



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2017 – 08:09 AM EDT

PDB ID : 2RGU
Title : Crystal structure of complex of human DPP4 and inhibitor
Authors : Nar, H.; Himmelsbach, F.; Eckhardt, M.
Deposited on : unknown
Resolution : 2.60 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

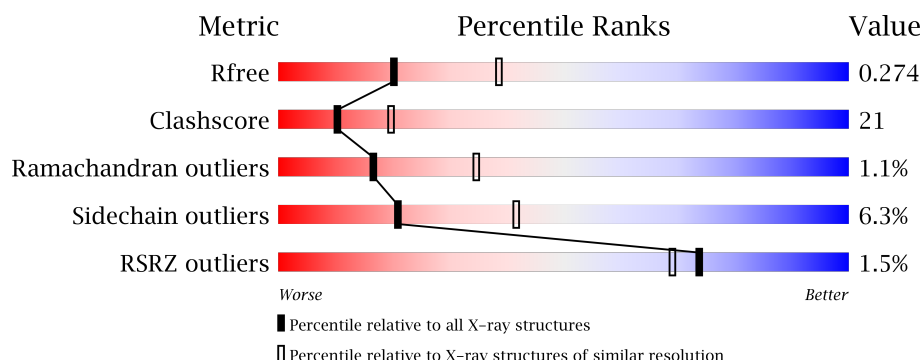
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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	734	<div> <div>2%</div> <div>60%</div> <div>35%</div> <div>..</div> </div>
1	B	734	<div> <div>%</div> <div>64%</div> <div>32%</div> <div>..</div> </div>

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	NAG	A	795	X	-	-	-
2	NAG	A	796	X	-	-	-
2	NAG	B	793	X	-	-	-
2	NAG	B	794	X	-	-	-
2	NAG	B	796	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12323 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	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			
1	B	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			

There are 12 discrepancies between the modelled and reference sequences:

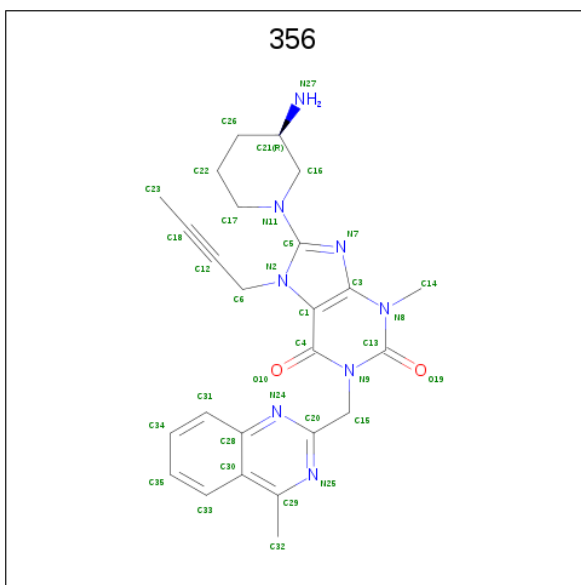
Chain	Residue	Modelled	Actual	Comment	Reference
A	767	HIS	-	EXPRESSION TAG	UNP P27487
A	768	HIS	-	EXPRESSION TAG	UNP P27487
A	769	HIS	-	EXPRESSION TAG	UNP P27487
A	770	HIS	-	EXPRESSION TAG	UNP P27487
A	771	HIS	-	EXPRESSION TAG	UNP P27487
A	772	HIS	-	EXPRESSION TAG	UNP P27487
B	767	HIS	-	EXPRESSION TAG	UNP P27487
B	768	HIS	-	EXPRESSION TAG	UNP P27487
B	769	HIS	-	EXPRESSION TAG	UNP P27487
B	770	HIS	-	EXPRESSION TAG	UNP P27487
B	771	HIS	-	EXPRESSION TAG	UNP P27487
B	772	HIS	-	EXPRESSION TAG	UNP P27487

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is 8-[(3R)-3-Aminopiperidin-1-yl]-7-but-2-yn-1-yl-3-methyl-1-[(4-methylquinazolin-2-yl)methyl]-3,7-dihydro-1H-purine-2,6-dione (three-letter code: 356) (formula: C₂₅H₂₈N₈O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 35	C 25	N 8	O 2	0	0
3	B	1	Total 35	C 25	N 8	O 2	0	0

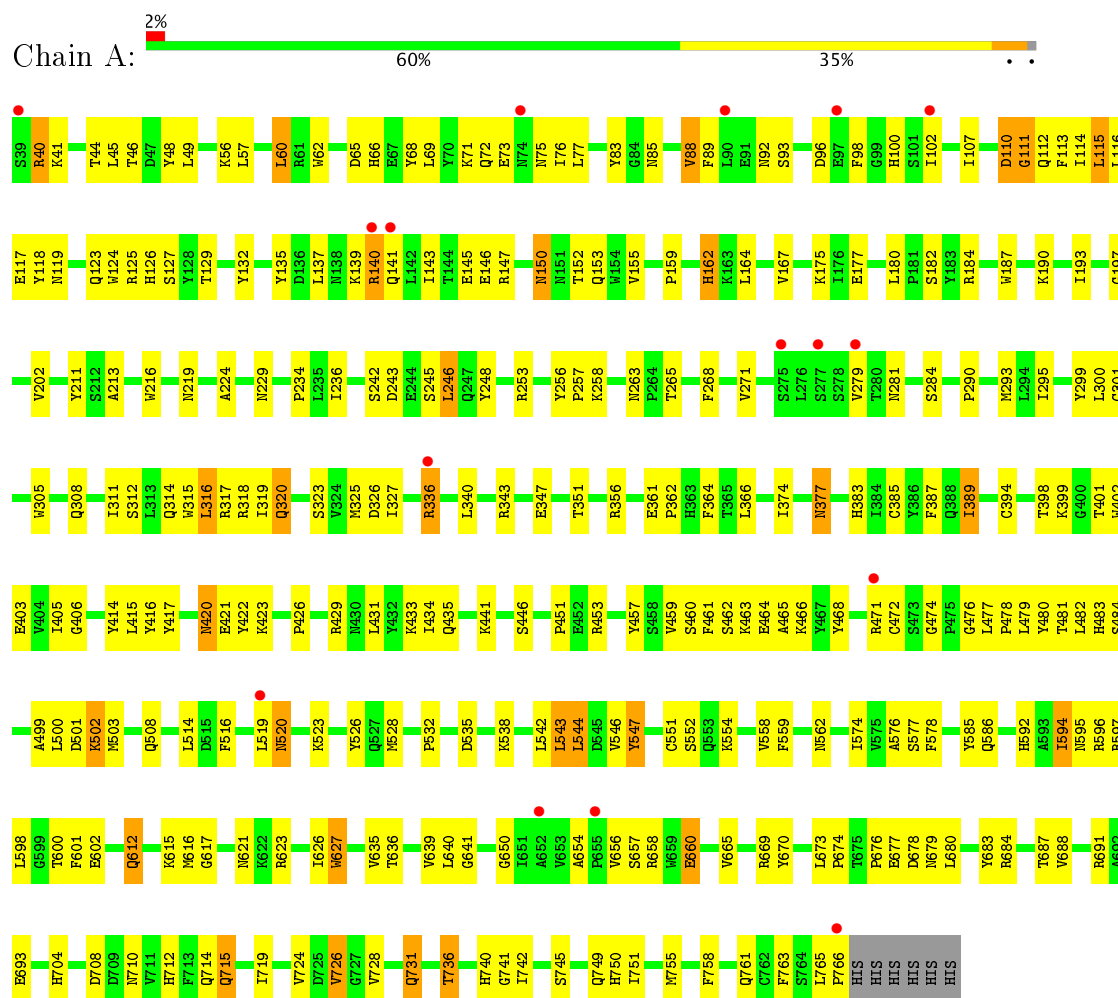
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	96	Total O 96 96	0	0
4	B	111	Total O 111 111	0	0

