:HA	1.86	0.56
1:B:403:TRP:CE3	1:B:422:GLU:HB2	2.40	0.56
1:B:632:TYR:O	1:B:635:TYR:HB3	2.04	0.56
1:A:415:TYR:HD2	1:A:436:GLN:HA	1.70	0.56
1:B:415:TYR:HD2	1:B:436:GLN:HA	1.70	0.56
1:B:277:THR:HG22	1:B:278:THR:N	2.20	0.56
1:B:58:LEU:H	1:B:58:LEU:HD12	1.70	0.56
1:A:264:VAL:HG12	1:A:265:LYS:N	2.21	0.56
1:B:320:TYR:CE2	1:B:322:VAL:HG23	2.41	0.56
1:B:403:TRP:CD2	1:B:422:GLU:HB2	2.40	0.56
1:A:178:LEU:HB3	1:A:179:PRO:HD2	1.87	0.56
1:B:462:LEU:N	1:B:462:LEU:HD12	2.21	0.56
1:A:632:TYR:O	1:A:635:TYR:HB3	2.05	0.56
1:A:707:THR:HG22	1:A:738:ASP:H	1.68	0.55
1:B:709:ASP:OD2	1:B:741:HIS:HA	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:ARG:HG2	1:A:524:ARG:HH11	1.71	0.55
1:B:116:TYR:O	1:B:117:ASN:HB2	2.06	0.55
1:A:483:LEU:CB	1:A:495:LEU:HD11	2.36	0.55
1:B:267:PHE:CE2	1:B:284:GLN:HB2	2.42	0.55
1:A:317:ILE:HG22	1:A:319:ASN:HB2	1.89	0.55
1:A:386:GLN:HG3	1:A:390:LYS:HE3	1.88	0.55
1:B:47:LEU:HD22	1:B:750:GLN:HA	1.88	0.55
1:A:320:TYR:CE2	1:A:322:VAL:HG23	2.41	0.55
1:B:524:ARG:HH11	1:B:524:ARG:HG2	1.71	0.55
1:A:125:SER:O	1:A:126:TYR:HB3	2.06	0.55
1:B:94:GLU:O	1:B:94:GLU:HG2	2.06	0.54
1:A:403:TRP:CD2	1:A:422:GLU:HB2	2.42	0.54
1:A:267:PHE:CE2	1:A:284:GLN:HB2	2.43	0.54
1:A:658:SER:H	1:A:716:GLN:HE21	1.54	0.54
1:A:767:ARG:HD2	1:A:767:ARG:C	2.27	0.54
1:A:460:VAL:CG2	1:A:461:SER:N	2.70	0.54
1:A:447:SER:HB2	1:A:458:TYR:CE1	2.42	0.54
1:B:125:SER:O	1:B:126:TYR:HB3	2.06	0.54
1:B:483:LEU:CB	1:B:495:LEU:HD11	2.37	0.54
1:A:601:THR:HG22	1:A:602:LEU:N	2.23	0.54
1:A:709:ASP:OD2	1:A:741:HIS:HA	2.08	0.54
1:B:267:PHE:CD2	1:B:284:GLN:HB2	2.43	0.54
1:A:228:ASP:OD1	1:A:262:PRO:HB3	2.07	0.54
1:A:256:LYS:HZ3	1:A:713:HIS:HD2	1.55	0.53
1:A:292:THR:HG22	1:A:292:THR:O	2.08	0.53
1:A:726:ASP:HA	1:B:747:THR:CG2	2.38	0.53
1:A:146:ILE:HD12	1:A:153:ILE:HD12	1.91	0.53
1:A:415:TYR:CD2	1:A:436:GLN:HA	2.43	0.53
1:A:403:TRP:CE3	1:A:422:GLU:HB2	2.43	0.53
1:A:707:THR:HG21	1:A:738:ASP:H	1.73	0.53
1:A:267:PHE:CD2	1:A:284:GLN:HB2	2.43	0.53
1:B:174:ILE:H	1:B:174:ILE:CD1	2.02	0.53
1:A:712:VAL:CG2	2:A:901:XIH:H21	2.39	0.53
1:A:455:CYS:HA	1:A:475:GLY:HA3	1.91	0.53
1:B:386:GLN:HG3	1:B:390:LYS:HE3	1.90	0.53
1:A:147:PRO:HB2	1:A:166:TRP:CD1	2.44	0.52
1:A:547:VAL:HG23	1:A:628:TRP:O	2.08	0.52
1:B:292:THR:HG22	1:B:292:THR:O	2.09	0.52
1:B:317:ILE:HG22	1:B:319:ASN:HB2	1.91	0.52
1:B:584:SER:O	1:B:585:GLY:O	2.27	0.52
1:A:174:ILE:HD12	1:A:174:ILE:N	2.04	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:SER:HB2	1:B:458:TYR:CE1	2.45	0.52
1:A:462:LEU:N	1:A:462:LEU:HD12	2.25	0.52
1:B:742:GLY:O	1:B:743:ILE:C	2.48	0.52
1:A:47:LEU:HD22	1:A:750:GLN:HA	1.91	0.52
1:B:80:GLU:H	1:B:493:ARG:HH22	1.58	0.52
1:A:688:THR:HG21	1:A:690:MET:HG2	1.92	0.52
1:A:485:ARG:HB3	1:A:492:LEU:HD21	1.91	0.52
1:B:60:TRP:CE3	1:B:66:TYR:HB3	2.45	0.52
1:A:421:ASN:ND2	1:A:427:PRO:HA	2.25	0.52
1:A:94:GLU:HG2	1:A:94:GLU:O	2.08	0.52
1:B:256:LYS:HZ3	1:B:713:HIS:HD2	1.58	0.52
1:B:415:TYR:CD2	1:B:436:GLN:HA	2.44	0.52
1:A:116:TYR:O	1:A:117:ASN:HB2	2.09	0.52
1:A:612:ARG:NH1	1:A:612:ARG:HG3	2.24	0.52
1:B:228:ASP:OD1	1:B:262:PRO:HB3	2.10	0.52
1:B:659:ARG:HG2	1:B:662:TYR:CE2	2.44	0.52
1:A:381:HIS:CD2	1:A:399:THR:HG22	2.45	0.52
1:B:146:ILE:HD12	1:B:153:ILE:HD12	1.90	0.52
1:A:299:CYS:SG	1:A:357:PRO:HD2	2.50	0.51
1:A:314:LEU:CD1	1:A:321:SER:HB2	2.41	0.51
1:A:699:VAL:HG12	1:A:700:GLU:N	2.24	0.51
1:B:95:ILE:C	1:B:97:GLY:H	2.13	0.51
1:B:455:CYS:HA	1:B:475:GLY:HA3	1.92	0.51
1:A:742:GLY:O	1:A:743:ILE:C	2.49	0.51
1:B:601:THR:HG22	1:B:602:LEU:N	2.25	0.51
1:B:547:VAL:HG23	1:B:628:TRP:O	2.09	0.51
1:B:688:THR:HG21	1:B:690:MET:HG2	1.92	0.51
1:A:314:LEU:HD12	1:A:321:SER:HB2	1.92	0.51
1:A:699:VAL:CG1	1:A:700:GLU:N	2.73	0.51
1:B:147:PRO:HB2	1:B:166:TRP:CD1	2.46	0.51
1:B:314:LEU:HD12	1:B:321:SER:HB2	1.91	0.51
1:A:122:TRP:CH2	1:A:252:ILE:HD11	2.45	0.51
1:A:412:THR:CG2	1:A:413:SER:H	2.23	0.51
1:B:598:ARG:HD3	1:B:598:ARG:O	2.10	0.51
1:A:95:ILE:C	1:A:97:GLY:H	2.13	0.51
1:B:485:ARG:HB3	1:B:492:LEU:HD21	1.92	0.51
1:A:121:GLN:O	1:A:122:TRP:HB2	2.11	0.51
1:B:612:ARG:NH1	1:B:612:ARG:HG3	2.24	0.51
1:B:421:ASN:ND2	1:B:427:PRO:HA	2.27	0.50
1:B:314:LEU:CD1	1:B:321:SER:HB2	2.41	0.50
1:B:699:VAL:HG12	1:B:700:GLU:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:ARG:HD3	1:A:598:ARG:O	2.11	0.50
1:B:699:VAL:CG1	1:B:700:GLU:N	2.74	0.50
1:B:766:LEU:O	1:B:767:ARG:O	2.30	0.50
1:B:767:ARG:HG3	1:B:767:ARG:NH1	2.27	0.50
1:A:584:SER:O	1:A:585:GLY:O	2.30	0.50
1:B:196:ILE:N	1:B:211:ALA:HB3	2.27	0.50
1:B:229:THR:HG22	1:B:230:GLY:N	2.27	0.50
1:A:584:SER:H	1:A:592:MET:HA	1.77	0.50
1:B:462:LEU:H	1:B:462:LEU:HD12	1.77	0.50
1:A:624:ARG:HB2	1:A:624:ARG:NH1	2.26	0.49
1:A:412:THR:HG23	1:A:413:SER:H	1.78	0.49
1:A:132:ILE:HG21	1:A:176:PRO:HB3	1.95	0.49
1:A:536:ASP:HB3	1:A:539:LYS:HE2	1.95	0.49
1:A:80:GLU:H	1:A:493:ARG:HH22	1.59	0.49
1:A:89:GLU:C	1:A:91:SER:N	2.63	0.49
1:B:122:TRP:CH2	1:B:252:ILE:HD11	2.48	0.49
1:A:334:VAL:HG12	1:A:335:TRP:N	2.28	0.49
1:A:767:ARG:HG3	1:A:767:ARG:NH1	2.28	0.49
1:B:412:THR:CG2	1:B:413:SER:H	2.25	0.49
1:B:121:GLN:O	1:B:122:TRP:HB2	2.13	0.49
1:A:659:ARG:HG2	1:A:662:TYR:CE2	2.48	0.49
1:B:511:PRO:HB2	1:B:531:LEU:O	2.13	0.49
1:A:342:GLU:O	1:A:343:HIS:HB2	2.13	0.49
1:B:132:ILE:HG21	1:B:176:PRO:HB3	1.94	0.48
1:A:234:ILE:O	1:A:234:ILE:HG13	2.12	0.48