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 ($\text{RSRZ} > 2$). 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



N679	T557	N450	N337	E232	Y135
L680	V558	Y456	N338	V233	D136
N684	F559	Y457	C339	P234	L137
N685	R560	Y458		N138	K139
N689	L561	V459	R343	I235	R140
	N562	S460	E361	I236	Q141
	T565	F461		E237	L142
A692		S462	I374	L246	L143
E593	I573	Y468	I375	Q247	N150
T695	Y585	Q469	S376	Y248	N151
N696		L470	N377	P249	T152
	I594	R471	E378		T153
I703		O472	E379	R253	N154
H704	T600	P478	G380	V254	V155
	F601	R479	R382	Y256	T156
N710	E602	Y480	R383		T157
V711		Y481	I384	V262	S158
H712	R611	L482	C385	M263	P159
	Q612	H483	Y386	V160	P160
Q715	F613		F387	V266	G161
S716	S614	V486	Q388	K267	H162
A717	K615		I389	F268	K163
Q718	M616	R492	D390	F269	L164
I719	G617	L500	R391		
	F618	L504	K392	T273	K175
A722	V619		D393	I176	I176
V726	D620	L507	C394	V279	E177
	N621	Q508			
K622		M509	I397	S284	L180
		P510	T398	I285	P181
D729	I626	G633	T401	K286	S182
	W627		W402	I287	
M733		K511	E403	A289	N196
G741	G633	K512			G197
I742		K513	G406	H298	V202
	L640	L514	Y414	Y299	V203
S745	K648	D515	L415	L300	
Q749	C649	I518	Y416	W305	E206
H750	G650	L519	Y417		V207
I751	I651	Q527	I418	Q308	Y211
		A654	S419		
M755	P655	V656	M420	I311	D214
	S657	S657	E421		W215
F758	R658			L316	W216
Q761			R429	I319	S217
C762	Y662	K538	M430	Q320	P218
	D663	P641	L431		N219
F766		L542	K433	D326	F222
HIS		L543	I434	I327	L223
HIS	R669	V546		C328	A224
HIS	P674	Y547	K441		Y225
HIS	T675			E332	A226
HIS	P676	Q553	L445	S333	Q227
HIS	E677	D556	S446	R336	F228
	D678				N229

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.30Å 67.10Å 419.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60 33.18 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.5 (40.00-2.60) 97.6 (33.18-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.217 , 0.276 0.217 , 0.274	Depositor DCC
R_{free} test set	2874 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	53.5	Xtriage
Anisotropy	0.654	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.034 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12323	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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: 356, NAG

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	0/6135	0.65	0/8344
1	B	0.41	0/6135	0.67	1/8344 (0.0%)
All	All	0.40	0/12270	0.66	1/16688 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	60	LEU	CA-CB-CG	5.47	127.89	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5963	0	5685	269	0
1	B	5963	0	5685	231	0
2	A	60	0	60	21	0
2	B	60	0	60	14	0
3	A	35	0	28	0	0
3	B	35	0	28	1	0
4	A	96	0	0	28	0
4	B	111	0	0	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12323	0	11546	492	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 21.

All (492) 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:B:85:ASN:ND2	2:B:794:NAG:H1	1.30	1.42
1:B:85:ASN:HD21	2:B:794:NAG:C1	1.43	1.31
1:A:229:ASN:HD21	2:A:796:NAG:C1	1.72	1.01
1:B:403:GLU:H	1:B:420:ASN:HD21	1.09	0.98
1:A:85:ASN:ND2	2:A:794:NAG:H1	1.79	0.96
1:B:229:ASN:ND2	2:B:796:NAG:H1	1.80	0.95
1:A:229:ASN:HD21	2:A:796:NAG:H1	1.28	0.94
1:A:113:PHE:HE2	1:A:162:HIS:HD1	1.12	0.92
1:B:116:LEU:HB3	4:B:1081:HOH:O	1.70	0.90
1:A:658:ARG:HG3	1:A:687:THR:HG22	1.51	0.90
1:B:229:ASN:HD21	2:B:796:NAG:C1	1.86	0.89
1:A:85:ASN:ND2	2:A:794:NAG:C1	2.37	0.87
1:A:295:ILE:HG12	4:A:1095:HOH:O	1.75	0.86
1:A:229:ASN:ND2	2:A:796:NAG:H1	1.91	0.84
1:B:657:SER:H	1:B:715:GLN:NE2	1.76	0.83
1:A:281:ASN:HD21	2:A:795:NAG:C7	1.92	0.82
1:B:177:GLU:HB2	1:B:180:LEU:HD23	1.59	0.82
1:B:693:GLU:HG3	1:B:726:VAL:HG11	1.63	0.80
1:B:229:ASN:ND2	2:B:796:NAG:C1	2.45	0.79
1:A:41:LYS:HD3	4:A:1072:HOH:O	1.81	0.79
1:A:69:LEU:HD13	1:A:107:ILE:HD12	1.64	0.79
1:A:281:ASN:ND2	2:A:795:NAG:H1	1.99	0.77
1:B:361:GLU:HB3	4:B:1019:HOH:O	1.84	0.77
1:A:177:GLU:HB2	1:A:180:LEU:HD23	1.67	0.77
1:B:85:ASN:CG	2:B:794:NAG:H1	2.04	0.77
1:B:71:LYS:HA	4:B:1089:HOH:O	1.83	0.76
1:A:320:GLN:OE1	1:A:669:ARG:HG3	1.86	0.75
1:B:486:VAL:HG23	4:B:1083:HOH:O	1.85	0.75
1:A:253:ARG:HD3	4:A:1031:HOH:O	1.88	0.74
1:A:403:GLU:H	1:A:420:ASN:HD21	1.34	0.74
1:B:85:ASN:HD21	2:B:794:NAG:H1	0.61	0.73
1:A:405:ILE:HD13	1:A:429:ARG:NE	2.03	0.73
1:A:499:ALA:O	1:A:502:LYS:HG3	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:ASN:C	1:A:377:ASN:HD22	1.92	0.73
1:A:657:SER:H	1:A:715:GLN:NE2	1.86	0.72
1:B:611:ARG:HD2	4:B:1064:HOH:O	1.88	0.72
1:B:46:THR:HG23	1:B:50:LYS:HD3	1.71	0.72
1:A:115:LEU:HD11	1:A:155:VAL:HG11	1.72	0.71
1:A:177:GLU:CB	1:A:180:LEU:HD23	2.19	0.71
1:A:57:LEU:HD22	1:A:471:ARG:HH21	1.54	0.71
1:A:751:ILE:HG12	1:A:755:MET:HE3	1.73	0.71
1:B:600:THR:HG22	1:B:601:PHE:N	2.06	0.70
1:A:69:LEU:CD1	1:A:107:ILE:HD12	2.20	0.70
1:A:736:THR:HG21	1:B:717:ALA:O	1.91	0.70
1:A:85:ASN:HD22	2:A:794:NAG:C1	2.04	0.70
1:B:481:THR:OG1	1:B:483:HIS:HE1	1.73	0.70
1:A:361:GLU:HB3	4:A:1014:HOH:O	1.92	0.69
1:A:502:LYS:HE2	1:A:503:MET:HG3	1.72	0.69
1:B:236:ILE:HD13	1:B:237:GLU:N	2.08	0.69
1:A:66:HIS:HB2	4:A:1064:HOH:O	1.91	0.69
1:A:83:TYR:HB2	1:A:85:ASN:OD1	1.92	0.69
1:A:656:VAL:HG13	1:A:715:GLN:HE22	1.56	0.69
1:A:44:THR:HG22	1:A:46:THR:H	1.57	0.69
1:B:386:TYR:HB2	1:B:397:ILE:HD11	1.75	0.68
1:A:140:ARG:N	1:A:140:ARG:HD2	2.07	0.68
1:A:595:ASN:ND2	1:A:596:ARG:HG3	2.09	0.68
1:A:65:ASP:HB2	4:A:1000:HOH:O	1.94	0.68
1:B:177:GLU:CB	1:B:180:LEU:HD23	2.24	0.68
1:B:196:ASN:OD1	1:B:227:GLN:HG3	1.94	0.68
1:B:514:LEU:HD12	1:B:557:THR:HG22	1.76	0.68
1:B:55:LEU:HD23	1:B:500:LEU:HD12	1.76	0.67
1:B:122:LYS:HE3	1:B:124:TRP:O	1.95	0.67
1:B:320:GLN:OE1	1:B:669:ARG:HD3	1.94	0.67
1:A:301:CYS:SG	1:A:316:LEU:HB2	2.34	0.67
1:B:326:ASP:OD2	1:B:339:CYS:HB3	1.95	0.67
1:A:674:PRO:HG2	4:A:1085:HOH:O	1.94	0.66
1:A:219:ASN:HB2	1:A:308:GLN:OE1	1.95	0.66
1:A:258:LYS:HD2	1:B:248:TYR:CZ	2.31	0.66
1:A:57:LEU:HD22	1:A:471:ARG:NH2	2.10	0.66
1:B:518:ILE:O	1:B:519:LEU:HD12	1.97	0.65
1:B:85:ASN:HD21	2:B:794:NAG:C2	2.07	0.65
1:A:464:GLU:HB2	4:A:1000:HOH:O	1.96	0.65
1:A:242:SER:HB3	1:A:246:LEU:HD12	1.80	0.64
1:A:463:LYS:C	1:A:465:ALA:H	2.00	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:657:SER:H	1:B:715:GLN:HE21	1.44	0.64
1:A:502:LYS:CE	1:A:503:MET:HG3	2.27	0.64
1:A:356:ARG:HD3	1:A:551:CYS:SG	2.38	0.64
1:A:542:LEU:C	1:A:542:LEU:HD23	2.19	0.63
1:B:377:ASN:HD22	1:B:377:ASN:C	1.99	0.63
1:A:626:ILE:HG12	1:A:636:THR:HG23	1.79	0.63
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.79	0.63
1:A:751:ILE:HG12	1:A:755:MET:CE	2.29	0.63
1:B:429:ARG:NE	4:B:1026:HOH:O	2.27	0.63
1:A:657:SER:H	1:A:715:GLN:HE21	1.47	0.62
1:A:461:PHE:CD1	1:A:468:TYR:HB3	2.34	0.62
1:A:520:ASN:N	4:A:1025:HOH:O	2.32	0.62
1:B:621:ASN:N	1:B:621:ASN:HD22	1.96	0.62
1:A:673:LEU:HD21	4:A:1070:HOH:O	1.99	0.62
1:A:229:ASN:HD21	2:A:796:NAG:C2	2.12	0.62
1:B:648:LYS:HE3	1:B:762:CYS:O	2.00	0.61
1:B:403:GLU:OE1	1:B:585:TYR:HA	2.00	0.61
1:B:236:ILE:HG13	1:B:712:HIS:CE1	2.35	0.61
1:B:92:ASN:CG	2:B:797:NAG:O1	2.38	0.61
1:A:594:ILE:HD11	1:A:602:GLU:H	1.66	0.61
1:A:102:ILE:HD13	1:A:116:LEU:HD22	1.80	0.61
1:A:242:SER:OG	1:A:243:ASP:N	2.30	0.61
1:B:45:LEU:HG	1:B:49:LEU:HD22	1.83	0.61
1:A:271:VAL:HG22	1:A:284:SER:HA	1.83	0.61
1:B:336:ARG:HG2	1:B:336:ARG:HH11	1.65	0.61
1:B:85:ASN:ND2	2:B:794:NAG:C1	2.23	0.61
1:A:435:GLN:HE22	1:A:441:LYS:HD2	1.65	0.61
1:A:75:ASN:HD21	1:A:92:ASN:ND2	1.99	0.61
1:B:674:PRO:O	1:B:680:LEU:HD23	2.01	0.60
1:B:377:ASN:ND2	1:B:381:TYR:H	1.99	0.60
1:B:509:MET:HE3	1:B:510:PRO:HD2	1.82	0.60
1:A:600:THR:OG1	1:A:601:PHE:N	2.34	0.60
1:A:316:LEU:HD13	1:A:320:GLN:HG2	1.82	0.60
1:A:60:LEU:HD23	1:A:60:LEU:O	2.02	0.60
1:B:500:LEU:HD22	1:B:504:LEU:HG	1.84	0.60
1:A:145:GLU:HG2	1:A:146:GLU:HG2	1.84	0.60
1:A:416:TYR:CE2	1:A:433:LYS:HG3	2.37	0.60
1:A:544:LEU:HD23	1:A:576:ALA:O	2.02	0.60
1:B:387:PHE:CD2	1:B:394:CYS:HB3	2.37	0.59
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.84	0.59
1:A:403:GLU:OE1	1:A:585:TYR:HA	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:LYS:HG2	1:A:193:ILE:HD12	1.85	0.59
1:B:675:THR:HB	1:B:677:GLU:OE1	2.03	0.59
1:B:459:VAL:HG22	1:B:460:SER:N	2.16	0.59
1:A:44:THR:HG22	1:A:45:LEU:N	2.16	0.59
1:A:676:PRO:HG3	1:A:680:LEU:HD23	1.84	0.59
1:A:471:ARG:HB2	4:A:1040:HOH:O	2.03	0.59
1:A:481:THR:OG1	1:A:483:HIS:HE1	1.86	0.59
1:B:377:ASN:HD21	1:B:381:TYR:H	1.48	0.59