1:A:314:LEU:HG	1:A:318:GLN:HG2	1.94	0.48
1:A:430:ARG:HG2	1:A:457:TYR:CE1	2.48	0.48
1:A:749:HIS:CE1	1:A:753:TYR:CE1	3.01	0.48
1:B:658:SER:H	1:B:716:GLN:HE21	1.61	0.48
1:B:299:CYS:SG	1:B:314:LEU:HD22	2.53	0.48
1:B:314:LEU:HG	1:B:318:GLN:HG2	1.95	0.48
1:B:690:MET:HE3	1:B:720:ILE:CA	2.40	0.48
1:A:748:ALA:O	1:A:752:ILE:HG22	2.13	0.48
1:B:381:HIS:CD2	1:B:399:THR:HG22	2.48	0.48
1:B:474:ARG:O	1:B:475:GLY:O	2.31	0.48
1:B:707:THR:HG21	1:B:738:ASP:H	1.72	0.48
1:B:200:VAL:HG13	1:B:201:TYR:N	2.28	0.48
1:B:78:ASN:O	1:B:81:HIS:O	2.32	0.48
1:B:441:THR:O	1:B:443:LYS:N	2.44	0.48
1:B:624:ARG:NH1	1:B:624:ARG:HB2	2.28	0.48
1:A:60:TRP:CE3	1:A:66:TYR:HB3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:GLY:O	1:A:83:ASN:C	2.52	0.48
1:A:264:VAL:HG12	1:A:265:LYS:H	1.79	0.48
1:A:603:GLU:OE1	1:A:603:GLU:N	2.46	0.48
1:B:75:LEU:HB2	1:B:77:PHE:HE1	1.79	0.48
1:A:104:SER:HB3	1:A:113:LEU:HB2	1.96	0.47
1:A:299:CYS:SG	1:A:314:LEU:HD22	2.54	0.47
1:A:61:VAL:HG21	1:A:67:LEU:HG	1.96	0.47
1:A:148:ASN:HD22	1:A:148:ASN:HA	1.56	0.47
1:A:583:GLY:HA2	1:A:592:MET:O	2.14	0.47
1:B:430:ARG:HG2	1:B:457:TYR:CE1	2.49	0.47
1:A:601:THR:HG22	1:A:602:LEU:HD23	1.95	0.47
1:A:71:GLU:O	1:A:73:ASN:ND2	2.48	0.47
1:A:229:THR:HG22	1:A:230:GLY:N	2.30	0.47
1:A:543:LEU:HD12	1:A:575:ILE:O	2.15	0.47
1:B:299:CYS:SG	1:B:357:PRO:HD2	2.55	0.47
1:B:82:GLY:O	1:B:83:ASN:C	2.52	0.47
1:A:196:ILE:N	1:A:211:ALA:HB3	2.30	0.47
1:A:520:LEU:O	1:A:522:GLU:N	2.48	0.47
1:B:234:ILE:HG13	1:B:234:ILE:O	2.14	0.47
1:B:584:SER:H	1:B:592:MET:HA	1.79	0.47
1:B:334:VAL:HG12	1:B:335:TRP:N	2.29	0.47
1:B:529:MET:HB3	1:B:529:MET:HE2	1.70	0.47
1:A:216:PRO:C	1:A:218:GLY:H	2.18	0.47
1:A:467:LYS:C	1:A:486:SER:HB2	2.35	0.47
1:A:78:ASN:O	1:A:81:HIS:O	2.33	0.47
1:B:680:ASN:ND2	1:B:683:HIS:HB2	2.30	0.47
1:A:509:GLN:O	1:A:533:PRO:HG3	2.14	0.47
1:A:583:GLY:HA2	1:A:592:MET:HA	1.97	0.47
1:B:303:TRP:CE2	1:B:309:ILE:HD12	2.50	0.47
1:B:509:GLN:O	1:B:533:PRO:HG3	2.14	0.47
1:B:601:THR:HG22	1:B:602:LEU:HD23	1.97	0.47
1:A:216:PRO:C	1:A:218:GLY:N	2.69	0.46
1:A:529:MET:HB3	1:A:529:MET:HE2	1.65	0.46
1:B:467:LYS:C	1:B:486:SER:HB2	2.35	0.46
1:B:767:ARG:C	1:B:767:ARG:CD	2.84	0.46
1:B:216:PRO:C	1:B:218:GLY:N	2.68	0.46
1:B:342:GLU:O	1:B:343:HIS:HB2	2.15	0.46
1:B:75:LEU:HD23	1:B:86:ILE:HA	1.96	0.46
1:B:216:PRO:C	1:B:218:GLY:H	2.18	0.46
1:B:488:ASP:O	1:B:489:GLN:HB2	2.15	0.46
1:A:303:TRP:CE2	1:A:309:ILE:HD12	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:LEU:C	1:A:416:LEU:HD12	2.36	0.46
1:A:418:TYR:O	1:A:432:LEU:HD12	2.16	0.46
1:A:694:GLU:O	1:A:697:LYS:HG3	2.15	0.46
1:B:289:ALA:C	1:B:291:VAL:H	2.19	0.46