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.33	0.58
1:B:471:ARG:HB2	4:B:1009:HOH:O	2.02	0.58
1:B:298:HIS:HE1	4:B:1018:HOH:O	1.86	0.58
1:B:62:TRP:CG	1:B:462:SER:HA	2.39	0.58
1:A:478:PRO:HB2	4:A:1088:HOH:O	2.01	0.58
1:B:336:ARG:HG2	1:B:336:ARG:NH1	2.18	0.58
1:B:656:VAL:HG13	1:B:715:GLN:HE22	1.68	0.58
1:A:516:PHE:CD1	1:A:523:LYS:HG3	2.39	0.58
1:A:314:GLN:HG3	4:A:1012:HOH:O	2.04	0.58
1:B:403:GLU:H	1:B:420:ASN:ND2	1.90	0.58
1:B:415:LEU:HD23	1:B:415:LEU:C	2.25	0.57
1:A:526:TYR:HB3	1:A:578:PHE:HD1	1.68	0.57
1:B:562:ASN:HD22	1:B:562:ASN:C	2.07	0.57
1:B:613:PHE:HA	1:B:616:MET:HE3	1.86	0.57
1:A:318:ARG:NE	4:A:1070:HOH:O	2.34	0.57
1:A:677:GLU:N	1:A:677:GLU:OE1	2.34	0.57
1:B:55:LEU:HD23	1:B:500:LEU:CD1	2.34	0.57
1:A:472:CYS:HA	4:A:1071:HOH:O	2.04	0.57
1:B:143:ILE:HG13	1:B:143:ILE:O	2.03	0.57
1:B:217:SER:OG	1:B:222:PHE:HB2	2.05	0.57
1:A:596:ARG:HA	1:A:670:TYR:O	2.04	0.56
1:A:305:TRP:CE3	1:A:311:ILE:HG23	2.40	0.56
1:A:466:LYS:HG2	4:A:1000:HOH:O	2.04	0.56
1:A:597:ARG:HB3	1:A:597:ARG:NH1	2.21	0.56
1:B:751:ILE:O	1:B:755:MET:HG3	2.04	0.56
1:A:319:ILE:HG13	4:A:1026:HOH:O	2.06	0.56
1:B:127:SER:HB3	1:B:211:TYR:CD1	2.41	0.56
1:B:159:PRO:HG2	1:B:217:SER:O	2.06	0.56
1:B:654:ALA:HA	1:B:704:HIS:ND1	2.21	0.56
1:A:435:GLN:NE2	1:A:441:LYS:HD2	2.20	0.56
1:B:319:ILE:HD12	1:B:319:ILE:H	1.71	0.56
1:B:459:VAL:HG22	1:B:460:SER:H	1.71	0.55
1:A:544:LEU:O	1:A:546:VAL:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:ASN:ND2	1:B:420:ASN:H	2.04	0.55
1:A:159:PRO:HD3	1:A:216:TRP:HB3	1.87	0.55
1:A:471:ARG:HG3	1:A:480:TYR:CE2	2.41	0.55
1:B:433:LYS:HG3	1:B:445:LEU:HD11	1.89	0.55
1:A:125:ARG:HD2	1:A:126:HIS:NE2	2.21	0.55
1:B:633:GLY:HA3	1:B:655:PRO:HB3	1.89	0.55
1:B:414:TYR:CD1	1:B:433:LYS:HD2	2.41	0.55
1:B:420:ASN:H	1:B:420:ASN:HD22	1.54	0.55
1:B:471:ARG:HD3	1:B:480:TYR:HE2	1.71	0.55
1:B:689:MET:HG3	1:B:722:ALA:HB2	1.88	0.55
1:A:542:LEU:HD23	1:A:543:LEU:N	2.22	0.55
1:B:109:PRO:HG2	1:B:158:SER:O	2.07	0.55
1:A:340:LEU:HB2	1:A:343:ARG:HD3	1.89	0.54
1:A:724:VAL:HG22	1:B:750:HIS:CD2	2.42	0.54
1:B:450:ASN:HB3	4:B:1052:HOH:O	2.07	0.54
1:B:656:VAL:HA	1:B:715:GLN:NE2	2.23	0.54
1:A:315:TRP:O	1:A:323:SER:HB2	2.07	0.54
1:A:422:TYR:CZ	1:A:423:LYS:HE3	2.42	0.54
1:A:528:MET:CE	1:A:574:ILE:HG21	2.37	0.54
1:A:635:VAL:O	1:A:639:VAL:HG23	2.08	0.54
1:A:383:HIS:HB3	1:A:398:THR:OG1	2.08	0.54
1:A:89:PHE:CE2	1:A:107:ILE:HD13	2.42	0.53
1:B:626:ILE:O	1:B:650:GLY:HA2	2.08	0.53
1:A:459:VAL:HG22	1:A:460:SER:N	2.24	0.53
1:B:621:ASN:H	1:B:621:ASN:HD22	1.54	0.53
1:A:415:LEU:C	1:A:415:LEU:HD23	2.29	0.53
1:A:93:SER:HA	1:A:96:ASP:OD1	2.08	0.53
1:A:117:GLU:HB2	1:A:132:TYR:HE1	1.74	0.53
1:B:127:SER:HB3	1:B:211:TYR:CG	2.44	0.53
1:B:135:TYR:HD2	1:B:142:LEU:HD23	1.74	0.53
1:A:612:GLN:HA	1:A:612:GLN:HE21	1.74	0.52
1:A:127:SER:HB3	1:A:211:TYR:CD1	2.44	0.52
1:A:736:THR:HG22	4:A:1052:HOH:O	2.09	0.52
1:B:471:ARG:HD3	1:B:480:TYR:CE2	2.44	0.52
1:B:658:ARG:HH22	1:B:684:ARG:NH1	2.08	0.52
1:B:375:ILE:HD12	1:B:387:PHE:HZ	1.75	0.52
1:A:658:ARG:HG3	1:A:687:THR:CG2	2.33	0.52
1:A:85:ASN:ND2	2:A:794:NAG:O1	2.42	0.52
1:A:693:GLU:OE2	1:A:726:VAL:HG22	2.10	0.52
1:B:418:ILE:HA	1:B:430:ASN:O	2.09	0.52
1:B:402:TRP:CD1	1:B:421:GLU:HG3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:SER:HB2	1:A:457:TYR:CE2	2.45	0.52
1:A:89:PHE:HE2	1:A:107:ILE:HD13	1.75	0.52
1:B:562:ASN:HB2	4:B:1094:HOH:O	2.10	0.52
1:B:677:GLU:H	1:B:677:GLU:CD	2.12	0.52
1:B:285:ILE:N	1:B:285:ILE:HD12	2.24	0.51
1:B:41:LYS:NZ	1:B:41:LYS:HB2	2.26	0.51
1:B:125:ARG:HD2	1:B:126:HIS:CE1	2.46	0.51
2:B:796:NAG:H62	4:B:1037:HOH:O	2.10	0.51
1:A:140:ARG:HH11	1:A:140:ARG:HG3	1.76	0.51
1:A:44:THR:HG23	4:A:1039:HOH:O	2.09	0.51
1:B:377:ASN:C	1:B:377:ASN:ND2	2.63	0.51
1:B:482:LEU:HD23	1:B:492:ARG:NH1	2.26	0.51
1:A:56:LYS:O	4:A:1088:HOH:O	2.20	0.51
1:A:85:ASN:ND2	2:A:794:NAG:N2	2.58	0.51
1:A:547:TYR:CD1	1:A:552:SER:HB2	2.46	0.51
1:A:85:ASN:HB2	2:A:794:NAG:O1	2.11	0.51
1:A:420:ASN:H	1:A:420:ASN:HD22	1.59	0.50
1:B:471:ARG:CB	4:B:1009:HOH:O	2.57	0.50
1:A:312:SER:HB2	1:A:364:PHE:CZ	2.45	0.50
1:B:237:GLU:HG2	1:B:253:ARG:HG2	1.94	0.50
1:A:177:GLU:HB3	1:A:180:LEU:HD23	1.94	0.50
1:A:340:LEU:HD22	1:A:343:ARG:HH11	1.76	0.50
1:A:401:THR:HG22	1:A:401:THR:O	2.12	0.50
1:A:597:ARG:HB3	1:A:597:ARG:HH11	1.76	0.50
1:B:76:ILE:HA	4:B:1089:HOH:O	2.11	0.50
1:A:597:ARG:NH1	1:A:600:THR:OG1	2.44	0.50
1:A:44:THR:CG2	1:A:45:LEU:N	2.75	0.50
1:B:620:ASP:OD1	1:B:622:LYS:HB2	2.12	0.50
1:A:417:TYR:HE1	1:A:434:ILE:HG13	1.77	0.49
1:A:479:LEU:CD2	1:A:481:THR:HG23	2.42	0.49
1:A:554:LYS:HB3	1:A:577:SER:HB3	1.93	0.49
1:A:57:LEU:HD23	1:A:480:TYR:OH	2.12	0.49
1:A:594:ILE:CD1	1:A:601:PHE:HB2	2.42	0.49
1:A:684:ARG:HD3	4:A:1046:HOH:O	2.12	0.49
1:A:597:ARG:HH11	1:A:597:ARG:CB	2.25	0.49
1:B:89:PHE:CE2	1:B:107:ILE:HD13	2.47	0.49
1:A:229:ASN:HB3	1:A:265:THR:OG1	2.12	0.49
1:B:139:LYS:O	1:B:141:GLN:N	2.45	0.49
1:B:461:PHE:CD1	1:B:468:TYR:HB3	2.47	0.49
1:A:327:ILE:HD13	1:A:389:ILE:HG12	1.94	0.49
1:A:175:LYS:HG3	1:A:182:SER:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:MET:CE	1:A:317:ARG:HG3	2.43	0.48
1:A:72:GLN:O	1:A:73:GLU:HB2	2.12	0.48
1:B:696:LYS:HD2	1:B:696:LYS:C	2.32	0.48
1:A:731:GLN:HG2	4:A:1021:HOH:O	2.13	0.48
1:B:269:PHE:HB3	1:B:284:SER:HB3	1.95	0.48
1:B:513:LYS:O	1:B:527:GLN:HA	2.14	0.48
1:A:674:PRO:O	1:A:680:LEU:HB2	2.14	0.48
1:B:102:ILE:HG12	4:B:1081:HOH:O	2.13	0.48
1:B:431:LEU:HD23	1:B:470:LEU:HD21	1.94	0.48
1:A:508:GLN:HG2	1:A:532:PRO:HB2	1.96	0.48