1:B:603:GLU:OE1	1:B:603:GLU:N	2.48	0.46
1:B:694:GLU:O	1:B:697:LYS:HG3	2.16	0.46
1:B:748:ALA:O	1:B:752:ILE:HG22	2.16	0.46
1:A:277:THR:HG22	1:A:279:THR:H	1.81	0.46
1:A:536:ASP:OD2	1:A:538:SER:OG	2.34	0.46
1:B:121:GLN:O	1:B:122:TRP:CB	2.64	0.46
1:B:741:HIS:O	1:B:741:HIS:CG	2.69	0.46
1:A:511:PRO:HB2	1:A:531:LEU:O	2.15	0.46
1:B:41:TYR:CD2	1:B:566:THR:HG22	2.51	0.46
1:B:583:GLY:HA2	1:B:592:MET:HA	1.98	0.46
1:A:474:ARG:O	1:A:475:GLY:O	2.35	0.45
1:A:766:LEU:O	1:A:767:ARG:O	2.34	0.45
1:B:160:HIS:HB2	1:B:176:PRO:HD3	1.98	0.45
1:B:235:GLU:OE2	1:B:251:TRP:HB3	2.16	0.45
1:B:392:GLU:C	1:B:393:GLN:HG3	2.37	0.45
1:B:543:LEU:HD12	1:B:575:ILE:O	2.16	0.45
1:B:89:GLU:C	1:B:91:SER:N	2.66	0.45
1:B:264:VAL:HG12	1:B:265:LYS:H	1.81	0.45
1:B:488:ASP:OD1	1:B:490:LYS:HB2	2.16	0.45
1:A:121:GLN:O	1:A:122:TRP:CB	2.63	0.45
1:A:289:ALA:C	1:A:291:VAL:H	2.20	0.45
1:B:71:GLU:O	1:B:73:ASN:ND2	2.50	0.45
1:A:91:SER:OG	1:A:92:THR:N	2.50	0.45
1:B:104:SER:HB3	1:B:113:LEU:HB2	1.98	0.45
1:A:235:GLU:OE2	1:A:251:TRP:HB3	2.16	0.45
1:A:382:ILE:HG13	1:A:405:VAL:HG21	1.98	0.45
1:A:392:GLU:C	1:A:393:GLN:HG3	2.36	0.45
1:B:163:ALA:HB2	1:B:214:TRP:CZ2	2.52	0.45
1:A:690:MET:HE3	1:A:720:ILE:CA	2.42	0.45
1:B:290:SER:O	1:B:291:VAL:HG23	2.17	0.45
1:A:297:TYR:CE2	1:A:666:VAL:HG22	2.51	0.45
1:B:80:GLU:HA	1:B:492:LEU:HD13	1.99	0.45
1:A:383:CYS:HB3	1:A:397:PHE:CA	2.40	0.45
1:A:462:LEU:H	1:A:462:LEU:HD12	1.81	0.45
1:B:120:LYS:HG2	1:B:121:GLN:N	2.32	0.45
1:B:216:PRO:O	1:B:306:GLU:OE2	2.35	0.45
1:B:231:VAL:HG22	1:B:260:VAL:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ALA:HB2	1:A:214:TRP:CZ2	2.52	0.44
1:A:386:GLN:O	1:A:387:LYS:C	2.56	0.44
1:B:277:THR:CG2	1:B:279:THR:O	2.64	0.44
1:B:536:ASP:HB3	1:B:539:LYS:HE2	1.98	0.44
1:A:120:LYS:HG2	1:A:121:GLN:N	2.33	0.44
1:B:174:ILE:HD12	1:B:174:ILE:N	2.06	0.44
1:A:200:VAL:HG13	1:A:201:TYR:N	2.32	0.44
1:B:297:TYR:CE2	1:B:666:VAL:HG22	2.52	0.44
1:B:320:TYR:HE2	1:B:322:VAL:HG23	1.80	0.44
1:B:346:THR:HG23	1:B:347:SER:N	2.33	0.44
1:A:320:TYR:HE2	1:A:322:VAL:HG23	1.82	0.44
1:A:488:ASP:O	1:A:489:GLN:HB2	2.18	0.44
1:A:41:TYR:CD2	1:A:566:THR:HG22	2.52	0.44
1:B:193:PHE:O	1:B:225:GLN:HA	2.18	0.44
1:B:318:GLN:OE1	1:B:670:ARG:HD3	2.17	0.44
1:A:160:HIS:HB2	1:A:176:PRO:HD3	1.99	0.44
1:A:318:GLN:OE1	1:A:670:ARG:HD3	2.18	0.44
1:B:61:VAL:HG21	1:B:67:LEU:HG	1.99	0.44
1:A:84:SER:O	1:A:85:SER:CB	2.65	0.44
1:A:246:TYR:CZ	1:B:232:PRO:HB2	2.53	0.44
1:B:412:THR:HG23	1:B:413:SER:H	1.81	0.44
1:B:749:HIS:CE1	1:B:753:TYR:CE1	3.05	0.44
1:A:439:ASP:C	1:A:441:THR:H	2.21	0.44
1:A:680:ASN:ND2	1:A:683:HIS:HB2	2.33	0.44
1:B:215:SER:HB3	1:B:303:TRP:CZ2	2.53	0.44
1:B:545:ILE:HB	1:B:627:ILE:HG13	2.00	0.44
1:B:355:PHE:O	1:B:356:ARG:HB3	2.18	0.43
1:B:690:MET:HE2	1:B:719:GLN:C	2.39	0.43
1:A:103:TYR:HA	1:A:113:LEU:O	2.18	0.43
1:A:75:LEU:HD23	1:A:86:ILE:HA	2.00	0.43
1:B:277:THR:HG22	1:B:279:THR:H	1.83	0.43
1:B:707:THR:HG22	1:B:738:ASP:N	2.32	0.43
1:A:488:ASP:OD1	1:A:490:LYS:HB2	2.18	0.43
1:B:418:TYR:O	1:B:432:LEU:HD12	2.18	0.43
1:B:484:HIS:ND1	1:B:484:HIS:N	2.66	0.43
1:B:91:SER:OG	1:B:92:THR:N	2.50	0.43
1:B:382:ILE:HG13	1:B:405:VAL:HG21	2.00	0.43
1:B:75:LEU:HB2	1:B:77:PHE:CE1	2.53	0.43
1:A:193:PHE:O	1:A:225:GLN:HA	2.18	0.43
1:A:277:THR:CG2	1:A:279:THR:O	2.63	0.43
1:A:454:ARG:HD3	1:A:478:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:GLU:O	1:A:608:ILE:N	2.50	0.43
1:A:75:LEU:HB2	1:A:77:PHE:HE1	1.82	0.43
1:A:586:TYR:HD1	1:A:586:TYR:H	1.66	0.43
1:B:583:GLY:HA2	1:B:592:MET:O	2.18	0.43
1:B:688:THR:HG22	1:B:690:MET:N	2.34	0.43
1:B:714:PHE:O	1:B:715:GLN:C	2.57	0.43
1:A:372:ILE:HA	1:A:381:HIS:O	2.19	0.43
1:A:707:THR:O	1:A:707:THR:HG23	2.19	0.43
1:A:714:PHE:O	1:A:715:GLN:C	2.58	0.43
1:A:751:HIS:CD2	1:B:725:VAL:HA	2.53	0.43
1:B:200:VAL:CG1	1:B:201:TYR:N	2.82	0.43
1:B:355:PHE:O	1:B:670:ARG:NH1	2.51	0.43
1:B:416:LEU:C	1:B:416:LEU:HD12	2.39	0.43
1:B:548:TYR:O	1:B:549:ALA:HB3	2.19	0.43
1:A:332:THR:O	1:A:332:THR:HG22	2.19	0.42
1:B:120:LYS:CG	1:B:121:GLN:N	2.82	0.42
1:A:120:LYS:CG	1:A:121:GLN:N	2.82	0.42
1:A:306:GLU:HG2	1:A:306:GLU:O	2.19	0.42
1:B:194:ASN:OD1	1:B:225:GLN:HG3	2.19	0.42
1:B:341:GLN:OE1	1:B:387:LYS:HE3	2.20	0.42
1:B:745:SER:OG	1:B:748:ALA:HB3	2.19	0.42
1:A:334:VAL:CG1	1:A:335:TRP:N	2.83	0.42
1:B:595:ILE:O	1:B:595:ILE:CG2	2.67	0.42
1:A:332:THR:O	1:A:334:VAL:HG23	2.19	0.42
1:A:341:GLN:OE1	1:A:387:LYS:HE3	2.18	0.42
1:A:346:THR:HG23	1:A:347:SER:N	2.34	0.42
1:A:355:PHE:O	1:A:670:ARG:NH1	2.51	0.42
1:A:545:ILE:HB	1:A:627:ILE:HG13	2.02	0.42
1:A:741:HIS:CG	1:A:741:HIS:O	2.71	0.42
1:B:498:ASN:HB3	1:B:501:LEU:HB3	2.02	0.42
1:B:707:THR:HG23	1:B:707:THR:O	2.17	0.42
1:A:204:GLU:HA	1:A:204:GLU:OE1	2.20	0.42
1:A:220:PHE:HB3	1:A:268:ILE:CG2	2.49	0.42
1:B:680:ASN:HD21	1:B:683:HIS:HB2	1.84	0.42
1:A:167:LYS:O	1:A:168:ASN:HB2	2.19	0.42
1:A:416:LEU:HD12	1:A:417:TYR:N	2.35	0.42
1:B:439:ASP:C	1:B:441:THR:H	2.23	0.42
1:A:153:ILE:HG13	1:A:164:TYR:HB3	2.01	0.42
1:A:193:PHE:CE2	1:A:198:ASP:HA	2.53	0.42
1:A:688:THR:HG22	1:A:690:MET:N	2.34	0.42
1:B:680:ASN:HD21	1:B:683:HIS:CG	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:VAL:HG22	1:A:260:VAL:O	2.19	0.42
1:A:370:TYR:CE2	1:A:384:GLN:CG	3.03	0.42
1:A:194:ASN:OD1	1:A:225:GLN:HG3	2.20	0.42
1:A:381:HIS:CG	1:A:399:THR:HG22	2.54	0.42