1:A:543:LEU:HD21	1:A:627:TRP:HD1	1.78	0.48
1:A:728:VAL:O	1:B:750:HIS:HE1	1.97	0.48
1:B:500:LEU:CD2	1:B:504:LEU:HG	2.44	0.48
1:B:594:ILE:CD1	1:B:601:PHE:HB2	2.44	0.48
1:B:397:ILE:HD12	1:B:397:ILE:N	2.28	0.48
1:B:504:LEU:HA	1:B:507:VAL:HG12	1.95	0.48
1:B:558:VAL:HG22	1:B:560:ARG:NH1	2.29	0.48
1:A:236:ILE:HG12	1:A:712:HIS:CE1	2.48	0.48
1:B:110:ASP:OD1	1:B:161:GLY:HA2	2.14	0.48
1:B:77:LEU:HD23	1:B:88:VAL:HA	1.96	0.48
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.49	0.48
1:A:414:TYR:CE1	1:A:433:LYS:HD2	2.49	0.48
1:A:69:LEU:HD22	1:A:76:ILE:HG22	1.95	0.48
1:A:76:ILE:O	1:A:89:PHE:HB3	2.13	0.48
1:B:164:LEU:HB2	1:B:175:LYS:HB2	1.96	0.47
1:A:245:SER:HA	4:B:1080:HOH:O	2.14	0.47
1:A:253:ARG:HH22	1:B:253:ARG:NH1	2.12	0.47
1:A:741:GLY:O	1:A:742:ILE:C	2.52	0.47
1:B:657:SER:N	1:B:715:GLN:NE2	2.55	0.47
1:A:281:ASN:ND2	2:A:795:NAG:C1	2.73	0.47
1:A:41:LYS:HE3	4:A:1015:HOH:O	2.14	0.47
1:A:60:LEU:HD22	4:A:1078:HOH:O	2.14	0.47
1:B:159:PRO:HD3	1:B:216:TRP:HB3	1.96	0.47
1:B:758:PHE:O	1:B:761:GLN:HG3	2.14	0.47
1:A:398:THR:O	1:A:399:LYS:HG3	2.14	0.47
1:B:139:LYS:O	1:B:141:GLN:HG3	2.14	0.47
1:A:229:ASN:ND2	2:A:796:NAG:C1	2.54	0.47
1:A:77:LEU:CD2	1:A:88:VAL:HA	2.44	0.47
1:B:175:LYS:HG3	1:B:182:SER:HB3	1.96	0.47
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.50	0.47
1:B:600:THR:HG22	1:B:601:PHE:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:758:PHE:O	1:A:761:GLN:HG3	2.14	0.47
1:A:150:ASN:OD1	2:A:793:NAG:C1	2.62	0.47
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.50	0.47
1:B:472:CYS:O	1:B:478:PRO:HA	2.13	0.47
1:B:654:ALA:HA	1:B:704:HIS:CE1	2.49	0.47
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.44	0.47
1:A:150:ASN:OD1	2:A:793:NAG:H1	2.15	0.47
1:A:543:LEU:HD23	1:A:544:LEU:N	2.30	0.47
1:A:519:LEU:N	4:A:1025:HOH:O	2.45	0.47
1:B:163:LYS:HZ3	1:B:273:THR:HG22	1.78	0.47
1:B:745:SER:O	1:B:749:GLN:HG3	2.15	0.47
1:A:508:GLN:HE21	1:A:532:PRO:HB2	1.78	0.47
1:A:463:LYS:C	1:A:465:ALA:N	2.68	0.47
1:B:538:LYS:O	1:B:618:PHE:HA	2.15	0.47
1:A:113:PHE:HE2	1:A:162:HIS:ND1	1.94	0.46
1:A:528:MET:HE3	1:A:574:ILE:HG21	1.96	0.46
1:B:219:ASN:HB2	1:B:308:GLN:OE1	2.15	0.46
1:B:420:ASN:N	1:B:420:ASN:HD22	2.12	0.46
1:B:611:ARG:O	1:B:614:SER:HB2	2.15	0.46
1:A:361:GLU:HG3	1:A:362:PRO:HD2	1.97	0.46
1:A:654:ALA:HA	1:A:704:HIS:ND1	2.30	0.46
1:A:750:HIS:HE1	1:B:729:ASP:HA	1.80	0.46
1:A:543:LEU:HD21	1:A:627:TRP:CD1	2.51	0.46
1:B:386:TYR:CB	1:B:397:ILE:HD11	2.42	0.46
1:A:708:ASP:OD2	1:A:740:HIS:HA	2.16	0.46
1:B:203:TYR:HA	1:B:207:VAL:HG23	1.97	0.46
1:A:281:ASN:HD21	2:A:795:NAG:H1	1.75	0.46
1:A:327:ILE:CD1	1:A:389:ILE:HG12	2.46	0.46
1:B:163:LYS:HD3	1:B:273:THR:HG21	1.96	0.46
1:B:319:ILE:HD12	1:B:319:ILE:N	2.31	0.46
1:B:662:TYR:CZ	3:B:902:356:H233	2.51	0.46
1:A:453:ARG:HG3	1:A:476:GLY:HA3	1.96	0.46
1:A:472:CYS:O	1:A:478:PRO:HA	2.15	0.46
1:A:299:TYR:CZ	1:A:665:VAL:HG22	2.50	0.46
1:B:115:LEU:HD11	1:B:155:VAL:HG11	1.97	0.46
1:A:402:TRP:CD2	1:A:421:GLU:HB2	2.50	0.46
1:B:692:ALA:O	1:B:695:PHE:HB2	2.16	0.46
1:B:235:LEU:HD23	1:B:255:PRO:HA	1.98	0.46
1:B:401:THR:O	1:B:401:THR:HG22	2.16	0.46
1:A:152:THR:HG23	1:A:167:VAL:O	2.17	0.45
1:A:422:TYR:CE2	1:A:423:LYS:HE3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:LYS:HD3	1:B:123:GLN:O	2.17	0.45
1:B:562:ASN:ND2	1:B:565:THR:H	2.14	0.45
1:A:547:TYR:CD2	1:A:547:TYR:C	2.88	0.45
1:A:65:ASP:OD2	1:A:66:HIS:ND1	2.48	0.45
1:A:623:ARG:HB3	1:A:763:PHE:CD1	2.51	0.45
1:B:288:THR:HG22	1:B:289:ALA:N	2.31	0.45
1:B:553:GLN:NE2	1:B:585:TYR:HD2	2.14	0.45
1:A:281:ASN:ND2	2:A:795:NAG:C7	2.72	0.45
1:B:150:ASN:O	1:B:151:ASN:HB2	2.17	0.45
1:B:326:ASP:OD2	1:B:339:CYS:CB	2.64	0.45
1:A:626:ILE:O	1:A:650:GLY:HA2	2.16	0.45
1:A:147:ARG:HB2	2:A:793:NAG:C8	2.46	0.45
1:B:594:ILE:O	1:B:594:ILE:HG23	2.15	0.45
1:B:111:GLY:O	1:B:137:LEU:HD12	2.17	0.45
1:B:232:GLU:HB2	1:B:262:VAL:HG11	1.98	0.45
1:B:305:TRP:CZ3	1:B:311:ILE:HG12	2.52	0.45
1:B:479:LEU:HD22	1:B:481:THR:HG23	1.99	0.45
1:A:114:ILE:O	1:A:114:ILE:HG23	2.16	0.45
1:A:40:ARG:NE	1:A:40:ARG:HA	2.32	0.45
1:B:150:ASN:ND2	2:B:793:NAG:C1	2.79	0.45
1:A:594:ILE:HD11	1:A:602:GLU:N	2.31	0.45
1:A:229:ASN:CG	2:A:796:NAG:H1	2.36	0.45
1:B:433:LYS:HE2	1:B:445:LEU:HD21	1.99	0.45
1:A:202:VAL:HG13	1:A:257:PRO:HD2	1.99	0.45
1:A:320:GLN:CD	1:A:669:ARG:HG3	2.38	0.45
1:A:615:LYS:O	1:A:616:MET:C	2.54	0.45
1:B:308:GLN:OE1	1:B:308:GLN:HA	2.17	0.45
1:B:715:GLN:HB3	1:B:715:GLN:HE21	1.65	0.45
1:B:93:SER:HA	1:B:96:ASP:OD2	2.17	0.45
1:A:197:GLY:C	1:A:213:ALA:HB3	2.37	0.45
1:A:714:GLN:NE2	1:B:249:PRO:HD3	2.32	0.45
1:A:98:PHE:CE2	1:A:100:HIS:HB2	2.52	0.45
1:B:60:LEU:CD1	1:B:469:GLN:NE2	2.80	0.45
1:B:180:LEU:N	1:B:180:LEU:HD22	2.32	0.44
1:A:139:LYS:C	1:A:140:ARG:HD2	2.37	0.44
1:A:308:GLN:HA	1:A:308:GLN:OE1	2.17	0.44
1:B:266:VAL:HG22	1:B:267:LYS:N	2.32	0.44
1:B:328:CYS:HA	1:B:338:ASN:O	2.17	0.44
1:B:397:ILE:HG22	1:B:434:ILE:HD13	1.99	0.44
1:B:558:VAL:CG2	1:B:560:ARG:CZ	2.95	0.44
1:B:741:GLY:O	1:B:742:ILE:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:VAL:HG11	1:A:719:ILE:HD13	2.00	0.44
1:B:236:ILE:HG13	1:B:712:HIS:ND1	2.31	0.44
1:B:382:ARG:HG2	1:B:382:ARG:HH11	1.81	0.44
1:B:69:LEU:HD13	1:B:107:ILE:HD12	2.00	0.44
1:A:660:GLU:HG3	1:A:683:TYR:CD2	2.53	0.44
1:B:703:ILE:HA	1:B:733:MET:O	2.18	0.44
1:A:387:PHE:CD2	1:A:394:CYS:HB3	2.53	0.44
1:A:516:PHE:CE1	1:A:523:LYS:HE2	2.53	0.44
1:A:528:MET:HE2	1:A:574:ILE:HG21	2.00	0.44
1:A:336:ARG:NH1	1:A:336:ARG:HG2	2.33	0.44
1:A:477:LEU:HD11	1:A:501:ASP:HA	1.99	0.44