1:A:690:MET:HE2	1:A:719:GLN:C	2.40	0.42
1:B:103:TYR:HA	1:B:113:LEU:O	2.20	0.42
1:B:68:TYR:HB3	1:B:77:PHE:CE1	2.55	0.42
1:A:518:ILE:HD13	1:A:519:VAL:H	1.84	0.41
1:B:220:PHE:HB3	1:B:268:ILE:CG2	2.49	0.41
1:A:80:GLU:HA	1:A:492:LEU:HD13	2.01	0.41
1:A:613:GLN:O	1:A:617:MET:HG3	2.20	0.41
1:B:628:TRP:CE3	1:B:756:MET:HE1	2.55	0.41
1:B:256:LYS:HZ1	1:B:713:HIS:HD2	1.68	0.41
1:A:484:HIS:ND1	1:A:484:HIS:N	2.68	0.41
1:A:254:TYR:CE1	1:A:713:HIS:CE1	3.08	0.41
1:B:152:TRP:CD1	1:B:212:LEU:HD12	2.55	0.41
1:B:193:PHE:CE2	1:B:198:ASP:HA	2.55	0.41
1:B:332:THR:O	1:B:332:THR:HG22	2.21	0.41
1:B:372:ILE:HA	1:B:381:HIS:O	2.21	0.41
1:B:471:LEU:HA	1:B:471:LEU:HD23	1.92	0.41
1:A:130:TYR:HB2	1:A:146:ILE:HD13	2.02	0.41
1:B:164:TYR:CE1	1:B:171:TYR:HB2	2.56	0.41
1:B:306:GLU:O	1:B:306:GLU:HG2	2.21	0.41
1:B:41:TYR:CD2	1:B:566:THR:CG2	3.03	0.41
1:B:529:MET:HE1	1:B:531:LEU:HD21	2.01	0.41
1:A:520:LEU:O	1:A:521:ASN:C	2.59	0.41
1:A:548:TYR:O	1:A:549:ALA:HB3	2.19	0.41
1:B:520:LEU:O	1:B:522:GLU:N	2.53	0.41
1:B:639:MET:HE3	1:B:689:VAL:CA	2.49	0.41
1:A:363:THR:HG23	1:A:368:SER:O	2.20	0.41
1:B:536:ASP:OD2	1:B:538:SER:OG	2.38	0.41
1:B:547:VAL:HG12	1:B:548:TYR:N	2.36	0.41
1:A:152:TRP:CD1	1:A:212:LEU:HD12	2.55	0.41
1:A:473:CYS:HB3	1:A:480:LEU:O	2.20	0.41
1:B:479:PRO:HG2	1:B:498:ASN:OD1	2.21	0.41
1:B:61:VAL:CG2	1:B:67:LEU:HG	2.51	0.41
1:A:601:THR:HG22	1:A:602:LEU:CD2	2.51	0.41
1:B:88:LEU:HA	1:B:88:LEU:HD23	1.87	0.41
1:A:355:PHE:O	1:A:356:ARG:HB3	2.20	0.41
1:A:585:GLY:HA3	1:A:587:GLN:HE21	1.85	0.41
1:B:153:ILE:HG13	1:B:164:TYR:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:TYR:C	1:B:254:TYR:CD2	2.94	0.41
1:B:586:TYR:HD1	1:B:586:TYR:H	1.68	0.41
1:A:101:SER:HB3	1:A:115:GLU:HG2	2.03	0.41
1:A:499:SER:O	1:A:502:ASP:HB3	2.21	0.41
1:A:547:VAL:HG12	1:A:548:TYR:N	2.36	0.41
1:A:624:ARG:HG2	1:A:764:PHE:CD2	2.56	0.41
1:B:334:VAL:CG1	1:B:335:TRP:N	2.84	0.41
1:B:520:LEU:O	1:B:521:ASN:C	2.60	0.41
1:B:58:LEU:HD12	1:B:58:LEU:N	2.35	0.41
1:B:680:ASN:HD21	1:B:683:HIS:CD2	2.38	0.41
1:B:84:SER:O	1:B:85:SER:CB	2.65	0.41
1:A:467:LYS:HD3	1:A:468:TYR:HE1	1.86	0.41
1:A:61:VAL:CG2	1:A:67:LEU:HG	2.50	0.41
1:B:458:TYR:HA	1:B:472:GLY:O	2.20	0.41
1:A:315:ARG:HD2	1:A:320:TYR:HB3	2.03	0.40
1:B:251:TRP:CD1	1:B:251:TRP:N	2.89	0.40
1:B:481:TYR:O	1:B:495:LEU:HB2	2.21	0.40
1:B:585:GLY:HA3	1:B:587:GLN:HE21	1.86	0.40
1:A:312:GLN:HG2	1:A:323:MET:HG3	2.04	0.40
1:A:411:LEU:HD12	1:A:411:LEU:HA	1.79	0.40
1:A:479:PRO:HG2	1:A:498:ASN:OD1	2.21	0.40
1:A:749:HIS:CE1	1:A:753:TYR:HE1	2.39	0.40
1:A:75:LEU:HB2	1:A:77:PHE:CE1	2.57	0.40
1:B:624:ARG:HG2	1:B:764:PHE:CD2	2.56	0.40
1:A:41:TYR:CD2	1:A:566:THR:CG2	3.04	0.40
1:A:525:PHE:HB3	1:A:579:PHE:CZ	2.57	0.40
1:A:459:SER:HB3	1:A:474:ARG:HE	1.85	0.40
1:A:498:ASN:HB3	1:A:501:LEU:HB3	2.03	0.40
1:A:667:TYR:O	1:A:670:ARG:HB3	2.22	0.40
1:A:68:TYR:HB3	1:A:77:PHE:CE1	2.56	0.40
1:B:299:CYS:SG	1:B:314:LEU:HB2	2.62	0.40
1:B:339:THR:O	1:B:342:GLU:HB2	2.22	0.40
1:B:60:TRP:CG	1:B:463:SER:HA	2.56	0.40
1:B:679:ASP:OD1	1:B:680:ASN:N	2.54	0.40
1:B:254:TYR:CE1	1:B:713:HIS:CE1	3.10	0.40
1:A:383:CYS:HB2	1:A:396:THR:O	2.22	0.40
1:B:256:LYS:O	1:B:257:ALA:C	2.60	0.40
1:B:430:ARG:HA	1:B:430:ARG:HD3	1.88	0.40
1:B:525:PHE:HB3	1:B:579:PHE:CZ	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	728/730 (100%)	614 (84%)	80 (11%)	34 (5%)	3	19
1	B	728/730 (100%)	619 (85%)	76 (10%)	33 (4%)	3	20
All	All	1456/1460 (100%)	1233 (85%)	156 (11%)	67 (5%)	3	19

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	SER
1	A	92	THR
1	A	274	LEU
1	A	450	LEU
1	A	475	GLY
1	A	521	ASN
1	A	533	PRO
1	A	585	GLY
1	A	619	PHE
1	A	713	HIS
1	B	91	SER
1	B	92	THR
1	B	274	LEU
1	B	450	LEU
1	B	475	GLY
1	B	533	PRO
1	B	585	GLY
1	B	619	PHE
1	B	713	HIS
1	A	80	GLU
1	A	85	SER
1	A	149	ASN
1	A	159	GLY
1	A	714	PHE
1	B	80	GLU

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Mol	Chain	Res	Type
1	B	85	SER
1	B	521	ASN
1	B	714	PHE
1	A	147	PRO
1	B	149	ASN
1	B	159	GLY
1	A	83	ASN
1	A	318	GLN
1	A	440	HIS
1	A	442	ASN
1	B	83	ASN
1	B	147	PRO
1	B	148	ASN
1	B	318	GLN
1	B	424	LYS
1	B	442	ASN
1	A	143	GLU
1	A	148	ASN
1	A	537	LYS
1	A	695	ASN
1	B	121	GLN
1	B	143	GLU
1	B	440	HIS
1	B	461	SER
1	A	240	SER
1	A	290	SER
1	A	291	VAL
1	A	461	SER
1	A	464	LYS
1	B	290	SER
1	B	291	VAL
1	B	464	LYS
1	A	391	PRO
1	B	391	PRO
1	B	356	ARG
1	B	191	VAL
1	A	191	VAL
1	A	356	ARG
1	A	583	GLY
1	B	350	GLY
1	B	583	GLY
1	A	350	GLY

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	643/651 (99%)	590 (92%)	53 (8%)	13	44
1	B	643/651 (99%)	589 (92%)	54 (8%)	13	43
All	All	1286/1302 (99%)	1179 (92%)	107 (8%)	13	43

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LEU
1	A	90	ASN
1	A	94	GLU
1	A	108	ASP
1	A	122	TRP
1	A	139	GLN
1	A	143	GLU
1	A	146	ILE
1	A	148	ASN
1	A	149	ASN
1	A	160	HIS
1	A	180	SER
1	A	229	THR
1	A	234	ILE
1	A	251	TRP
1	A	254	TYR
1	A	300	ASP
1	A	319	ASN
1	A	340	THR
1	A	342	GLU
1	A	346	THR
1	A	394	VAL
1	A	395	CYS
1	A	413	SER
1	A	414	ASP
1	A	416	LEU
1	A	441	THR

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Mol	Chain	Res	Type
1	A	453	GLU
1	A	459	SER
1	A	470	GLN
1	A	474	ARG
1	A	483	LEU
1	A	485	ARG
1	A	486	SER
1	A	516	ASP
1	A	518	ILE
1	A	533	PRO
1	A	547	VAL
1	A	548	TYR
1	A	586	TYR
1	A	593	HIS
1	A	598	ARG
1	A	622	SER
1	A	624	ARG
1	A	664	ASP