1:B:456:TYR:O	1:B:472:CYS:HA	2.18	0.44
1:B:546:VAL:CG2	1:B:547:TYR:N	2.81	0.44
1:A:153:GLN:HB3	1:A:211:TYR:HE2	1.82	0.44
1:B:613:PHE:HD1	1:B:616:MET:HE1	1.82	0.44
1:A:586:GLN:NE2	4:A:1027:HOH:O	2.41	0.43
1:B:154:TRP:NE1	1:B:156:THR:OG1	2.50	0.43
1:B:163:LYS:NZ	1:B:273:THR:CG2	2.81	0.43
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.99	0.43
1:A:137:LEU:C	1:A:139:LYS:H	2.20	0.43
1:A:535:ASP:HB3	1:A:538:LYS:HB2	1.99	0.43
1:B:417:TYR:CE1	1:B:434:ILE:HD11	2.53	0.43
1:B:621:ASN:ND2	1:B:621:ASN:H	2.17	0.43
1:B:621:ASN:ND2	1:B:621:ASN:N	2.66	0.43
1:A:336:ARG:HG2	1:A:336:ARG:HH11	1.83	0.43
1:A:62:TRP:CG	1:A:462:SER:HA	2.54	0.43
1:A:558:VAL:HG12	1:A:559:PHE:N	2.33	0.43
1:A:731:GLN:CG	4:A:1021:HOH:O	2.65	0.43
1:A:140:ARG:HG3	1:A:140:ARG:NH1	2.33	0.43
1:A:314:GLN:HG2	1:A:325:MET:HG3	2.01	0.43
1:A:420:ASN:OD1	1:A:426:PRO:HA	2.19	0.43
1:A:477:LEU:HD12	1:A:501:ASP:HB2	1.99	0.43
1:B:614:SER:HA	1:B:619:VAL:CG2	2.48	0.43
1:A:111:GLY:O	1:A:137:LEU:HD12	2.18	0.43
1:A:224:ALA:HB1	1:A:268:PHE:CZ	2.54	0.43
1:A:528:MET:HG2	1:A:576:ALA:HB2	2.00	0.43
1:A:69:LEU:HD22	1:A:76:ILE:CG2	2.48	0.43
1:B:152:THR:HG21	1:B:155:VAL:HG22	2.01	0.43
1:A:745:SER:O	1:A:749:GLN:HG3	2.18	0.43
1:B:197:GLY:HA2	1:B:214:LEU:HD13	2.01	0.43
1:B:613:PHE:O	1:B:616:MET:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LYS:HD2	1:B:248:TYR:CE2	2.53	0.43
1:A:596:ARG:N	1:A:670:TYR:O	2.51	0.43
1:B:197:GLY:CA	1:B:214:LEU:HD13	2.49	0.43
1:B:417:TYR:HE1	1:B:434:ILE:HG13	1.84	0.43
1:A:113:PHE:CE2	1:A:162:HIS:ND1	2.77	0.43
1:B:225:TYR:CZ	1:B:269:PHE:HB2	2.54	0.43
1:B:377:ASN:ND2	1:B:379:GLU:H	2.16	0.43
1:B:456:TYR:CG	1:B:558:VAL:HG12	2.54	0.43
1:B:206:GLU:OE2	1:B:663:ASP:OD2	2.36	0.43
1:B:512:LYS:HE3	1:B:527:GLN:CD	2.39	0.42
1:A:110:ASP:O	1:A:112:GLN:N	2.52	0.42
1:A:543:LEU:CD2	1:A:627:TRP:HD1	2.32	0.42
1:A:420:ASN:C	1:A:420:ASN:ND2	2.73	0.42
1:B:387:PHE:CE2	1:B:394:CYS:HB3	2.54	0.42
1:B:383:HIS:CD2	1:B:398:THR:OG1	2.72	0.42
1:B:49:LEU:HA	1:B:49:LEU:HD12	1.80	0.42
1:A:327:ILE:HD13	1:A:389:ILE:CD1	2.50	0.42
1:A:596:ARG:NH2	1:A:679:ASN:HB2	2.35	0.42
1:A:140:ARG:N	1:A:140:ARG:CD	2.82	0.42
1:A:312:SER:HB2	1:A:364:PHE:HZ	1.84	0.42
1:B:263:ASN:HA	1:B:263:ASN:HD22	1.61	0.42
1:A:398:THR:C	1:A:399:LYS:HD2	2.39	0.42
1:A:48:TYR:CE1	1:A:562:ASN:HA	2.55	0.42
1:B:383:HIS:HD2	1:B:398:THR:OG1	2.02	0.42
2:B:793:NAG:O7	2:B:793:NAG:H1	2.19	0.42
1:B:229:ASN:ND2	2:B:796:NAG:O1	2.48	0.42
1:A:340:LEU:H	1:A:340:LEU:HD12	1.84	0.42
1:A:641:GLY:O	1:A:691:ARG:HD3	2.20	0.42
1:B:316:LEU:HD21	1:B:320:GLN:HG2	2.01	0.42
1:A:414:TYR:CD1	1:A:433:LYS:HD2	2.55	0.42
1:A:502:LYS:HD2	1:A:503:MET:N	2.34	0.42
1:B:441:LYS:NZ	4:B:1040:HOH:O	2.52	0.42
1:B:343:ARG:NH2	1:B:390:ASP:OD1	2.53	0.42
1:B:657:SER:HB3	1:B:719:ILE:HD11	2.01	0.42
1:A:153:GLN:HB3	1:A:211:TYR:CE2	2.55	0.41
1:A:765:LEU:HA	1:A:766:PRO:HD3	1.90	0.41
1:B:446:SER:HB2	1:B:457:TYR:CE2	2.55	0.41
1:A:180:LEU:HD22	1:A:180:LEU:N	2.36	0.41
1:B:269:PHE:CE1	1:B:286:GLN:HB2	2.55	0.41
1:B:562:ASN:HD22	1:B:565:THR:H	1.67	0.41
1:B:627:TRP:HB2	1:B:651:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:726:VAL:HG12	1:B:726:VAL:O	2.19	0.41
1:A:125:ARG:HD2	1:A:126:HIS:CE1	2.55	0.41
1:A:459:VAL:CG2	1:A:460:SER:N	2.84	0.41
1:B:389:ILE:HG22	1:B:390:ASP:N	2.35	0.41
1:B:374:ILE:HD11	1:B:406:GLY:HA2	2.01	0.41
1:A:123:GLN:HG2	1:A:124:TRP:N	2.35	0.41
1:A:597:ARG:O	1:A:600:THR:HG23	2.20	0.41
1:B:397:ILE:CD1	1:B:397:ILE:N	2.83	0.41
1:B:675:THR:C	1:B:680:LEU:HB2	2.40	0.41
1:A:60:LEU:HB2	1:A:68:TYR:CD1	2.56	0.41
1:B:327:ILE:HB	1:B:343:ARG:HG2	2.02	0.41
1:B:627:TRP:HA	1:B:651:ILE:O	2.21	0.41
1:A:140:ARG:C	1:A:141:GLN:HG3	2.40	0.41
1:A:184:ARG:HD3	1:A:187:TRP:CE2	2.56	0.41
1:A:202:VAL:HG11	1:A:257:PRO:CG	2.50	0.41
1:A:290:PRO:O	1:A:293:MET:HB2	2.21	0.41
1:A:461:PHE:CE1	1:A:468:TYR:HB3	2.55	0.41
1:B:383:HIS:HD2	1:B:398:THR:CB	2.33	0.41
1:A:479:LEU:HD22	1:A:481:THR:HG23	2.02	0.41
1:A:71:LYS:HA	1:A:75:ASN:O	2.19	0.41
1:B:246:LEU:HA	1:B:246:LEU:HD23	1.93	0.41
1:A:340:LEU:CD1	1:A:340:LEU:H	2.34	0.41
1:A:340:LEU:HD12	1:A:340:LEU:N	2.36	0.41
1:A:77:LEU:HD22	1:A:88:VAL:HA	2.02	0.41
1:B:134:ILE:HG22	1:B:135:TYR:N	2.35	0.41
1:B:507:VAL:HG13	1:B:509:MET:HG2	2.03	0.41
1:B:434:ILE:HG23	4:B:1079:HOH:O	2.20	0.41
1:B:602:GLU:N	1:B:602:GLU:OE1	2.50	0.41
1:B:562:ASN:ND2	1:B:562:ASN:C	2.74	0.41
1:A:118:TYR:CE2	1:A:119:ASN:ND2	2.89	0.41
1:A:596:ARG:NH2	1:A:678:ASP:OD1	2.54	0.41
1:B:298:HIS:CE1	4:B:1018:HOH:O	2.67	0.40
1:B:459:VAL:CG2	1:B:460:SER:N	2.83	0.40
1:B:534:PHE:HZ	1:B:618:PHE:CD1	2.39	0.40
1:B:541:PRO:HG2	1:B:573:ILE:HG12	2.03	0.40
1:A:598:LEU:HD11	1:A:670:TYR:HB2	2.03	0.40
1:B:225:TYR:CE1	1:B:269:PHE:HB2	2.57	0.40
1:A:405:ILE:HD13	1:A:429:ARG:CD	2.51	0.40
1:A:420:ASN:HD22	1:A:420:ASN:C	2.25	0.40
1:A:457:TYR:HA	1:A:471:ARG:O	2.22	0.40
1:A:480:TYR:HE1	4:A:1088:HOH:O	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:TYR:CE1	1:B:433:LYS:HD2	2.56	0.40
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.51	0.40
1:A:118:TYR:CD2	1:A:119:ASN:ND2	2.90	0.40
1:A:281:ASN:HD21	2:A:795:NAG:C1	2.34	0.40
1:A:374:ILE:HD11	1:A:406:GLY:HA2	2.04	0.40
1:A:474:GLY:HA2	1:A:476:GLY:O	2.22	0.40
1:B:134:ILE:HD11	1:B:164:LEU:HD11	2.03	0.40
1:B:512:LYS:HE2	1:B:556:ASP:O	2.22	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	726/734 (99%)	657 (90%)	59 (8%)	10 (1%)	13	26
1	B	726/734 (99%)	662 (91%)	58 (8%)	6 (1%)	22	44
All	All	1452/1468 (99%)	1319 (91%)	117 (8%)	16 (1%)	17	35