1	A	680	ASN
1	A	686	ASN
1	A	690	MET
1	A	707	THR
1	A	716	GLN
1	A	740	ASP
1	A	747	THR
1	A	767	ARG
1	B	58	LEU
1	B	90	ASN
1	B	94	GLU
1	B	108	ASP
1	B	122	TRP
1	B	139	GLN
1	B	143	GLU
1	B	146	ILE
1	B	148	ASN
1	B	149	ASN
1	B	160	HIS
1	B	180	SER
1	B	229	THR
1	B	234	ILE
1	B	251	TRP
1	B	254	TYR

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Mol	Chain	Res	Type
1	B	300	ASP
1	B	319	ASN
1	B	340	THR
1	B	342	GLU
1	B	346	THR
1	B	394	VAL
1	B	395	CYS
1	B	413	SER
1	B	414	ASP
1	B	416	LEU
1	B	441	THR
1	B	453	GLU
1	B	459	SER
1	B	470	GLN
1	B	474	ARG
1	B	483	LEU
1	B	484	HIS
1	B	485	ARG
1	B	486	SER
1	B	516	ASP
1	B	518	ILE
1	B	533	PRO
1	B	547	VAL
1	B	548	TYR
1	B	586	TYR
1	B	593	HIS
1	B	598	ARG
1	B	622	SER
1	B	624	ARG
1	B	664	ASP
1	B	680	ASN
1	B	686	ASN
1	B	690	MET
1	B	707	THR
1	B	716	GLN
1	B	740	ASP
1	B	747	THR
1	B	767	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	148	ASN
1	A	177	HIS
1	A	319	ASN
1	A	384	GLN
1	A	484	HIS
1	A	498	ASN
1	A	587	GLN
1	A	593	HIS
1	A	607	GLN
1	A	680	ASN
1	A	698	GLN
1	A	713	HIS
1	A	715	GLN
1	A	716	GLN
1	A	719	GLN
1	A	749	HIS
1	B	90	ASN
1	B	148	ASN
1	B	177	HIS
1	B	319	ASN
1	B	384	GLN
1	B	484	HIS
1	B	498	ASN
1	B	587	GLN
1	B	593	HIS
1	B	607	GLN
1	B	680	ASN
1	B	698	GLN
1	B	713	HIS
1	B	715	GLN
1	B	716	GLN
1	B	719	GLN
1	B	749	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

1 ligand is 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	XIH	A	901	-	24,32,32	3.57	4 (16%)	29,47,47	2.30	5 (17%)

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	XIH	A	901	-	-	0/6/20/20	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	XIH	C19-C18	2.06	1.43	1.39
2	A	901	XIH	C23-C18	3.93	1.46	1.40
2	A	901	XIH	C3-C5	5.60	1.51	1.41
2	A	901	XIH	C6-N7	15.30	1.47	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	XIH	C17-C18-C19	-4.21	111.73	121.17
2	A	901	XIH	C22-C23-C24	-3.23	113.54	119.41
2	A	901	XIH	C18-C17-N16	2.83	118.00	113.31
2	A	901	XIH	C18-C23-C24	5.96	126.13	120.24
2	A	901	XIH	C17-C18-C23	8.12	131.40	120.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	XIH	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 [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	730/730 (100%)	-0.38	1 (0%) 95 96	4, 31, 79, 187	0
1	B	730/730 (100%)	-0.34	2 (0%) 93 93	5, 37, 92, 161	0
All	All	1460/1460 (100%)	-0.36	3 (0%) 94 95	4, 33, 88, 187	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	767	ARG	3.6
1	B	392	GLU	3.3
1	B	393	GLN	2.3

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	XIH	A	901	29/29	0.92	0.25	2.24	48,48,48,48	0

6.5 Other polymers ⓘ

There are no such residues in this entry.