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	320	GLN
1	B	140	ARG
1	B	333	SER
1	B	393	ASP
1	A	111	GLY
1	A	143	ILE
1	A	617	GLY
1	B	392	LYS
1	B	320	GLN
1	A	520	ASN

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Mol	Chain	Res	Type
1	A	40	ARG
1	A	110	ASP
1	A	389	ILE
1	B	389	ILE
1	A	279	VAL
1	A	451	PRO

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	653/659 (99%)	611 (94%)	42 (6%)	20	40
1	B	653/659 (99%)	613 (94%)	40 (6%)	22	43
All	All	1306/1318 (99%)	1224 (94%)	82 (6%)	21	42

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	LEU
1	A	60	LEU
1	A	88	VAL
1	A	115	LEU
1	A	129	THR
1	A	140	ARG
1	A	150	ASN
1	A	162	HIS
1	A	164	LEU
1	A	246	LEU
1	A	256	TYR
1	A	263	ASN
1	A	300	LEU
1	A	316	LEU
1	A	326	ASP
1	A	336	ARG
1	A	347	GLU

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Mol	Chain	Res	Type
1	A	351	THR
1	A	366	LEU
1	A	377	ASN
1	A	385	CYS
1	A	420	ASN
1	A	431	LEU
1	A	482	LEU
1	A	484	SER
1	A	500	LEU
1	A	502	LYS
1	A	514	LEU
1	A	543	LEU
1	A	544	LEU
1	A	547	TYR
1	A	592	HIS
1	A	594	ILE
1	A	612	GLN
1	A	621	ASN
1	A	627	TRP
1	A	660	GLU
1	A	710	ASN
1	A	715	GLN
1	A	726	VAL
1	A	731	GLN
1	A	736	THR
1	B	40	ARG
1	B	41	LYS
1	B	49	LEU
1	B	51	ASN
1	B	60	LEU
1	B	63	ILE
1	B	65	ASP
1	B	90	LEU
1	B	100	HIS
1	B	122	LYS
1	B	202	VAL
1	B	214	LEU
1	B	223	LEU
1	B	236	ILE
1	B	246	LEU
1	B	256	TYR
1	B	263	ASN

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Mol	Chain	Res	Type
1	B	300	LEU
1	B	326	ASP
1	B	332	GLU
1	B	377	ASN
1	B	385	CYS
1	B	420	ASN
1	B	472	CYS
1	B	479	LEU
1	B	500	LEU
1	B	514	LEU
1	B	515	ASP
1	B	543	LEU
1	B	547	TYR
1	B	558	VAL
1	B	562	ASN
1	B	621	ASN
1	B	655	PRO
1	B	679	ASN
1	B	685	ASN
1	B	696	LYS
1	B	710	ASN
1	B	715	GLN
1	B	761	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	119	ASN
1	A	123	GLN
1	A	141	GLN
1	A	150	ASN
1	A	169	ASN
1	A	229	ASN
1	A	247	GLN
1	A	263	ASN
1	A	281	ASN
1	A	298	HIS
1	A	377	ASN
1	A	420	ASN
1	A	430	ASN
1	A	435	GLN

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Mol	Chain	Res	Type
1	A	483	HIS
1	A	508	GLN
1	A	592	HIS
1	A	595	ASN
1	A	612	GLN
1	A	621	ASN
1	A	679	ASN
1	A	710	ASN
1	A	715	GLN
1	A	731	GLN
1	A	748	HIS
1	A	750	HIS
1	B	85	ASN
1	B	123	GLN
1	B	126	HIS
1	B	169	ASN
1	B	229	ASN
1	B	263	ASN
1	B	298	HIS
1	B	377	ASN
1	B	383	HIS
1	B	420	ASN
1	B	483	HIS
1	B	487	ASN
1	B	533	HIS
1	B	553	GLN
1	B	562	ASN
1	B	621	ASN
1	B	679	ASN
1	B	685	ASN
1	B	710	ASN
1	B	715	GLN
1	B	750	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	793	-	15,15,15	0.29	0	21,21,21	0.63	0
2	NAG	A	794	-	15,15,15	0.44	0	21,21,21	0.83	1 (4%)
2	NAG	A	795	-	15,15,15	0.42	0	21,21,21	0.55	0
2	NAG	A	796	-	15,15,15	0.43	0	21,21,21	0.71	1 (4%)
3	356	A	901	-	28,39,39	1.66	9 (32%)	33,57,57	1.82	9 (27%)
2	NAG	B	793	-	15,15,15	0.47	0	21,21,21	0.62	0
2	NAG	B	794	-	15,15,15	0.34	0	21,21,21	0.65	0
2	NAG	B	796	-	15,15,15	0.32	0	21,21,21	0.91	1 (4%)
2	NAG	B	797	-	15,15,15	0.46	0	21,21,21	0.70	0
3	356	B	902	-	28,39,39	1.90	8 (28%)	33,57,57	1.82	7 (21%)

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	NAG	A	793	-	-	0/6/26/26	0/1/1/1
2	NAG	A	794	-	-	0/6/26/26	0/1/1/1
2	NAG	A	795	-	1/1/6/7	0/6/26/26	0/1/1/1
2	NAG	A	796	-	1/1/6/7	0/6/26/26	0/1/1/1
3	356	A	901	-	-	0/6/22/22	0/5/5/5
2	NAG	B	793	-	1/1/6/7	0/6/26/26	0/1/1/1
2	NAG	B	794	-	1/1/6/7	0/6/26/26	0/1/1/1
2	NAG	B	796	-	1/1/6/7	0/6/26/26	0/1/1/1
2	NAG	B	797	-	-	0/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	356	B	902	-	-	0/6/22/22	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	902	356	C3-N7	-4.95	1.28	1.33
3	B	902	356	C5-N7	-3.69	1.28	1.34
3	A	901	356	C3-N7	-3.65	1.30	1.33
3	A	901	356	C5-N7	-2.81	1.30	1.34
3	A	901	356	C17-N11	-2.25	1.43	1.46
3	B	902	356	C17-N11	-2.16	1.43	1.46
3	A	901	356	C26-C21	2.01	1.57	1.51
3	A	901	356	C34-C35	2.18	1.43	1.38
3	A	901	356	C32-C29	2.20	1.52	1.50
3	A	901	356	C29-N25	2.54	1.35	1.32
3	B	902	356	C34-C35	2.58	1.44	1.38
3	A	901	356	C22-C26	2.60	1.60	1.53
3	B	902	356	C29-N25	2.61	1.35	1.32
3	B	902	356	C26-C21	2.64	1.58	1.51
3	A	901	356	C30-C28	2.84	1.46	1.42
3	B	902	356	C22-C26	2.86	1.60	1.53
3	B	902	356	C30-C28	3.51	1.47	1.42

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	902	356	C22-C17-N11	-4.43	102.38	111.09
3	A	901	356	C4-C1-C3	-3.90	117.23	119.92
3	A	901	356	C30-C28-N24	-3.89	118.82	122.84
3	B	902	356	C4-C1-C3	-3.84	117.27	119.92
3	B	902	356	C30-C28-N24	-3.76	118.96	122.84
3	A	901	356	C22-C17-N11	-3.63	103.95	111.09
3	B	902	356	N24-C20-N25	-3.42	122.36	126.33
3	A	901	356	N24-C20-N25	-3.34	122.45	126.33
3	A	901	356	C20-C15-N9	-2.27	107.54	111.44
3	B	902	356	C20-C15-N9	-2.06	107.91	111.44
2	A	796	NAG	C1-C2-C3	-2.05	107.75	110.54
3	A	901	356	C26-C22-C17	2.04	113.64	110.96
2	A	794	NAG	O5-C1-C2	2.04	111.56	109.52
3	A	901	356	C15-C20-N25	2.23	120.12	116.53
2	B	796	NAG	O5-C1-C2	2.40	111.92	109.52
3	A	901	356	C20-N25-C29	2.75	122.18	117.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	902	356	C32-C29-N25	2.82	120.31	115.67
3	A	901	356	C32-C29-N25	2.88	120.41	115.67
3	B	902	356	C20-N25-C29	2.90	122.47	117.07

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	796	NAG	C1
2	B	794	NAG	C1
2	B	793	NAG	C1
2	B	796	NAG	C1
2	A	795	NAG	C1

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	793	NAG	3	0
2	A	794	NAG	6	0
2	A	795	NAG	6	0
2	A	796	NAG	6	0
2	B	793	NAG	2	0
2	B	794	NAG	6	0
2	B	796	NAG	5	0
2	B	797	NAG	1	0
3	B	902	356	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	728/734 (99%)	-0.10	16 (2%) 62 56	36, 55, 82, 98	0
1	B	728/734 (99%)	-0.23	6 (0%) 86 83	34, 48, 72, 86	0
All	All	1456/1468 (99%)	-0.17	22 (1%) 74 69	34, 51, 77, 98	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	39	SER	5.0
1	B	279	VAL	3.5
1	A	279	VAL	3.2
1	B	97	GLU	3.1
1	A	97	GLU	3.0
1	A	39	SER	2.9
1	A	140	ARG	2.9
1	A	766	PRO	2.9
1	A	102	ILE	2.4
1	A	90	LEU	2.4
1	A	655	PRO	2.3
1	B	40	ARG	2.3
1	B	655	PRO	2.3
1	A	652	ALA	2.3
1	A	141	GLN	2.2
1	B	336	ARG	2.2
1	A	471	ARG	2.2
1	A	275	SER	2.2
1	A	74	ASN	2.1
1	A	336	ARG	2.0
1	A	519	LEU	2.0
1	A	277	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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(Å ²)	Q<0.9
2	NAG	B	794	15/15	0.94	0.16	1.40	50,52,54,57	0
2	NAG	B	793	15/15	0.81	0.22	0.98	98,99,100,100	0
3	356	B	902	35/35	0.94	0.23	0.97	34,36,45,48	0
2	NAG	B	796	15/15	0.91	0.17	0.68	65,65,66,67	0
2	NAG	A	796	15/15	0.86	0.19	0.55	79,80,81,82	0
3	356	A	901	35/35	0.93	0.20	0.32	40,42,45,46	0
2	NAG	A	794	15/15	0.93	0.18	0.27	68,68,69,69	0
2	NAG	A	793	15/15	0.92	0.17	-0.25	95,96,96,97	0
2	NAG	B	797	15/15	0.88	0.14	-	92,93,93,93	0
2	NAG	A	795	15/15	0.82	0.32	-	99,99,100,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.